

## BIBLIOGRAPHY OF ATOMIC AND MOLECULAR INNER-SHELL EXCITATION STUDIES

**Adam P. Hitchcock**

Department of Chemistry  
Brockhouse Institute for Materials Research  
McMaster University, Hamilton, Ontario  
CANADA L8S 4M1

THIS DOCUMENT is available from  
[http://unicorn.mcmaster.ca/corex/core\\_exit\\_bib.html](http://unicorn.mcmaster.ca/corex/core_exit_bib.html)

### Codes

**P** - photon impact (photoabsorption, ionic photofragmentation)

**E** - electron impact (electron energy loss, (e,e+ion), (e,2e) coincidence)

**R** - review

**T** - theory, calculation

**Molecular formulas in BOLD** indicate that core excitation spectra are available for download from  
[http://unicorn.mcmaster.ca/corex/corex\\_read-me.html](http://unicorn.mcmaster.ca/corex/corex_read-me.html)

Please send additions, corrections and (p)reprints relevant to this bibliography to me at [aph@mcmaster.ca](mailto:aph@mcmaster.ca)

**an update of: A.P. Hitchcock and D.C. Mancini, J. Electron Spectrosc. 67 (1994) 1-132.**

supercedes: 26-Sep-09 update of the 25-Jun-93 published edition. (Other updates: 24-Aug-98, 28-Feb-94, 21-Sep-95; 15-Jul-96)

Previously UPDATED on unicorn.mcmaster.ca website: 18-June-2016; 24-Oct-04, 03-Jan-05, 15-Jul-06, 26-Sep-09

## ATOMS

Atom/ Level	Ref	Energy (eV,keV)	Code	Comments
Al 2p	CTS82	77- 83	P	relative, absorption by Al I in flash pyrolysis plasma
	S85	77- 83	P,R	Al I in plasma
	BKM88	72-100	P	laser plasma absorption; laser X-rays; compared to other Na I series
	CE&92	60-240	P,T	Al <sup>+</sup> ; relative, laser generated and probed; MC-SCF calc.
	KMC96	80-100	P	laser plasma study of Al <sup>+</sup> ; comp. to Mg, Si <sup>++</sup>
	CK&98	76-82	P,T	Al(0); dual plasma; ab initio calc.
	W01	48-100	P,R	review of atom and ion photoionization
	WA&01	80-160	P,T	absolute; Al <sup>+</sup> , Al <sup>++</sup> cross-sections
				FIRST ATOMIC CORE EXCITATION MEASUREMENT
Ar 2p	P34	200-300	P	absolute
	LZ63	50-4000	P	absolute
	S66	200-300	R	absolute
	FC68	50-810	T	absolute, ab initio calculation
	NS&68	243-252	P	photographic, Rydberg analysis IP (248.52, 250.55)
	AG&69	0-450	E	angular dependence of inelastic scattering, differential X-section
	D69	238-262	P	absolute
	WM69	155-305	P	photographic, Rydberg analysis IP (248.5, 250.6)
	HK&71	250-260	P	relative, comp to solid Ar
	WW71	20-400	E	absolute, multiple ionisation
	ZG71	50-810	R	review of atomic photoionization
	WB72	200-300	E	absolute, TRK sum rule normalisation
	C73	200-300	P,R	review of atomic photoabsorption
	WWT76	240-280	E	ion yields, post-collision interaction, quadrupole transition
	KT&77	242-252	E	Rydberg analysis IP (248.628(4), 250.776(1)), Z+1 analogy, <70meV res.
	R78	244-250	E	Rydberg analysis IP (see KT&77), Z+1 analogy
	GHF81	243-252	P	0.1 eV FWHM
	SC82	253	E	(e,2e) Auger-ELS coincidence, anisotropic angular correlation
	SK&82	243-248	E	dipole forbidden transitions, 2p->4p intensity as f(K)
	SD&83	243-267	T	absolute, comp. to expt.(NS&68), core-hole relaxation emphasized
	HM&84	243-253	P	absolute, total and ion yield spectra, P.C.I.
	K84	243-248	E	k-dependence of 4p/4s intensities; I(4p)>I(4s) for k>2bohr <sup>-1</sup>
	SB84	244.37(2)	E	calibration standard(2p <sub>3/2</sub> >4s)
	SC84	254	E	in-plane ang. variation of (e,2e) Auger-loss, PCI distorts alignment
	SV84	253	E	out-plane ang. variation (e,2e) Auger-loss, PCI distorts alignment
	SA&86a	256,308	E	(e,e',Auger), (e,2e) coincidences, PCI
	YK&86b	245-260	T	absolute; ab initio, radial correlation only, comp. to expt [NS+68]
	HL&87	240-260	P	threshold PES, shake-off at discrete res.
	AA&88	244-248	P	DES, shake-up (spectator decay dominates)
	EB&88	242-256	P	Ar+ and Ar2+ yield, PCI, shake-down (to 2 eV above L2)
	HM&88	242-258	P	(threshold e-, photoion coincidence); multiple ionisation
	C89	254-260	T	ang. dist. of resonant Auger; res. of multiplets
	CM&89	244,246	P	resonant Auger, ang. dist.; comp. of Ar,Kr,Xe
	PK89	100-300	T	absolute, MBPT, comp. to expt. (NS&68, LZ63, D69), double ionisation
	SS&89	242-256	P	relative, res. check (0.4 eV FWHM), apparatus description (CSRF)
	AA&90a	244,245	P,T	DES, shake-up fraction comp. of Ne1s, Ar2p, Kr3d, Xe4d
	DC&90	400-2000	E	(Auger-ej.e-) coinc.; both 205 eV KE; angular distr.; strong threshold spike
	HMS90	243-254	P	ZEKE yield, ZEKE-ion coincidence
	KY90	247-248	T	absolute; HF-multi config; 3% monopole redist.; 2p63d lineshape

Ar 2p ..	M90	245-270	P	ion desorption, AI spectrum (DES), comp. to gas
	PB90	242-255	T	relative, sol. Ar, comp. to expt. (HK&71), shape res.!
	VM&90	244	P	(hv,2e); 2-step autoionization decay of discrete states in Ar, Kr, Xe
	HM&91b	249-254	P	ZEKE at 0.15 eV fwhm; PCI (Niehaus) line shape; Ryd. res.
	II&91	>250	E	PCI shift of Auger, comp. of Ar LMM, Kr MNN, Xe NOO
	MR&91	245-248	P	DES, 3d-collapse, shake prob. of spectator type strong function of n
	RJ&91	240-320	P	atomic vs. cluster (Nbar to 3); Ar <sub>2</sub> <sup>+</sup> yield, EXAFS of clusters, 4s exciton
	S91a	240-270	P,R	autoionisation of Rydberg res., comp. to Xe 4d
	AA&92b	244-250	P	resonant AI; ion branching ratios; comp. of Ar, Kr
	RS&92d	240-390	P,T	absolute; comp to Ar <sub>n</sub> clusters, 4s, EXAFS at 6 sol.
	CC&92	200-400	E	absolute; comp. of Ar, Kr, Xe
	DM&92	243-251	P	high res. (70 meV); SX-700II characterization
	GE&92	243-251	P	resonant Auger (AI); post collision effect; comp.to theory
	ZKP92	200-290	T	anomalous scattering factor; reflects Ar 2p resonance edge structure
	HM&92a	240-290	P	ZEKE-TIY; shake-up vs. 2-electron
	SS92d	44-1300	P	PIY and BR for multi-charge ions of Ne, Ar, Kr, Xe; ΔBR at edges
	C93	100-5000	T	X-sect; β; comp. of all rare gases; ang. cor. correct.; dipole breakdown
	MB93	244.4	T	ab initio, GOS calc., OOS=0.0078); comp. to all earlier calc.
	MB&93	242-250	T	GOS calculation of Ar 2p →nd Ryd.
	RH&93a	240-290	P	comp. of atom, cluster, solid; Ryd.-exciton; EXAFS
	AD&94	243-256	P	ZEKE; small 4s, large 3d resonance; PCI shift 0.28 eV
	AK&94	243-248	P	50 meV fwhm; SX700 performance test; obs. 135 mV; nat. 116 mV
	GE&94	244-252	P	3s/3p partial PI yields; coupled to 3d res.; Fano lineshape; comp to Kr 4s
	KJ&94	240-260	P	comp. of threshold (zeke) of Ar, Ar <sub>n</sub> ; PCI lineshape analysis
	LH&94	245-255	P	zeke spectrum, apparatus for (azepeco)
	SS94	240-280	P	BR of multiple PI; Auger; comp. of 2e- ionization of Ne,Ar,Kr,Xe
	AK&95c	240-260	P	SX700 pgm performance at MAX; Ar 2π* mat. width <110 meV
	BF&95	243-248	P	partial ion yields; comp. of atoms & clusters
	CC&95	240-260	P	SGM at SRBC performance test; high resolution
	GE&95	247-252	P,T	L <sup>3</sup> M <sup>23</sup> M <sup>23</sup> resonant Auger at Ar 2p res.; PCI and time dep. model of decay of Rydberg states needed; new interference lineshape predicted
	IK&95a	240-370	P	absolute; Beers law determination; corr. for stray light, higher order, optics
	QO&95	243-251	P	high resolution (19 meV estimated); SGM 5-grating system (17-900 eV)
	SK&95c	244-249	P	accurate natural linewidths; partial ion yields
	BA&96	190-260	P	partial ion yield, pre-edge ioniz. tails to ~20 eV below IP; 2p/1s comp.
	BS96	100-500	P,R	absolute, partial cross-sect.
	FH&96	245-260	P	high resolution (E/dE~4000); variable line spacing PGM
	HZ96	242-256	P,R	relative, partial & total ion yields; review ion yield spect. of atoms
	KT&96	250-252	P	TPEPICO of Ar <sup>2+</sup> , Ar <sup>3+</sup> ; PCI at L <sub>2</sub> edge
	L96a	250-450	E,R	Auger-scattered electron coincidence; angular distribution
	RK&96	240-265	P	comp to clusters, TIY, AEY
	SK&96	243-253	P	high res.; Γ(4s)=114(2)eV up to Γ(6d)=139(10) eV; comp. to SK&82
	SS&96	242-253	P,T	absolute; PCI at Ar 2p threshold; fluorescent yield; width as f(n)
	TH&96	244-254	P	ZEKE; Lorentzian lineshapes; channel effects on natural linewidth (120 meV)
	AEB97b	242-253	P	TIY, PIY, charge state mapping
	FH&97	243-250	P	angular-resolved Auger; β values
	LB&97	244,246	P	resonant, non-res. Auger at 4s, 3d; angular dist.; test of spectator models
	SLS97	248-253	P	Auger, ion yield; fluorescence; PCI effects on PES
	WW97	248-268	E	(e,2e) EELS-Auger coincidence; angle-dependent interference; β values
	HK&98	250	E	resonant Auger excited by EI; weak
	SS98a	240-270	P	charge state PIY; PE-PI coincidence
	US&99a	244	P	4s Auger; lifetime-interference effect on ang. Dist.; ‘second step’ Auger

Ar 2p ..	VP&99	244	P	lifetime 111(3) meV, comp. to others (113 -121 meV)
	FL00	240-255	E	GOS; comp to theory (MB93); 4s structured; areas used; no geom. overlap correction; 1.5 to 9.5° scattering angle
	SP&00	244-254	P	SB7 LURE beamline tests; $\Delta E/E > 8500$
	MB&01	243-245	P	DES; Fano profiles vary with AI channel; classic channel interference
	US&01	244-246	P	resonant Auger; angular distribution
	GT&03b	240-260	P	60 meV; BL4B UVSOR commissioning
	HNK04	244-252	P	PEY, FY, comp to solid and Ar:Kr, Ar:Xe, Ar:N <sub>2</sub> matrices.
	K04	243-253	P,T	Ar(g) comp to Xe, Kr, N <sub>2</sub> matrices; S-O split & Ryd-val. Exchange
	KHS05	250	P	AEICO electron-ion coincidence, charge state mapping
	KS&05	244-251	P	resonant Auger decay, comp. to Ar <sub>n</sub>
	FN&06	246	P	(3p,2p) interference at $2p_{1/2} \rightarrow 4s$ ; relative PES, $\beta$ -parameter
	KM&07	242-253	P	absolute, hi-res; natural linewidths deduced; IP from Rydberg series
	NS&07	453	E	(e,2e)-(e,3e); competition of single Ar 2p & direct double
	SL&10	246	P	post-collision interaction effect on Ar 2p PES line
	CM12	246	P, R	review of lifetime-limited linewidths (many small mol. & atoms)
	PK&17	300	E	triple electron coincidence decay, time-resolved, KE-resolved
Ar 2s	LS&87	320-380	T	absolute, effect of correlation and core-hole relax.; comp to expt. (LZ63)
	KY97	320-340	T	RPAE calc.; virtual Auger decay; comp. to expt.
	LP&00	240-335	P,T	Auger threshold coinc; resonance enhanced double ionization; Coster-Kronig; sub-natural linewidths; ‘continuum’ resonance Raman Auger
	SK&02	321-330	P	detailed line shape analysis, Coster-Kronig spectroscopy
	LS&12	252	P	post-collision interaction effect on Ar 2s PES line
Ar 1s	P39	3.2 keV	P	10eV about edge, photographic
	SS59	3.2 keV	P	relative; comp. of gas-solid
	S63	3.2 keV	P	35eV about K-edge, double excitation (KM)
	W65	1.5-6.2	P	photographic, absolute
	Wa65	3.2 keV	T	fit to lineshapes of S63
	SP66	3.1-3.2	P	absolute
	SBB68	3.2 keV	P	40 eV about edge, gas-solid comparison
	AP74	3.2 keV	P,R	review of analyses
	H77a	3.1-3.6	P	double excitation structure
	SD&79	3.1-3.2	T	absolute, comp. to expt. (SP66), inner-shell relaxation
	B80	3.2 keV	P,R	review, (P39 data)
	BC&80	3.2 keV	P	Rydberg series analysis
	AIK81	3.2 keV	T	absolute, compared to experiment (S63)
	BQB81	3.2 keV	T	ab initio calculation, compared to experiment (BC&80)
	DLR82	3.2 keV	E	test of modified Bethe sum rule, 25 keV impact, #1s e-'s =1.54(6)
	DL&83	3.18-4.55	P	(1s,3p) and (1s,3s) double excitation, emission, absorption compared
	TA85	3.2 keV	T	post-collision interaction
	YK&85	3.20-3.24	T	absolute, HF-multi config.; E,f calc; comp. to expt. (SP66)
	CH86	3.20-3.26	P	double excitation (1s2p)
	D86b	3.2-3.3	P	absolute, photon-selected emission spectra; KM transitions
	DL86	3.20-3.27	T	interpretation of (1s3p) double excitation via Ar K-β satellites
	LG&86	3.20-3.36	P	double excitation (1s3p); gas ionisation detector; ppm sensitivity
	YK&86b	3.2 keV	T	ab initio, radial correlation only, comp to expt
	KYP87	3.20-3.24	T	absolute; HF-MC; E,f calc; comp to expt (SP66)
	C88	3.20-3.26	T	absolute, double excitation, comp. to expt. (DL&83)
	V88	3.2-5.2	T	shake-up/off; comp to expt (AA&85)
	LB&90	3.2-3.24	P	Auger-ion coinc in discrete, cont., double Auger, PCI-recapture
	S90a	3.20-3.26	T	near threshold, multiple excit. (2e) in first 50 eV of continuum
	LB&91	3.19-3.22	P	Auger-ion coinc, PCI, charge state yields
	KH91	3.48-3.54	P	KL double excit., 0.3% of 1e- continuum

Ar 1s ...	US&91	3.19-3.22	P	total and partial ion yields, Ar <sup>+</sup> to Ar <sup>6+</sup> ; threshold effects
	DMD92	3.20-3.60	P,T	absolute; KM, KL double excit.; HF & DF calc.
	S92	3.20-3.26	P,R	KL double excitation
	C93	100-5000	T	X-sect; β; comp. of all rare gases; ang. cor. correct.; dipole breakdown
	DA&93	3.19-3.22	P	relative yields of all ions at threshold; non-diagram trans; double PI
	RH&93c	3.1-3.8	P	comp. of atomic, cluster, solid XANES and XAFS
	TK&93	3.21-3.22	P,T	relative; treats unresolved Ryds as quasi-continuum; 6p Ryd=IP=3216.34 eV
	HW&94	3.19-3.34	P	threshold yields; PCI lineshape; shake-up model for KM satellites
	LM&94	3.19-3.22	P	(e,ion) coinc.; total and partial ion yields
	SK&94	3.49-3.52	P,T	KL double excitation; 3d <sup>2</sup> mixes with (1s,2p) <sup>-1</sup> 4p <sup>2</sup> - doublet structure
	BA&95	3.19-3.23	P	average charge state; PIPICO; enhanced higher charge down to 100 eV below 1s IP; virtual 1s states
	HM&95b	3.20-3.22	P	TIY, threshold e-; PIY; 2-step decay ~70% in 4p resonance; comp. to US&91
	KJ&95	3.21-5.21	P	β (photoioniz.); <230 eV KE 6 significant direct quadrupole; comp. to theory
	MBS95	3.19-3.21	P,T	relative; partial & total IY; PCI, mean ion charge increases 30 eV < Ar 1s IP due to lifetime & expt'l resolution; IE jumps 2.7 to 3.8 above edge
	A96	3.1-3.2	T,R	partial P.I. cross-sections
	ABZ96	3.19-3.22	T	comp. to K 1s; nuclear screening affects intensities; I(Ar1s63p) < I(K1s63p)
	ALS96	3.19-3.22	P,T	absolute; Auger-ion coincidence; PCI; cascades
	BA&96	3.1-3.2	P	partial ion yield, pre-edge ioniz. tails to ~60 eV below IP; 2p/1s comp.
	BS96	3.2-3.4	P,R	absolute, partial cross-sect. comp. to total
	KY96	3.1-3.6	P	many electron 'shake' structure
	ADB97	3.1-5	P	filtered white light; (e,ion), (e,e) coinc.; decomposition of Auger cascade
	AL&97	3.1-3.2	P,T	X-ray fluorescence, Auger e- coinc; vacancy cascade; HF calc.; PCI shifts
As 1s	H31	11.86	P	1 <sup>st</sup> chemical state XAS s; photographic; As, AsBr <sub>3</sub> , AsCl <sub>3</sub> , AsH <sub>3</sub> As <sub>2</sub> O <sub>3</sub>
Au 5p	KC&95	40-120	P,T	dual lasers; ground & (5d <sup>9</sup> 6s <sup>2</sup> )-valence excited Au; RHF calc; Fano profiles
	MSZ96	45-85	P,T	photoion yield; comp. of SR to dual laser plasma; Fano resonances
Au 4f	KC&95	40-120	P,T	dual lasers; ground & (5d <sup>9</sup> 6s <sup>2</sup> )-valence excited Au; RHF calc; Fano profiles
B 1s	LC&92b	190-220	P	laser generated; laser plasma X-rays, comp. of B I & II; DF calc.
	BPS97	190-200	T	shake-up/off is 30% of total PI; ioniz. only
Ba 4d	CM64b	90-140	P	photographic, continuum res.
	CM74	60-1200	P	photographic
	CT&74	80-160	P,T	compared to theory, continuum res.
	EL&74	80-160	P	continuum res., Rydberg analysis IP (98.3, 101.0)
	LW74	95-110	T	ab initio calculation, continuum res.
	PRW74	80-160	P,T	gas-solid comparison, compared to theory
	RRW74	90-140	P	gas-solid comparison
	EL&75	90-105	P	Rydberg analysis IP (98.25, 101.02)
	HFK75	90-105	T	alternate assignment of EL&75, ab initio calculation
	W75	85-160	T	ab initio calculation, continuum res., comp. to expt.(RRW74)
	W76	90-110	T	ab initio calculation, location of 4d <sub>9</sub> 4f <sup>1</sup> level
	C78	90-140	P,R	review, continuum res.
	WS78	90-110	T	ab initio calculation, continuum res.
	ZS80	90-140	T	absolute, time-dependent density functional theory
	HL81	95-135	P	absolute continuum X-section, normalized to theory (ZS80), sol. spectrum
	LM&81	85-150	P	collapse of d->f continuum res. in Ba Ba <sup>+</sup> Ba <sup>2+</sup> series, absolute
	C82a	90-140	T	collapse of 4d->4f continuum res. in Ba, Ba <sup>+</sup> , Ba <sup>2+</sup> series
	CM82	90-140	T	ab initio, potential barrier, relativistic effects, (Ba, Ba <sup>+</sup> , Ba <sup>2+</sup> )
	KCN82	90-140	T	absolute X-section, Ba and Ba <sup>2+</sup> , compared to expt (HL81)
	NSZ82	80-180	T	absolute cross-section, Ba, Ba <sup>+</sup> Ba <sup>2+</sup> , density functional method
	C83	90-155	T	quantum defect theory calc., compared to expt (LM&81)
	CF83	60-220	T	4d->f (Xe, Cs <sup>+</sup> , Ba <sup>2+</sup> etc), comp. to (LM81), cent. barr.; 4f collapse
	C84	60-220	T	res. width/energy relation

Ba4d . . .	BC&86	40-140	P,T	absolute, excitation of Ba*(6s6p <sup>1</sup> P), compared to LDRA theory
	BC&89	116-180	P	absolute, partial PI, comp. to theory
	HB&89	100-150	P	laser plasma, Ba <sup>2+</sup> , 4f res., 4f partially collapsed
	NI&89	90-210	P	part. & tot. IY; comp. to Cs; calc.; cascade scheme; strong mult. ion.
	RM&89a	90-140	P	absolute, total and partial, comp. to theory
	RM&89b	100-150	P	EY absorption, comparison of Ba..Tb; PES of Sm, Eu, Gd
	AC&90	100-150	T	RPAE, similar extend of single and double PI, comp to expt [HL81]
	KR&90	95-150	T	absolute, various approx.; comp. to expt.
	NY&90	60-220	P	total and partial ion yield; comp. across RE series
	R90	0-300	T	absolute; ion (1 <sup>+</sup> , 2 <sup>+</sup> ); absorption; comp of Ba 4d, Xe4d, Kr3d
	SZ92	80-160	R	absolute; comp. to Ba II; calc; review
	PN&93	80-180	P	absolute; comp. of atomic and BaC <sub>60</sub> - inside cage; EXAFS
	KWM93	40-1000	T	RPA(E) cacl. of $\sigma$ , BR and $\beta$ for all alkaline earths
	BC94	80-160	R	collapse of giant resonances in Ba, Ba <sup>+</sup> , Ba <sup>2+</sup> spectra
	BF&95c	80-140	P,T	absolute; laser plasma; comp. to ZS80, AC&90, KR&90
	KI&95a	90-140	P	photoabsorption and PI of ions; Ba <sup>2+</sup> , Ba <sup>3+</sup> yields
	R95	80-160	P,R	comp. of Ba, Ba <sup>+</sup> , Ba <sup>++</sup> ; 4d collapse
	KA&96c	90-140	P	partial ion yields; comp. of Xe, Ba, Eu 4d
	KCM96	90-140	P,R	comp. of Ba, Ba <sup>+</sup> , Ba <sup>++</sup> ; laser plasma
	BT97	90-150	T	absolute; MC-Dirac-Fock; comp. to expt.; only ion final states
	W01	80-160	P,R	review of atom and ion photoionization
	KA&02a	40-160	P	absolute, Ba <sup>+</sup> , Ba <sup>++</sup> PIY; 4f collapse mapped; isonuclear identical; $\Sigma(OOS) \sim 10$ suggests little cross-shell correlation
Ba 3d	CM74b	60-1200	P	photographic
	SN&84	770-810	P	relative, collapse of f-continuum, compared to theory
	KWM93	40-1000	T	RPA(E) cacl. of $\sigma$ , BR and $\beta$ for all alkaline earths
	AI&99	780-815	P,T	relative, TIY, 4f collapse; HF-calc; comp of Xe, Cs, BaBa 2p
	KM&84	5.2,5.6	P,T	heat pipe atomic vapour, IP(L3)=5256; (L2)=5633
Ba 2s	KM&84	6.0	P,T	heat pipe atomic vapour, IP(L1)=5998, natural line width = 1.9eV
Be 1s	ME74	110-140	P	photographic, Rydberg analysis IP (123.345), autoionization of Be I,II
	AC&76	130-320	T	ab initio calculation, continuum shape
	KC87a	120-145	P	Auger yield, strong shake-up satellites, partial X-sect., comp to solid
	KC87b	120-200	P	total and partial yields, relative, de-excitation (AI)
	K88	120-144	P	relative; 2e- (KL) transitions; strong threshold resonance
	C90	100-120	T	resonant decay of (1s,2p), comp. to Ne-like series
	CF&90	106	P	AI decay of (1s,2p); spectator dominates
	VS&92	120-145	T	absolute, R-matrix, comp. to expt. (KC87a,b)
	KWM93	40-1000	T	RPA(E) cacl. of $\sigma$ , BR and $\beta$ for all alkaline earths
	BPQ97	20-125	T	Be <sup>+</sup> ; absolute; R-matrix; e- and hv impact cross-sections
	LHC02	25-122	T	absolute; $\Gamma(Be1\sigma^{-1}) = 36.6$ eV; comp. to expt.
Br 3d	MP81	63-66	P	photographic, 3d->4p, 3 lines, Fano parameters
	NM91	62-83	P	relative, total ion yield, laser diss. of IBr; 0.118 eV fwhm
	NMC92	64-66	P	total ion yield, laser dis.. Br <sub>2</sub> , 50 meV fwhm
	CS96	50-800	P,T	Br, Br <sup>+</sup> , Br <sup>++</sup> ; dual laser plasma; ab initio MC-HF calc; 3d 6f resonances
C 1s	RM79	300-1000	T	absolute: K-shell absorption X-sec. for many astrophysical species
	JNT87	250-480	P	C <sup>4+</sup> , soft X-ray plasma source and sample generator
	JNT90	260-480	P	C <sup>I</sup> , C <sup>II</sup> , C <sup>III</sup> , C <sup>V</sup> , soft X-ray source & sample; strong Ryd.&cont.; like CH <sub>4</sub>
	GJ91	297.4	T	IP.; f calc of common interstellar elements; KL structure
	HK&92	275-500	P	laser-ionized; laser continuum source; C <sup>2+</sup> , C <sup>3+</sup> , C <sup>4+</sup> spectra identified
	TG&93	300-500	P,T	C <sup>2+</sup> (C II); absolute; laser generated ion and light source; comp. to Cowan HF calc.; strong discrete lines
	JN&95	300-600	P	absolute; dual lasers; C <sup>III</sup> , C <sup>IV</sup> , C <sup>V</sup> lines; C <sup>IV</sup> PI X-sect; comp. to RM79

C1s . . .	MBH97	300-500	T	absolute PI for C(IV); comp to JN&95
	W01	280-480	P,R	review of atom and ion photoionization
	PB&20	280-1000	P,T	C <sup>-</sup> photodetachment; m <sup>-</sup> removed (m-2-5); double K-shell ionization
	MB&23	290-350	P,T	C <sup>2+</sup> ; absolute; single photon absorption, double excitation
C 2s	CM&04	40	T	GOS
Ca 3p	SH&85	30-35	P	Ca <sup>+</sup> , Ca <sup>2+</sup> yields at 3p threshold
	BG&87	40-150	P	absolute, partial X-sections, comp. to theory
	CBS87	30- 40	P	revised assignments, MCQD theory
	SZ92	30-40	R	Ca <sup>+</sup> , partial cross-section
	KWM93	40-1000	T	RPA(E) cacl. of $\sigma$ , BR and $\beta$ for all alkaline earths
	GA&97	30-400	T	partial PI for 3p resonances in 3d-excited Ca <sup>+</sup>
	HH99	25-40	T	absolute; ab initio CI; compare to GA&97; core-core correlation needed
Ca 2p	M76a	100-1200	P	photographic
	MR&89	342-368	P	partial 3p (CIS), matches absorption, DES, breakdown of spectator model
	KK&92	348-368	P	relative, oven, photoion yield, comp. of (Ca,K,Mn,Fe)
	MH&92a	330-550	P	partial Ca <sup>+</sup> , Ca <sup>2+</sup> , Ca <sup>3+</sup> yields; cascade Auger from shake-up/off
	OH&02	345-360	P	TIY, PIY, resonant PES, configuration mixing
Ca 1s	AL&93	4.03-4.06	P,T	absolute; strong 1s 6 3p white line; LSD-HF-CI calc.
	KM&02b	100-2000	T	absolute, realxation effects; comp. of Ca, Mg, Sr
	MY&02b	8.0-35.0	P	inter-shell effects from X-ray emission; comp. of Ca, Ti, V K-shell
Cd 3d	CM&72	390-420	P,T	photographic, compared to theory
	CMT74	400-730	P,T	photographic, continuum res.
	CM77a	400-730	P	photographic, correction to CMT74 theory comparison
	C84	400-700	T	res. width/energy relation
Cd 4d	CHW78	30-250	P,T	absolute, continuum res., compared to theory
	BA&94	30-100	P	high resolution; Ryd. series and interchannel coupling identified
Ce 4d	WB&76	100-150	P	gas-solid comparison, continuum res.
	ZS80	110-134	T	ab initio calculation, continuum res., compared to expt (WB&76)
	MP&86	100-150	P	relative, partial X-sect, comp to theory (ZS80)
	RM&89a	100-160	P	absolute, total and partial, comp to theory
	RM&89b	100-150	P	EY absorption, comparison of Ba..Tb; PES of Sm, Eu, Gd
	SZ92	80-180	R	comp. of rare earth 4d edges; partial X-sections; comp. to calc.
	HZ96	90-150	P,R	relative, partial & total ion yields; review ion yield spect. of atoms
Ce 3d	TL&85	870-930	P,T	electron yield (solid), comp to multiplet calc, full RE series
Ce 2p	MST83	5.73,6.17	P	L3,L2, gas-solid comparison, (atom - metal)shift = 2.6(3)
	AM&90	5.7-6.4	P	gas-sol. comp.; comp of 2p spectra of Ce, Er, Gd, Sm, Yb
Ce 2s	MST83	6.56	P	gas-solid comparison, (atom - metal)shift = 5.3(6)
Cl 2p	CK&98a	202-212	P,T	TIY; high res. (20 meV); 16-22 meV natural linewidths; Slater-Condon calc
	CK&99	198-212	P,T	TIY; discharge in HCl; HF-Cl; intermediate coupling; 21 meV fwhm; $\Gamma$ = 16 meV – much less than expected (85 meV from KO79 – empirical)
	M01	202-212	T	relativistic CI; absolute, Rydberg excitations
Cl 1s	MI80	2.81-2.88	T	calculation of structured near edge continuum shape in atoms (8<Z<30)
Co 3p	DF76	50-90	T	interference lineshape, multiplet effects, compared to solid
	BSW79	50-90	P	photographic, gas-solid comparison
	MP&86	50-70	P	relative, comp. to other TM 3p spectra
	SZ92	80-180	R	comp. of rare earth 4d edges; partial X-sections; comp. to calc.
	FF&96	54-57	P,T	absolute; total and partial (Co <sup>++</sup> , Co <sup>+</sup> ) yields; initial state CI
	HZ96	40-60	P,R	relative, partial & total ion yields; comp. of 3d TM element PA and PI
	W01	45-65	P,R	review of atom and ion photoionization
Cr 3p	DF76	30-80	T	interference lineshape, multiplet effects, compared to solid
	M77	30-70	P	photographic
	BS&82	30-70	P	absolute, Rydberg analysis IP's (P(9/2:7/2:5/2) = 46.365,46.725,47.050)
	ADI83	30-70	T	ab initio (RPAE), total 3d X-section

Cr 3p ..	MP&86	38-60	P	relative, comp. to other TM 3p spectra, partial X-sect, comp calc [ADI83]
	CC&89	42-48	P	comp to Mn, $Mn^+$ ; Ryd. series plus discrete 3p63d res., Ryd. intensity from R-V mixing; IP's; 30 meV fwhm res.
	CK&91a	40-70	P	laser-plasma, relative, Cr vs. $Cr^+$ , comp. to metallic and molecular solids
	CM&91	40-70	P,R	laser-plasma, comp to $Cr^+$
	SZ92	30-80	R	comp. of 3p edges of 3d-transition metal atoms
	D93b	40-100	T	absolute; comp. to (MP&86); Ryd/3p6nd mixing affects decay dynamics
	DB&96	39-42	P,T	laser aligned ground state; linear dichroism up to 30% in discrete 3p 6 d res.
	HZ96	40-60	P,R	relative, partial & total ion yields; comp. of 3d TM element PA and PI
	KC&99	40-65	P,T	dual laser plasma, multiplets
	MM&99a	35-65	P,T	absolute; laser plasma $Cr^+$ ; metastable excitation line detected by comp. to HF calc
	MM&00	35-70	P,T	laser plasma $Cr^{++}$ ; HF calc; time-resolved
	CM&01	60-160	P,T	relative; laser plasma $Cr^{++}$ ; HF calc;
	CS&01	64-130	P,T	relative; laser plasma $Cr^{++}$ , $Cr^{3+}$ , $Cr^{4+}$ ; discrete lines; giant resonance collapse
	GR*03	60-130	P	PIY, $Cr^+$ , $Cr^{++}$ , Fano profiles
Cr 2p	AI&95	570-590	P,T	total ion yield, HF calc
Cr 1s	AL&93	5.98-6.01	P,T	absolute; strong white line; LSD-HF-CI calc.
Cs 4d	RS74	78-92	P	compared to theory
	PR&75	75-180	P	photographic, continuum res. compared to theory, (4d+5p) excitations
	C78	75-180	P,R	review, continuum res.
	C82b	75-180	T	intermediate valence modelled by 4d->4f excitation, pot. barrier effects
	PR&86	50-130	P	absolute total & partial yields, collective d-->f, satellite X-sections
	HB&89	100-150	P	laser plasma, $Cs^+$ , 4f res. collapse
	NI&89	70-190	P	partial & total ion yield; comp. to abs., calc., Ba4d; cascade decay scheme
	NY&90	60-220	P	total and partial ion yield; comp. across RE series
	CS97	80-150	P,T	relative; photographic; dual plasma; ab initio calc.; comp. to $Ba^{2-} \dots La^{3+}$
	KA&02a	40-160	P	absolute, $Cs^+$ PIY; 4f collapse mapped; isonuclear identical; $\Sigma(OOS) \sim 10$ suggests little cross-shell correlation
	AI&99	780-815	P,T	relative, TIY, 4f collapse; HF-calc; comp of Xe, Cs, Ba
Cs 4p	PR&75	158-180	P	photographic, Rydberg structure
Cs 3d	CM76a	700-850	P	photographic, continuum res.
	SN&84	730-760	P	relative, collapse of f-continuum, compared to theory
	AI&99	725-760	P,T	relative, TIY, 4f collapse; HF-calc; comp of Xe, Cs, Ba
Cu 3p	BSW79	50-90	P	photographic, gas-solid comparison
	DF81	70-90	T	Fano line-shape effects, compared to experiment (BSW79)
	C82c	35-90	T	partial and total X-sect, comp to Xe 3d, La 3p
	C86	35-90	T	R-matrix CI, partial & total X-sect, comp to (BSW79), 3p63d ang. dist.
	DS&91	40-130	P,T	state-selective decay; $V6Cu^+$ , Ryd 6 $Cu^{2+}$
	SZ92	60-85	R	comp. of 3p edges of 3d-transition metal atoms
	VD&98	60-95	T	absolute; comp. to BSW79; R-matrix
	VW&00	68-90	P	relative; CIS resonant photoemission; Rydberg series; comp to theory
Cu 2p	AI&94	925-975	P,T	absolute; TIY and abs. very similar; HF (Cowan) calc; comp. to Cu(sol)
Cu 1s	SZ92	8.97-8.99	R	relative, comp. to solid.
	AL&93	8.97-8.99	P,T	absolute; strong white line; LSD-HF-CI calc.
Dy 4d	DF&89	80-180	P,T	absolute, partial ion X-sections; comp. to calc.
	SZ92	80-180	R	comp. of rare earth 4d edges; partial X-sections; comp. to calc.
	HZ96	80-180	P,R	relative; 4d excitation; partial ion yields; comp. to TDLDA calc.
Dy 3d	TL&85	1.28-1.34	P,T	electron yield (solid), comp to multiplet calc, full RE series
Er 4d	BK&93	140-200	P,T	relative; total and partial ion yields; comp. of Er, Ho, Tm; HF calc
Er 3d	TL&85	1.40-1.45	P,T	electron yield (solid), comp to multiplet calc, full RE series
Er 2p	MST83	6.98,7.62	P	L23, gas-solid comparison, (atom - metal)shift = 3.7(3)
	AM&90	7.0-8.0	P	gas-sol. comp.; comp of 2p spectra of Ce, Er, Gd, Sm, Yb

Er 2s	MST83	8.06	P	gas-solid comparison, (atom - metal)shift = 3.6(7)
Eu 4d	MC76	41-310	P,T	photographic, continuum res., compared to theory
	C84	50-300	T	res. width/energy relation
	BK&86	120-200	P	total and partial yield, compared to calc [C84] and 3d
	PCK87	110-200	T	partial and total yields, 4d6ef res.
	NY&90	60-220	P	total and partial ion yield; comp. across RE series
	PCK&91	100-200	T	partial & total yield; MBPT; 4d6ef reson.; comp. to expt (BK&86)
	SZ92	80-180	R	comp. of rare earth 4d edges; partial X-sections; comp. to calc.
	KA&94	120-145	P	partial AI yields at giant res.; differ from direct ioniz. Auger; comp. of Eu,Sm
	BS96	110-160	P,R	absolute, partial cross-sect. comp. to total
	KA&96c	110-140	P	partial ion yields; comp. of Xe, Ba, Eu 4d
	KSP96	110-160	P,T	(e,ion) coinc. predicted; vacancy cascades; 4d 6 4f forbidden decay
	LG&96	132-148	P	partial PI X-sect.; ( $\text{Eu}^{2+}$ - $\text{Eu}^{4+}$ ) true PEPICO - ions & PE (TOF-CMA)
	SS&97	125-150	E	relative; excitation and e- emission spectra; 300 & 173 eV impact; 4d giant res.
	KO&98	110-160	P	$\text{Eu}^+$ ionized by SR; partial ion yild spectra; 4d6ef res.
	TK&00	120-160	T	spin-dependent density functional (TDLSDA); spin down broad; spin-up sharp
	TK&01	110-160	T	$\text{Eu}^0$ , $\text{Eu}^+$ cross-sections; DFT
	SW&02	133-152	P, T	linear dichroism by electron analysis, HF-CI, LS coupling model; comp. to Gd(s)
Eu 3d	TL&85	1.12-1.16	P,T	electron yield (solid), comp to multiplet calc, full RE series
	BK&86	1.10-1.18	P	total and partial yield, strong cross-channel coupling, orbital collapse
	RM&89b	120-180	P	EY absorption, comparison of Ba..Tb; PES of Sm, Eu, Gd
F 1s	SK&90	677	P	atomic FL of $(1s, 2p^6)^2S$ from HF; ultrafast decay
	KNS90	670-820	T	calc. of KL ioniz. in F; strong 2e- complication to F-K EXAFS
Fe 3p	DF76	50-90	T	interference lineshape, multiplet effects, compared to solid
	BSW77	50-90	P	photographic, gas-solid comparison
	BSW79	50-90	P	photographic, gas-solid comparison
	N79	50-90	T	ab initio calculation, compared to experiment (BSW77)
	MP+86	40-80	P	relative, comp to other TM (3p), partial X-sect, Fano fit
	TLP90	50-700	T	partial X-sect. for $\text{Fe}^{n+}$ , n=0 to 13; evolution of 3p63d res.
	SZ92	30-80	R	comp. of 3p edges of 3d-transition metal atoms
	FF&96	50-70	P,T	absolute; total and partial ( $\text{Fe}^{++}$ , $\text{Fe}^+$ ) yields; initial state CI
	HZ96	50-70	P,R	relative, partial & total ion yields; comp. of 3d TM element PA and PI.
	L98a	45-65	T	absolute; rel. TD local spin; comp. to expt; circular pol. response predicted
	BB01a	30-75	T	absolute; $\text{Fe}^+$ , $\text{Fe}^{++}$ ionization/absorption; R-matrix
	KK&02	30-180	P	absolute; $\text{Fe}^+$ ionization/absorption; comp. to BB01
	WW&02	47-68	P	relative, partial PE cross-sections; 3d giant resonances
	BG&12	50-70	P	photodetachment (2e-) from $\text{Fe}^-$
Fe 2p	KK&92	701-725	P	relative, oven, photoion yield, comp. of (Ca,K,Mn,Fe)
	B00a	701-720	T	absolue; R-matrix; electron impact cross-section for $\text{Fe}^{15+}$ (plasma)
	B00b	0.02-10 kV	T	absolue; R-matrix; threshold structure in EI cross-sections
	BB01b	100-1300	T	absolute; FeIII, FeVIII ionization/absorption; R-matrix
	BBB01	0.5-10 kV	T	absolute; Li-like, Be-like Fe; modelling for Chandra
Fe 1s	GJ91	7123.6	T	IP,; f calc of common interstellar elements; KL structure
Ga3d	CJKJ88	20-100	P	partial PI cross sections; $\beta$ 's; Cooper minimum
	KCF83	19-22	P	decay of 3d $\rightarrow$ 3p resonance; CIS PES
Gd 4d	CP84	120-200	P	4d-->f continuum res., fit to C84 lineshape, compared to $\text{GdF}_3$
	RM&89b	130-160	P	EY absorption, comparison of Ba..Tb; PES of Sm, Eu, Gd; AI (DES)
	SZ92	80-180	R	comp. of rare earth 4d edges; partial X-sections; comp. to calc.
Gd 3d	TL&85	1.14-1.22	P,T	electron yield (solid), comp to multiplet calc, full RE series
Gd 2p	MST83	7.25,7.94	P	L3,L2; gas-solid comparison, (atom - metal)shift = 2.8(3); 2.9(3)
	AM&90	7.0-8.2	P	gas-sol. comp.; comp of 2p spectra of Ce, Er, Gd, Sm, Yb
Gd 2s	MST83	8.06	P	gas-solid comparison, (atom - metal)shift = 4.7(4)

Hf 4p	GBP82	>380	T	inner-shell excitation contributions to total cross-section calculated
Hg4f,5s	CM73	100-620	P	photographic, transmission maximum around 160eV
Hg 1s	H31	12.2 – 14.0	P	1 <sup>st</sup> chemical state XAS ; photographic; compare Hg, HgCl <sub>2</sub>
Hg 2p	KM&84	12.2,14.2	P,T	heat pipe atomic vapour, IP(L3) = 12292, IP(L2) = 14219
Hg 2s	KM&84	14.8	P,T	heat pipe atomic vapour, IP(L1) = 14849, line width = 6.2eV
Ho 4d	BK&93	130-200	P,T	relative; total and partial ion yields; comp. of Er, Ho, Tm; HF calc
Ho 3d	TL&85	1.34-1.40	P,T	electron yield (solid), comp to multiplet calc, full RE series
I 4d	MPT81	60-120	P	photographic, d-->f res.
	ND&90	45-54	P,T	laser dissociated I <sub>2</sub> , strong 4d-65p ( <sup>2</sup> D) res.
	NM91	44-60	P	total ion yield, PES, DES, laser produced I, Br
	NSM91	60-130	P,T	absolute; total & partial X-sect.; laser-generated I atoms; PES; ion KE; centr. barr. effects?; sum rule, N <sub>eff</sub> < 10
	MNN92	44-60	P	laser produced I from I <sub>2</sub> ; PES, DES
	NMC92	44-60	P	TIY, PES, DES, laser diss. I <sub>2</sub> ; 4d 6 5d
	SM&96	45-300	P,T	laser plasma; I, I <sup>+</sup> , I <sup>++</sup> absorption; MCI-HF calc; 4d 6 f dominates
	AC&00b	40-136	T	absolute, I <sup>0</sup> , I <sup>+</sup> , I <sup>++</sup> ; RPAE; com to NSM91; x3 deviation = unknown physics ?
	KA&00	40-140	P	absolute; I <sup>+</sup> , I <sup>++</sup> PIY; giant resonances
	W01	50-120	P,R	review of atom and ion photoionization
	AC&02	40-150	T	absolute; I <sup>0</sup> , I <sup>+</sup> , I <sup>++</sup> excitaiton; GRPAE, comp. to KA&00
	DT02	60-130	T	absolute; I <sup>0</sup> , I <sup>+</sup> , I <sup>++</sup> excitaiton; DFT, comp. to KA&00
	KA&02a	40-160	P	absolute, I <sup>+</sup> , I <sup>+</sup> , I <sup>++</sup> PIY; 4f collapse maaped; isonuclear identical; Σ(OOS) ~10 suggests little cross-shell correlation
I 3d	KG&18	610-680	P,T	I <sup>+</sup> , PIY, compare PIY for I <sup>+</sup> and HI <sup>+</sup>
	SG&19	610-670	P,T	I <sup>+</sup> , PIY, DFT calc; compare CH <sub>x</sub> I <sup>+</sup> (x = 0–3)
In 4d	LOL84	20-240	P,T	abs.; sol.; comp. to I <sub>2</sub> (CNS73) Xe(HK&69), 4d Cooper min.; struct. 4d->εf
Ir 5p,4f	MS&97a	40-70	P,T	relative; atomic beam; Ir <sup>+</sup> , Ir <sup>++</sup> yields; Fano profie
K 2p	M75	270-350	P	photographic
	MH&92	270-400	P	K <sup>+</sup> , K <sup>2+</sup> , K <sup>3+</sup> yield, cascade Auger and shake processes
	KK&92	292-315	P	relative, oven, photoion yield, comp. of (Ca,K,Mn,Fe)
	BRK00	296-300	E	metastable state detection; K*
K 1s	BA&95	3.59-3.62	P	multicharge state yields, tail to low E of high charge states - virtual 1s
	ABZ96	3.59-3.62	T	comp. to Ar 1s; nucl. screening changes intensities; I(Ar1s63p) < I(K1s63p)
	PK&01	3.59-3.67	P	realitive, 1s3s3p doubly excited states
Kr 3d	CM64	80-105	P	photographic, Rydberg analysis IP (93.82, 95.04)
	LBZ64	30-620	P	absolute
	LZB64	88- 98	P	photographic
	CM65	60-180	P	photographic
	MC68	30-250	T	ab initio calculation, delayed onset
	AG&69	0-300	E	angular dependence of inelastic scattering, differential cross-section
	HK&69a	90-130	P	absolute, gas-solid comparison
	ZG71	40-300	P,T	review, continuum res.
	CM75a	90-250	P	photographic, absolute
	GM&76	90-95	P	Rydberg structure, no analysis
	CM77a	95-275	P	photographic, correction to CM75a theory comparison
	KT&77	90-96	E	Rydberg analysis IP (93.79, 95.04), Z+1 analogy, <70meV FWHM res.
	EKK78	90-120	P	Auger decay of res. lines
	C84	90-200	T	res. width/energy relation
	HM&84	90-96	P	absolute, total and ion yield spectra, no P.C.I. detected
	AA&86b	90-120	P	energy dependence of Auger and AI spectra
	DSK86	89-95	E	high res. (65 meV), d-->s quadrupole transitions
	AA&87	40-160	P	partial and total PI X-sections, 4s Cooper minimum
	HL&87	90-98	P	threshold PES, shake-off at discrete res.

Kr 3d . .	LH&87	90-93	P	DES, partial yields at 5p, 6p res., X-sections, $\beta$ s
	CM&88a	91	P	anisotropy of DES (AI) at 3d63p; parity forbidden transitions
	K88	20-160	P	partial PI X-sections
	AA&89b	91-94	P,T	DES, shake-up intensities
	CM&89	91-94	P	resonant Auger, ang. dist.; comp. of Ar,Kr,Xe
	MLL89	91-94	P	ionic yields, direct double ionis. versus 1- and 2-step autoionisation
	AA&90a	91-94	P,T	DES, shake-up fraction comp. of Ne1s, Ar2p, Kr3d, Xe4d
	BS90	91-94	P,R	DES at 5p Ryd; comp. of Kr, Ne, Ar DES
	HY&90a	80-280	P	ion yield spectra ( $\text{Kr}^{2+}, \text{Kr}^{3+}, \text{Kr}^{4+}$ )
	HY&90b	89-99	P	partial and total ion yields; (ZEKE,ion) coinc; PCI
	MH&90	80-280	P	absolute, partial ion yields, multiple ionis. ratios ( $\text{Kr}^+ - \text{Kr}^{4+}$ )
	R90	90-400	T	absolute; ion (1+, 2+); absorption; comp of Ba 4d, Xe4d, Kr3d
	VM&90	91	P	(hv,2e); 2-step autoionization decay of discrete states in Ar, Kr, Xe
	AH&91	90-97	E	near threshold; triplets; PCI shifts; lineshape analysis; comp. to theory
	HM&91a	90-130	P	threshold EY vs. total ion; strong conjugate shake-up
	II&91	>95	E	PCI shift of Auger, comp. of Ar LMM, Kr MNN, Xe NOO
	LM91	88-98	P	absolute; total & partial IYs; 1-(22%) & 2-(57%) step decay; direct DI
	AA&92b	91-94	P	resonant AI; ion branching ratios; comp. of Ar, Kr
	CC&92	80-200	E	absolute; comp. of Ar, Kr, Xe
	CW&92	90-94	P,T	$\text{Kr}^+, \text{Kr}^{2+}$ resonant PES; spectator shake process; 2-step AI; PCI
	DM&92	90-95	P	high res. (20 meV); SX-700II characterization
	SS92d	44-1300	P	PIY and BR for multi-charge ions of Ne, Ar, Kr, Xe; $\Delta$ BR at edges
	TA&92	95-260	P,T	absolute, partial 3d, 4s, 4p X-sect.; $\beta$ , 5/2:3/2 branch. ratios, MMDF calc
	C93	100-5000	T	X-sect; $\beta$ ; comp. of all rare gases; ang. cor. correct.; dipole breakdown
	AK&94	90-95	P	<20 meV fwhm; instrument test on Rydbergs
	GE&94	90-96	P	4s,4p partial PI yields; 5p resonance dominated; com. to Ar 2p; Fano lineshape
	SS94	80-120	P	BR of multiple PI; Auger; comp. of 2e- ionization of Ne,Ar,Kr,Xe
	A95	91	P,R	resonant Auger; high resolution
	AK&95	80-100	P	SX-700 pgm at MAX performance, 2e4 resolving power
	SK&95c	90-95	P	accurate natural linewidths; partial ion yields
	HZ96	90-95	P,R	relative, partial & total ion yields; review ion yield spect. of atoms
	KAA96	91	P	Auger resonant Raman; line narrowing; influence of finite photon bandwidth; lifetime interference
	SK&96	243-253	P	high res.; 4 meV/eV E-scale comp.; $\Gamma(6p) = 83(1)$ up to $\Gamma(10p) = 68(8)$
	AK&97b	92-94	P	resonant Auger; PCI studied; shake transitions
	KA&97	92-93	P,T	resonant Auger; lifetime interference of 2 channels
	SA97	95	P,R	angle-resolved Auger resonant Raman
	SS98a	90-120	P	charge state PIY; PE-PI coincidence
	BA&01	105-127	P	threshold EY, ion coincidence
	DH&02	~90	P	time-domain inner shell spectroscopy; 2 atto-sec probe of Kr 3d decay
	YZ&02	90-110	E	absolute, OOS from EELS
	SA&06	90-91	P,T	relative, $\beta$ -spectrum, interference with 4p <sup>4</sup> np direct; 10 meV resolution, ab initio
	CM12	95	P, R	review of lifetime-limited linewidths (many small mol. & atoms)
	WM69	150-305	P	photographic, Rydberg analysis IP (215.0)
	HM&86	200-230	P	abs.; tot.& part. IY (to $\text{Kr}^{4+}$ ); Ryd. series in $\text{Kr}^{4+}$ ; C-K Auger cascade
	SDM88	220-350	T	absolute; comp. various methods; non-EXAFS, non-Cooper min. osc. in ATOMS
	SW&99	220-230	P	gas-cluster-solid comparison; Rydberg – exciton conversion
	MY&02a	205-235	P	TIY, PIY, threshold yield; PCI; Auger cascade; branching ratios
	CH&01	400-1400	P,T	absolute; 3d, 3p, 3s cross-sect. far above threshold; ang. dist.; channel coupling
	H31	1650-120	P	photographic; compare atoms and vapors
	KNY93	1670-1760	T	HF-MC; multi-electron effects at L <sub>3</sub> and L <sub>2</sub> thresholds in Kr 2p and Xe 2p
	SG&95a	1660-1760	P	gas, cluster comparison, 3d exciton in cluster is 0.5 eV above gas

Kr2p ...	HT&99	1660-1720	P,T	TIY, threshold ion coinc to Kr <sup>7+</sup> , PCI (up to 8 eV)
	NI&00	1650-1800	P	TIY, resonant Auger; ang. Dist
	KM&07	1640-1780	P	absolute cross-section
Kr 2s	C93	100-5000	T	X-sect; $\beta$ ; comp. of all rare gases; ang. cor. correct.; dipole breakdown
Kr 1s	S40	14.1-14.5	P	Rydberg lineshape analysis
	KE75	14.1-15.1	P	absence of extended fine structure (EXAFS)
	HK83	14.1-14.5	P	ion yields for different charge states
	KE&83	14.3-14.4	P	relative, gas-solid (Kr, KrF <sub>2</sub> ) comp., near-edge shape res. in solid
	MN&84	14.3-14.4	P	relative
	DH86a	14.1-14.6	P	accurate cross-section, compared to calc.
	DH86b	14.3-16.3	P,T	double excitation (1s + 3d,3p,3s,2p,2s)
	BB87	14.2-14.4	P	multiple ionization, partial X-sects simulated by absorption derivative
	YKD90	14.3-14.5	T	absolute; HF-MC; E,f calc; comp to MN&84
	DK92	14.3-15.0	P	multiple excitation
	IN&92	14.3-16.3	P	multiple-excitation; (1s3p), (1s3d), (1s,4p) double; (1s3d4p) triple
	LBB92	14.3-14.7	P	double ionisation continua identified; complication of ME to EXAFS
	SK&93a	14.3-14.8	T	single & multiple excitation; compt to DH86a,b
	HF&00	1.43-1.44	P	relative, PIY, TPEPICO, PCI, cascades
	KA&02b	14.3-14.7	P	absolute; multi-electron thresholds identified
La 4d	H72	110-150	T	ab initio calculation, location of 4f levels
	R77	90-150	P	continuum res., gas-solid comparison
	WS78	110-150	T	ab initio calculation, continuum res.
	R79	95-145	P	compared to solid
	CP&80	95-145	P	compared to metal, LaF <sub>3</sub>
	C82c	80-150	T	correlation effects at res.
	HM&87	100-150	P,T	partial and total; 4d6 $\epsilon$ f giant res.
	HB&89	100-150	P,T	laser plasma, La <sup>3+</sup> abs., 4f collapse
	RM&89a	100-160	P	absolute, partial and total, comp. to theory
	RM&89b	100-150	P	EY absorption, comparison of Ba..Tb; PES of Sm, Eu, Gd
	SZ92	80-180	R	comp. of rare earth 4d edges; partial X-sections; comp. to calc.
	KK&95a	90-150	P,T	dual lasers; La <sup>3+</sup> ; 4d 6 4f giant res.; HF-CI calc.
	K96	100-200	P,R	absolute; calc of 4f 6 d resonance
	KMC96	90-150	P,R	laser plamsa; La <sup>3+</sup>
	SK&96	243-253	P	high res.; $\Gamma(6p)=83(1)$ up to $\Gamma(10p)=78(8)$ ; comp. to SK&82
La 3d	EK&83	820-870	P,T	absorption, XPS (sol.) and multiplet calc. compared
	W84	810-860	T	non-relativistic RPA, non-stat. spin-orbit intensities, cont. res.
	TL&85	820-870	P,T	absorption (sol) comp. to calc.
Li 1s	FN67	55-90	E	metastable lifetimes
	ELM70	50-70	P	photographic, Li <sub>2</sub> lines observed
	CP75	60-80	T	pre-edge structure
	ZBS75	50-70	P	core-excited states from H <sup>+</sup> ,He <sup>+</sup> ion-impact-excited Auger spectra
	AC&76	60-120	T	absolute, continuum shape
	MW76	60-80	P	photographic
	CP&77	60-80	P	photographic, flash pyrolysis produced Li, Li <sup>+</sup>
	CS77	55-70	T	CI calculation of core-excited states, comp. to expt (ELM70, ZBS75)
	ML77	40-120	P	excitation of 2s to 2p excited Li, optically forbidden states
	ME&78	62-72	P	absolute
	SB&78	56-62	P,T	photographic, Z+1 analogy, compared to theory
	B79	40-120	T	ab initio theory, compared to ML77
	RM79	60-120	T	absolute, continuum shape
	GB81	40-120	T	ab initio theory, compared to ML77
	MCS82	70-115	P	absolute, Fano profiles, TRK-sum rule tested, comp. to (CP75,AC&76,RM79)

Li 1s . . .	SSE82	55-70	T	ab initio, line structure
	S85	60-80	P,R	heat pipe and laser plasma techniques
	DYM87	55-70	T	valence bond, ab initio, comp to LiH
	FL&87	70-100	P	absolute, partial and total X-sect, Fano profile (1s3s3p)
	MM&87	58-65	P	core excitation, decay of laser-valence excited, aligned atoms
	S87	60-63	P,R	comp. of absorption and AI spectra (ML77)
	LBH90	72-200	T	absolute; R-matrix; decay X-sections; comp. to FL&87
	LV&91	60-140	P	partial X-sections, satellite line branching ratios; conjugate shake-up
	S91a	50-75	P,R	angle-resolved autoionis. of laser-aligned-Li
	FM92	50-130	T	absolute, multi-electron processes, general considerations
	L92	50-100	T	R-matrix; complex structure above IP predicted
	SZ92	50-140	R	absolute, comp. to calc., AI resonances (polarised)
	CC94	60-70	T	absolute; CI; $1s^0 2p^3$ ; Fano resonance; R-matrix calcs.
	CD&96	140-147	P,T	PI line; 19 meV resolution; 118 meV natural linewidth
	DC&96	143-154	P,T	absolute; partial X-sect. for $2s^2 2p$ ionization; Li KK double excitation; 'hollow lithium'; R-matrix calc.; resonances in $1s2s$ and $1s2p$ $Li^+$ X-sect.
	JC&96	140-144	P,T	absolute; absorption; $Li^+$ yields; high res. (<10 meV); compares Rydberg structure at $Li^{K+}$ , $Li^{KV++}$ thresholds; R-matrix calc; window resonances
	KL&96	62-76	P,T	laser plasma; comp of Mg, Al <sup>+</sup> , Si <sup>++</sup>
	KMC96	54-64	P,R	absolute, photoionization cross-section
	VF&96	60-180	T	Auger decay of hollow Li
	DC&97a	150-175	P,T	absolute; partial X-sections; triply excited states = hollow Li; extended Rydberg series; 2 core-excited electrons are strongly bound, 3rd weakly bound.
	DC&97b	148-153	P,T	29 term R-matrix, hollow lithium ( $Li\ 2l2l'$ ) state; comp. to expt. (DC&97)
	KF&98	140-167	T	relative, dual laser plasma, comp. to theory (VF&96)
	MC&00	60-180	P	lineshapes for creating hollow $Li^+$ ( $2s^2$ ) states
	LM01	174-176	T	threshold for $Li^{++}$ ; Wannier theory compared
	WBW02	81-83	P	TIY,autoionization. Fano profile analysis,
	LWW09	70-77	P	absolute, $Li^-$ core excited states
Li <sup>-</sup> 1s	Z99	55-75	T	absolute, photodetachment involving $Li^- \rightarrow Li^+(1s^*)$
Mg 2p	KA&01	55-70	P	photographic, Rydberg analysis IP's (57.544,57.822)
	N71b	16-62	P	photographic, compared to theory, Rydberg analysis
	EM74	55-70	P,T	resonant AI; branching ratios
	WCK91	55-60	P	resonant AI; shake and PCI effects
	WTA91	55-60	P	RRPA, MBPT calc; ang. dist. for PE, Auger; expt-theory comp.
	KH&92	60-130	T,P	RPA(E) calc. of $\sigma$ , BR and $\beta$ for all alkaline earths
	KWM93	40-1000	T	absolute OOS, GOS; HF-CI; Born approx.
	MB97	50-100	T	partial cross-sections; R-matrix calculations
	WD&97	140-160	P,T,R	resonant AI; Mg <sup>++</sup> , dual laser plasma
	KC&99	95-120	P,T	review of atom and ion photoionization
	W01	40-160	P,R	IP.; f calc of common interstellar elements; KL structure
Mg 1s	GJ91	1310.6	T	$Mg^{7+}$ -Mg <sup>10+</sup> K-shell absorption in plasma; X-ray emission
	BD&92	1.3-1.7kV	P	absolute OOS, GOS; HF-CI; Born approx.
	MB97	1.30-1.31	T	absolute, realxation effects; comp. of Ca, Mg, Sr
	KM&02b	100-2000	T	photographic, comparison to solid Mn, MnF <sub>2</sub> , MnCl <sub>2</sub> , MnBr <sub>2</sub>
Mn 3p	CMM76	40-70	P	interference lineshape, multiplet effects, compared to solid
	DF76	50-90	T	photographic, gas-solid comparison
	BSW78	40-60	P	photographic, compared to theory
	CGM71	20-85	P,T	RPAE calculation, compared to experiment (BSW78)
	AIC81	40-70	T	absolute (4s,3d,3p), MBPT, compared to expt (BSW78)
	GB&83	40-100	T	res. width/energy relation
	C84	40-100	T	comparison of absorption (BSW78) with sum of partial cross-sections
	SS&85	40-70	P	

Mn 3p . .	MP&86	40-70	P	relative, comp. to other TM (3p)
	S86	43-63	P	3p,3d, photoabsorption and sum of PES compared
	K88	20-260	P	partial PI X-sections
	CC&89	45-70	P	comp. to Mn <sup>+</sup> and Cr 3p; v. weak Ryd.; strong 3p63d res.; IPs; 30 meV
	JK&89	65-230	P,R	part. X-sect (3p, 3s, 3d); β's; comp. to theory; multiplets; lit. review
	ADM90	47-90	P,T	4s( <sup>7</sup> S/ <sup>9</sup> S) BR; spin-pol. RPAAE; matches expt. (Sonntag unpublished); strong 3p63d, 4s62p coupling
	CK&91a	40-70	P	laser-plasma, relative, Mn, Mn <sup>+</sup> , comp. to metal and molecules (sol)
	CM&91	40-70	P	laser-plasma, Cr, Mn, Mn <sup>+</sup> compared
	KY91	45-70	T	absolute, p 6 ed resonance; effect of AI; PCI effect on position & width
	D92b	47-54	T	comp. of Mn <sup>+</sup> , Mn <sup>*+</sup> ; spin-resolved X-sections
	SZ92	30-80	R	comp. of 3p edges of 3d-TM atoms; partial X-sect; Mn <sup>2+</sup> , βs, calc.
	D93a	47-54	T	comp. of Mn <sup>+</sup> , Mn <sup>*+</sup> , Mn; SP-RPAAE; (3d+4s) X-sect.
	WK&94	80-120	P	partial 3d/4s and satellite X-sections; 3d giant res. in all channels
	A96	44-70	T	virtual 3p excitations; ratio of spin-up/spin-down 4s X-sect. in 3p region
	BS96	44-80	P,R	absolute, partial cross-sect. comp. to total
	CD96	44-60	T	RPAAE of 3p64s & 3p63d res.; reversal in PA (4s < 3d) relative to β(3d) (3d < 4s)
	DBH96	32-46	P,T	R-matrix; Mn <sup>+</sup> calcs; comp. to CC&89
	HZ96	35-65	P,R	relative, partial & total ion yields; comp. of 3d TM element PA and PI.
	K96	40-65	R	absolute; 3p resonances in 3d sub-shell cross-section
	DM98	45-65	T	ab initio; absolute; comp. to CK&91a
	L98a	40-60	T	absolute; rel. TD local spin; comp. to expt; circular pol. response predicted
	W01	45-70	P,R	review of atom and ion photoionization
Mn 2p	AF&92	635-660	P,T	comp. to solid (atomic); HF-calc (2p <sup>-1</sup> , 3d) single config. in int. coupling
	KK&92	633-654	P	relative, oven, photoion yield, comp. of (Ca,K,Mn,Fe)
Mn 1s	SZ92	6.53-6.56	R	relative, comp. to solid Mn
	AL&93	6.53-6.56	P,T	absolute; strong white line; LSD-HF-CI calc.
N 1s	G83	400-2000	T	absolute calculation
	PV87	40-440	T	absolute, compared to N <sub>2</sub> , origin of σ* res.
	GJ91	412.4	T	IP; f calc of common interstellar elements; KL structure
	BI&19	390-435	P,T	HN <sup>+</sup> ; PIY, XMolecule calc, compare N <sup>+</sup> , HN <sup>+</sup> , H <sub>2</sub> N <sup>+</sup> , H <sub>2</sub> N <sup>+</sup> nEXAFS
N <sup>+</sup>	GB&11	399-402	E,T	absolute, ion-photon merged beam
Na 2p	GC&69	20-90	P	photographic
2s	M70	35-160	T	calc. of levels and continuum cross-sections
	CGM71	20-90	P	photographic
	WR&72	30-160	P	absolute, gas-solid comp., Na2s structure & calc., comp. to theory (M70)
	CHW77	45-250	P	absolute, compared to theory (M70), expt (WR&72)
	LMS81	65-80	P	Na2s pe-edge and double excitation features, Fano profiles
	AP88	120-260	T	absolute; continuum intensity; large 3s63p shake-up
	CD&90	33-35	P	laser excited Na, (2p,2s) excitation; val. & core excit. independent
	ZB93	45-60	T	CI, uses semi-empirical (Z+1) core potential; autoionization rates, X-ray laser
	TMM94	64-72	T	ab initio CI; comp to WR&72; Fano profiles; AI resonances
	WJ&94	55-250	P,T	X-sect. for (2p,3s) (LV) satellites; direct double ioniz.; MBPT calc.
	R95	50-90	P,R	σ(++)/σ(TOT) in laser excited Na*
	CV&98	20-400	P,T	absolute; selected total and partial X-sects; PE partial X-sect.
	KC&99	68-82	P,T	dual laser plasma
	W01	44-48	P,R	review of atom and ion photoionization
	CM&04	40	T	GOS
Na 1s	L79	1.07-1.1	P	photographic, Z+1 analogy
	TLE82	1.07-1.1	P	1s63p line width = 0.30(5) eV
	STB83	1.07-1.1	T	semiempirical, comparison to TLE82
	S85	1.07-1.1	P,R	heat pipe and plasma techniques, analysis of TLE82

Na1s ...	YK&86b	1.07-1.08	T	ab initio, double excitation ( <u>1s</u> ,3pes; <u>1s</u> 4sep), comp. to TLE82
	YP&86	1.07-1.08	T	ab initio, comp to TLE82, relaxation and multiplet effects
	Y93	1.07-1.08	T	ab initio, CI; comp. to YP&86; modifies assignments
	TE&00	1.06-1.09	P	relative, compared to Na <sub>n</sub> in Ar matrix; Na(s); atom – solid
Nd 4d	RM&89b	100-150	P	EY absorption, comparison of Ba..Tb; PES of Sm, Eu, Gd
	SZ92	80-180	R	comp. of rare earth 4d edges; partial X-sections; comp. to calc.
	GG&98	100-160	P	relative, partial PI cross-sections; shape resonances in Pr, Nd
Nd 3d	TL&85	0.97-1.02	P,T	electron yield (solid), comp to multiplet calc, full RE series
Ne 2s	DM&92	45-49	P	high resolution (55 meV)
Ne 1s	B18	870	P	photographic
	B54	863-871	P	photographic, Rydberg analysis IP (870.79)
	L65	866-876	P	Ni L emission as source
	C05	879	T	DFT, small molecue BE and excitation energies
	W65	1.5-6.2	P	photographic, absolute
	W70	862-878	P	photographic, Rydberg analysis IP (870.2)
	W71	860-880	P	photographic, Rydberg analysis IP (870.3)
	WK74	100-2000	E,T	absolute, partial X-sections, comp. to calc.
	DK75	865-870	T	ab initio calculation, compared to experiment (B18, L65)
	SD&79	865-895	T	absolute, comp. to expt. (L65)
	B80	860-878	P,R	review, (W70 data)
	HB80c	863-878	E	Rydberg analysis IP (870.1), dipole forbidden transitions
	BQB81	865-872	P	ab initio calculation, compared to experiment (HB80c, W70)
	BD&82	863-878	E,R	dipole forbidden transitions, calibration (3p=867.23 eV)
	AVZ82b	532-540	P	comparison of H <sub>2</sub> O, NH <sub>3</sub> , CH <sub>4</sub> , Ne isoelectronic sequence
	EG&83	865-915	P	(1s,3p) line width 0.30(4)eV, 1s,2p double excit. Rydberg IP (870.28)
	LDR83	0-3 keV	E	Compton profile (E <sub>0</sub> = 25keV, 7° and 17° spectra shown)
	KS84	865-874	P	partial Auger (AI) yields; βs
	SB84	867.13(7)	E	calibration standard (1s->3p)
	KYP87	860-910	T	absolute; HF-MC; E,f calc; comp to (EG&83); KL excit.
	K88	100-2000	P	absolute; partial X-sect (from WK74)
	V88	860-900	T	absolute; shake-off cross-sects, comp. to XPS (PR 140 (1965) 1057)
	AA&89a	857,865	P,T	DES, comp. to calc. of Auger, AI
	LWP89	0.78-1.78	P	absolute; comp. to expt (W71); CI; enhanced near threshold; dynamic screening
	AA&90	870	P,T	DES, shake-up fraction comp. of Ne1s, Ar2p, Kr3d, Xe4d
	BS90	865-915	P,R	relative (from EG&83); DES at 3p; comp. of Kr, Ne, Ar
	H90a	860-900	E,R	absolute, comp. of Ne, NH <sub>3</sub> , N <sub>2</sub> H <sub>4</sub> , N <sub>2</sub> ; Ryd. vs. valence
	ST90	0-3000	E	absolute, double diff. (angle, E <sub>0</sub> ), X-sect (Bethe surface); Auger-loss coinc.
	GJ91	869.4	T	IP.; f calc of common interstellar elements; KL structure
	HF91	864-1200	P	comp. of gas-sol.; (unanalysed) EXAFS strong in solid; 1.2 eV exciton shift
	DM&92	865-872	P	high res. (70 meV); SX-700II characterization
	HM&92b	862-875	P	threshold e-; I(4p)>I(3p) interpreted as 2-stop vs. shakeoff
	S92	855-895	E,P,R	comp to NH <sub>n</sub> series
	SI&92	860-980	P,T	gas,solid, theory comp.; Ne <sub>87</sub> cluster gives good match to solid spectrum
	SS92a	810-1340	P	Ne <sup>x+</sup> partial ion yields
	SS92d	44-1300	P	PIY and BR for multi-charge ions of Ne, Ar, Kr, Xe; ΔBR at edges
	YM&92	865-871	P	220 meV fwhm; instrument paper
	ZKP92	0-1600	T	anomalous scattering factor exhibits Rydberg resonances
	SI&93	860-980	P,T	gas (W65), solid comp; identification of 2e- processes; 3p (1.2eV), 4p (0.8 eV)
				exciton shifted lower in sol. relative to gas
	TK&93	865-871	P,T	relative; treats unresolved Ryds as quasi-continuum; 6p~IP= 869.75(2) eV
	FB&94	865-871	P	comparison of atom, Ne <sub>n</sub> (25-3000) clusters and solid
	LB&94b	865-870	P	270 mV fwhm (1st), 195 mV fwhm (2nd order); 220 meV nat. linewidth
	SS94	860-900	P	BR of multiple PI; Auger; comp. of 2e- ionization of Ne,Ar,Kr,Xe

Ne 1s ...	BM&95	866-880	P	HERMON at SRC; 1e5 resolving power
	CC&95	860-875	P	SGM at SRBC performance test; high resolution
	HM&95a	865-871	P	PIY, Auger-ion coincidence; 2-step channels identified
	QO&95	865-871	P	Elettra; high resolution (190 meV estimated); natural LW of 310 meV
	RN&96	865-870	P,T	TIY, autoionization; electronic-state-lifetime interference; 1-step model
	JA&97	865-872	E,T	relative, 130 meV fwhm based on observed width of 250 meV
	MSB97	865-872	P	TIY, PIY, branching ratio in 3p resonance; small PCI
	RL&97	865-870	P,T	relative; TIY; {excitation, emission} interfere; RIXS; Stokes doubling in 3p DES
	CA&99	846-871	P,T	100 meV fwhm; 3p line 270 meV; Fano lineshapes
	PV&99	870	P	lifetime width = 250(10) meV
	SA&99	860-900	E,T	absolute, GOS (2.5 keV, 2.4 – 24°); double excitation; Bethe theory, CI
	G00	865-871	P,T	absolute, close-coupled with optical potential to treat spectator Auger
	SP&00	865-871	P	SB7 LURE beamline tests; $\Delta E/E > 8500$ ; 280 meV fwhm
	SY&00	870	P	resonant Auger Raman at 1s → 3p; 100 meV fwhm; $\beta$
	SO&01	870	P	sub-natural linewidths by resonant Auger
	FS&02	865-872	P	high res. (66 meV); Fano profile; interchannel interference
	KY&02	852-873	P,T	relative, $N^{4+}$ from $Ne^{3+}$ ; MCDF calculation
	NH02	840-1050	T	absolute; double core excitation/ionization – shake-up/off
	RR&12	800-1000	P	<b>FIRST TRUE X-RAY LASER !</b>
	YO&02	840-880	P,T	relative; $Ne^{x+}$ ( $x=1-3$ ) ion photoionization; MC-Dirac-Fock gets E right
	MB&17	700-920	P,T	$Ne, Ne^+$ PI cross-sections, absolute; 9-E's compared - 0.2 eV spread; $\sigma^{++}$ of $Ne^+$
	SK&22a	866-870	P	high accuracy E-caib (1s → 3p 867.278), $Ne, CO_2-O1s, SF_6-F1s$
Ni 3p	DF76	60-100	T	interference lineshape, multiplet effects, compared to solid
	BSW79	50-90	P	photographic, gas-solid comparison
	CB80	60-100	T	R-matrix, coupled channel
	FB80	35-200	T	R-matrix, CI, partial and total X-sect, compared to BSW79
	D86a	60-100	T	summary of TM calc by Davis and Feldkamp
	MP&86	60-100	P	relative, comp. to TM (3p), partial X-sect, Fano fit, comp. to [CB80,D86]
	SZ92	30-80	R	comp. of 3p edges of 3d-TM atoms, rel. part. X-sect.; comp. to calc.
	C93	100-5000	T	X-sect; $\beta$ ; comp. of all rare gases; ang. cor. correct.; dipole breakdown
	FF&96	54-82	P,T	absolute; total and partial ( $Ni^{++}, Ni^+$ ) yields; initial state CI
	HZ96	60-80	P,R	relative, partial & total ion yields; comp. of 3d TM element PA and PI
O 1s	SG82	530-1200	T	absolute calc. 1s->2p res. claimed at edge, compared to expt(BB&79)
	GJ91	500-700	T	absolute; IP; $E_{th}$ , f calc of common interstellar elements; KL structure
	KC&96	525-555	P	ion yield; compound to atom (1s 6 3p at 527.8 eV)
	MB&96	525-560	P,T	TIY; discharge mix of $O_2/O$ ; $\Gamma = 140(9)$ meV; HF calc.; 1s → $\pi^*$ at 527.8(1) eV
	SL&97	525-553	P	PIY ( $O^+, O^{++}$ ) from O atom; strong 2p line; PCI
	MK98	520-560	T	absolute; R-matrix; comp to SL&97, MB&96
	GM00	520-560	T	absolute; R-matrix; comp to SL&97, MB&96; 1s → 2p at 527 eV
	AC&01	525-550	P	relative; XAS and XPS; metastable O atom & molecules
	KY&02	524-540	P,T	relative, $O^{++}$ from $O^+$ ; MCDF calculation
	ZY02	526-535	T	absolute; CI, R-matrix; 1s-valence interaction
	SH&22	525-1500	P,T	$O^-$ anion; multiple photodetachment
Pb 4f	CDM76	120-310	P	photographic
Pr 4d	RM&89b	100-150	P	EY absorption, comparison of Ba..Tb; PES of Sm, Eu, Gd
	SZ92	80-180	R	comp. of rare earth 4d edges; partial X-sections; comp. to calc.
	GG&98b	100-140	P	relative, partial PI cross-sections; shape resonances in Pr, Nd
Pr 3d	TL&85	920-960	P,T	electron yield (solid), comp to multiplet calc, full RE series
Pt 5p,4f	CK&91b	40-90	P	laser plasma generated and source; 5p 6 5d resonances
	SM&94	40-90	P,T	partial PI ( $Pt^+, Pt^{2+}$ ); TIY; rel-HF; $I(5p+4f)/I(5d+6s)$ related to $Pt^{2+}/Pt^+$ ratio
	BG&12	40-90	P	(2e-) photodetachment from $Pt^-$

Rb 3d,3p	MC75a	120-280	P	photographic
	KH&87	112-125	P	total and partial ion yields, no Rb <sub>+</sub> , matches absorption (MC75a)
	CM76b	110-280	P	photographic, delayed continuum onset
	CM77a	120-280	P	photographic, correction to MC75a theory comparison
	MJ81	130-150	T	Z+1 analogy, ab initio calculation, analysis of CM76b
	MC82	105-135	T	inadequacy of Z+1 analysis, compared to expt (CM76)
	KH&87	110-150	P	multiple ionization yields, 0.2 shake probability
	AL&88	113	P	resonant Auger (DES), strong spectator signal (Auger shake-up)
	KH&90	110-280	P	multiple ionization yields, 0.2 shake probability
	L98b	110-120	P,T	resonant Auger; MC-DF calc.
Rb 1s	KA&02b	15.2-15.8	P	absolute; multi-electron thresholds identified
Re 5p,4f	MS&97	35-70	P,T	absolute; TIY & PIY; relativistic; fused wire TOF
Rn 1s	T85	98-170	T	relativistic calc., PCI small, no oscillation (cf. MI80)
S 2p	KA&02c	30-200	P	absolute; S <sup>+</sup> →S <sup>++</sup> , S <sup>3+</sup> ; x2 deviations with accepted astrophysics values
	BG&12	218-228	P	multi-electron photodetachment from S <sup>-</sup>
S 1s	GJ91	2479.9	T	IP; f calc of common interstellar elements; KL structure
Sb 4d	BC94	20-120	P,R	relative; comp. to general. shape for atomic giant res.; comp. to solid, Sb <sub>5</sub>
	DC99	30-40	P,T	relative, dual plasma, HF calc; metastable; Sb, Sb <sup>+</sup> , Sb <sup>++</sup> , Sb <sup>3+</sup>
	AC&00c	30-100	P,T	relative, dual plasma, HF calc; metastable; Sb, Sb <sup>+</sup> , Sb <sup>++</sup> , Sb <sup>3+</sup> , Sb <sup>4+</sup> ; 4f continuum
Sc 3p	MP&86	30-50	P	comp. of 3p edges of 3d-transition metal atoms
	SZ92	30-50	R	comp. of 3p edges of 3d-transition metal atoms, rel. partial X-sections
	HZ96	30-50	P,R	relative, partial & total ion yields; comp. of 3d TM element PA and PI.
	KS98	50-70	P,T	Si <sup>3+</sup> ; dual laser plasma; RPAB calc.
	W01	28-48	P	absolute; dual plasma
	WK&01	29-40	P	CIS PES, relative PI cross sections
	M02	28-45	T	absolute; CI, strong correlation effects; compare to W01
	SM&02b	28-45	P,T	absolute; Sc <sup>++</sup> →Sc <sup>+++</sup> ; test of microscopic reversibility
Sc 2p	RO&01	397-410	P,T	relative, TIY, PIY, HF calculation agrees
	RO&03	397-410	P	relative, partial ion yields; photoelectron spectra – DES
Si 2p	PVZ82	100-140	T	multiple scattering calc. of continuum shape, compared to SiH <sub>4</sub> , SiF <sub>4</sub>
	SK&95a	105-140	P,T	(Si <sup>2+</sup> ); dual plasma; HF-CI calc.
	KMC96	110-140	P,R	laser plasma; comp. of Mg, Al <sup>+</sup> , Si <sup>++</sup>
	CK&98a	93-113	P,T	relative; dual laser plasma; absorption from metastable Si <sup>*+</sup> , Si <sup>2+</sup> ; HF calc
	CK&98b	105-190	P, T	Si <sup>+</sup> ; dual laser plasma; ab initio calc.; comp. to Al
	KC&99	100-130	P,T	dual laser plasma
	W01	143-165	P,R	Si <sup>+</sup> excitation; review of atom and ion photoionization
Si 1s	GJ91	1.849	T	IP; f calc of common interstellar elements; KL structure
	PB&21	1.83-1.90	P,T	Si <sup>-</sup> photodetachment; m <sup>-</sup> removed (m-2-6)
	SS&22	1.6-1.9	P	(Si <sup>m+</sup> , m=1-3)
Sm 4d	R77	120-160	P	gas-solid comparison
	PR&86	120-160	P	absolute total and partial X-sections (4f,4d,5p), collective res.
	RM&89b	110-170	P	EY absorption, comparison of Ba..Tb; PES of Sm, Eu, Gd
	NY&90	60-220	P	total and partial ion yield; comp. across RE series
	SZ92	80-180	R	comp. of rare earth 4d edges; partial X-sections; comp. to calc.
	KA&94	115-140	P	partial AI yields at giant res.; differ from direct ioniz. Auger; comp. of Eu,Sm
	LG&96	124-144	P	partial PI X-sect.; (Sm <sup>2+</sup> - Sm <sup>4+</sup> ) true PEPICO - ions & PE (TOF-CMA)
Sm 3d	TL&85	1.02-1.12	P,T	electron yield (solid), comp to multiplet calc, full RE series
	SB&91	1060-1120	P,T	relative, gas-sol; theory (Dirac-Fock); intermediate-valence; comp of Sm, Tm
	BC94	1060-1120	P,R	relative; gas-sol. comp. (SB&91)
Sm 2p	MST83	6.72,7.32	P	L23, gas-solid comparison, (atom - metal)shift = 3.8(3); 3.9(3)
	AM&90	6.5-7.5	P	gas-sol. comp.; comp of 2p spectra of Ce, Er, Gd, Sm, Yb
Sm 2s	MST83	7.74	P	gas-solid comparison, (atom - metal)shift = 2.5(5)

Sn 3d	KPR81	485	T	ab initio, overlap of shape res. & Cooper minimum structure, $10^4$ eV > IP
Sr 4p	NW&86	25-32	P	$\text{Sr}^+$ , $\text{Sr}^{2+}$ yields at threshold
	KWM93	40-1000	T	RPA(E) cacl. of $\sigma$ , BR and $\beta$ for all alkaline earths
	JC&93	40-200	P	resonant Auger; cascade processes
	FB&01	38-45	P,T	dipole matrix elements
Sr 3d	MC75b	110-280	P	photographic, delayed onset
	KH&87	130-150	P	multiple ionization yields, 0.2 shake probability
	KH&90	130-280	P	multiple ionization yields, 0.2 shake probability
	KWM93	40-1000	T	RPA(E) cacl. of $\sigma$ , BR and $\beta$ for all alkaline earths
	MS&95a	135-300	P,T	dual laser; $\text{Sr}^0$ to $\text{Sr}^{3+}$ ; HF-CI calc; cont. X-sect. depends on charge
Sr 3p	IK&95b	130-200	P	relative; $\text{Sr}^+$ , $\text{Sr}^2$ , $\text{Sr}^3$ yields from $\text{Sr}^+$ ; 3d6ef giant res.; 4d orb. collapse
	KH&87	136-146	P	total and partial ion yields, no $\text{Sr}_+$ , matches absorption (MC75a)
	CM77a	110-280	P	photographic, correction to MC75b theory comparison
	MJ81	110-150	T	Z+1 analogy, ab initio calculation
	MC82	135-145	T	inadequacy of Z+1 analogy, compared to expt (MC75a)
	C84	50-300	T	res. width/energy relation
	KWM93	40-1000	T	RPA(E) calc. of $\sigma$ , BR and $\beta$ for all alkaline earths
Sr 1s	KM&02b	100-2000	T	absolute, realxation effects; comp. of Ca, Mg, Sr
Ta 5p,4f	MS&97	30-50	P,T	absolute; TIY & PIY; relativistic; fused wire TOF
Tb 4d	RM&89b	120-180	P	EY absorption, comparison of Ba..Tb; PES of Sm, Eu, Gd
	SZ92	80-180	R	comp. of rare earth 4d edges; partial X-sections; comp. to calc.
Tb 3d	TL&85	1.23-1.28	P,T	electron yield ( $\text{TbAl}_2$ (sol)), comp to multiplet calc, full RE series
Te4d	M99	70-102	P,T	$\text{Te}^{4+}$ , $\text{Te}^{5+}$ , dual plasma source; HF calculations
Ti 3p	MP&86	30-60	P	comp. of 3d transition metal atoms
	SZ92	30-80	R	comp. of 3p edges of 3d-transition metal atoms
	HZ96	35-60	P,R	relative, partial & total ion yields; comp. of 3d TM element PA and PI.
	KS98	50-100	P,T	$\text{Ti}^{3+}$ ; dual laser plasma; RPAE calc.
Ti 2p	GBP82	>450	T	inner-shell excitation contributions to total cross-section calculated
	MG&16	448-472	P	$\text{Ti}_{n+}^+$ , n=1-5,7,10; atoatomic ion to solid comparison, selected ion NEXAFS
Ti 1s	MY&02b	8.0-35.0	P	inter-shell effects from X-ray emission; comp. of Ca, Ti, V K-shell
Th 5d	W84	70-140	T	non-rel. RPA, non-stat. I(S-O), comp. to (J. Phys (Paris) 41 (1980) 603)
	CC&86	70-140	P	laser source & sample; comp. to sol.; $\text{ThF}_4$ (CP&80), calc. (W84)
	CM&91	80-140	P,R	laser-plasma, comp. to $\text{ThF}_4$ , solid; review
	BT92	80-120	P,T	relativistic calc, comp. of gas-metal for U, Th
	SZ92	80-140	R	relative (CC&86); comp. to calc.
Tl 4f	CM75b	120-275	P	photographic, continuum res.
Tm 4d	BK&93	140-200	P,T	relative; total and partial ion yields; comp. of Er, Ho, Tm; HF calc
Tm 3d	TL&85	1.46-1.52	P,T	electron yield (solid), comp to multiplet calc, full RE series
	BE&89	1.45-1.47	P	matrix isolated atoms; cluster vs. gas; size effect; multiplet changes as valency changes (initial state effect)
U 4f	SB&91	1450-1520	P,T	relative, gas-sol; theory (Dirac-Fock); intermediate-valence; comp of Sm, Tm
	KPR81	385	T	ab initio, overlap of shape res. & Cooper minimum structure, $10^4$ eV > IP
	PC83	110-120	P	photographic, sharp 5d-f above 5d threshold), comp. to solid, $\text{UF}_4$ (CP&80)
U 5d	W84	80-160	T	non-relativistic RPA, non-statistical f(S-O); cont. res., comp. to expt (UF <sub>4</sub> -CM&80; U(solid)-Cukier et al. J. Phys (Paris) 39 (1978) L315)
	CC87	70-150	P	relative, plasma continuum, compared to $\text{UF}_4$ (CM&80), U(sol)
	S87	70-145	P,R	comp. of solid, vapor, calc. (CC87)
	BT92	80-120	P,T	relativistic calc, comp. of gas-metal for U, Th
	SZ92	80-120	R	relative; CC87 comp. to calc.
V 1s	KG&00	15-150	P,T	relative, total and partial yields ( $\text{U}^+$ , $\text{U}^{++}$ $\text{U}^{3+}$ ); dual laser plasma
	MY&02b	8.0-35.0	P	inter-shell effects from X-ray emission; comp. of Ca, Ti, V K-shell

W 5p,4f	CK&91b	30-60	P,T	laser source & generation; 5p 6 5d res.; comp. to MBPT (Boyle, ICPEAC-91)
	SZ92	30-60	R	relative (CK&91b)
	BAK93	30-60	T	MBPT calc.
	SF&95	30-60	P,T	absolute; TIY, PIY; comp. to CK&91b; MBPT calc (BAK93); Fano profile
Xe 2p,2s	H31	1.6-1.8	P	photographic; compare atom and compound vapors
Xe 4d	C64	60-170	T	absolute, continuum res.
	CM64	60-75	P	photographic, Rydberg analysis IP (67.55, 69.52)
	E64	40-160	P	absolute, continuum res.
	LBZ64	30-620	P	absolute
	LZB64	64- 69	P	photographic
	CM65	60-180	P	photographic
	S66	60-200	R	absolute
	FC68	50-400	R	atomic oscillator strengths review
	MC68	40-1000	T	photographic, compared to experiment (S66), delayed onset
	RF68	50-140	T	ab initio calculation, continuum res.
	AG&69	50-140	E	angular dependence of inelastic scattering, differential cross-section
	HK&69a	60-150	P	absolute, gas-solid comparison
	HK&69b	60-150	P	absolute, gas-solid comparison
	ZG71	70-500	P,R	absolute, continuum res.
	KM72	50-350	P	ab initio calculation, continuum res.
	ABC75	50-140	T	RPAE calculation, continuum res., generalized oscillator strengths
	FTD76	50-140	T,R	electron-optical properties of atomic fields
	WW77	30-200	E	absolute photoionization, post-collision interaction
	KT&77	64-70	E	Rydberg analysis IP (67.55, 69.54), Z+1 analogy, <70meV FWHM res.
	EKK78	64-70	P	Auger decay of res. lines
	S80a	70-130	T,R	review, centrifugal barrier
	S80b	50-350	P,R	ab initio calculation, continuum res.
	C82c	64-70	T	resonant Auger effects in PES, compared to expt (EKK78)
	CF83	60-220	T	4d-f in Xe-like ions, centrifugal barrier, 4f collapse
	SB&83	50-100	P	PCI, autoionization decay (>90%), $\beta$ values, partial cross-sections
	SK&83	60-80	E	dipole forbidden transitions
	C84	60-100	T	res. width/energy relation
	HM&84	64-70	P	absolute, total electron and ion yield spectra, no P.C.I. detected
	DG85	60-200	T	dispersion ( $q=0.5 \text{ \AA}^{-1}$ ) of d-->ef giant res., 30eV shift, l=1 dominates
	AA&86a	60-140	P	energy dependence of Auger and AI spectra
	BP&86	60-140	P	DES; coupled-channel part. X-sect.; large shake-off at ef res.
	HM&86	138-152	P	absolute, partial & total ion yields; Ryd. series most visible in $\text{Xe}^{4+}$
	SKR86	63-70	E	high res. (65 meV), quadrupole d-->s at low impact E
	BK&87	200-1000	P	absolute partial and total ionisation X-sections; comp. to calc.
	HI&87	64-72	P	threshold PES, shake-off at discrete resonances, PCI
	AKK88	70-150	T	MBPT & relax; comp. to (total, 4d partial); $\beta$ s; enhanced 2+ at 4d giant res.
	LF&88	150-300	P	4p, 4d part. X-sect; rel; $\beta$ at Cooper min (185 eV); comp to calc (KM72)
	NML88	64- 72	P,R	partial ion and threshold e- yields; double ionisation via ISE
	BB89	70-140	P	absolute, partial, comp. to BP&86; lower double ioniz.
	BS&89a	64- 70	P	DES, large shake-off; increases with nd Rydberg (6p=30%; 7p=34%)
	BS&89b	40-1000	P	absolute, partial and total PI X-sections, $\beta$ s
	CM&89	63-65	P	resonant Auger, ang. dist.; comp. of Ar,Kr,Xe
	HB&89	100-150	P	laser plasma, 4f collapse (comparison of $\text{Cs}^+$ , $\text{Ba}^{2+}$ , $\text{La}^{3+}$ )
	KKS89	70-130	P	absolute, partial 4d PI; comp. to BP&86; smaller many e- contribution
	SD89	140-330	T	RPA, partial X-section and $\beta$ ; comp. to ext. (LF&88)
	AA&90a	66,68	P,T	DES, shake-up fraction comp. of Ne1s, Ar2p, Kr3d, Xe4d
	AC&90	70-150	T	RPAE; comparable single and double ionisation intensity; comp to HK&69

Xe 4d . . .	BS90	65	P,R	DES at 6p Ryd; comp. of Kr, Ne, Ar DES
	HY&90	60-160	P	partial ion yield spectra ( $\text{Xe}^{2+}/\text{Xe}^{3+}/\text{Xe}^{4+}$ )
	NY&90	60-220	P	total and partial ion yield; comp. across RE series
	OEK90	65,74	P	PEPICO, decay of Ryd. res.; ion kinetic energy dist.
	R90	60-160	T	absolute; comp. of Ba4d, Xe4d, Kr3d; ion (1+, 2+) vs. absorption
	VM&90	65	P	(hv,2e); 2-step AI of discrete states in Ar, Kr, Xe
	AH&91	64-74	E	near threshold excit.; triplets; PCI; lineshapes; comp. to theory
	HM&91a	75-100	P	threshold EY; strong conjugate shake-up
	II&91	>70	E	PCI shift of Auger, comp. of Ar LMM, Kr MNN, Xe NOO
	S91	65-90	P,R	autoionisation of Rydberg res., comp. to Xe 4d
	CC&92	50-200	E	absolute; comp. of Ar, Kr, Xe
	DM&92	64-70	P	high res. (12 meV); SX-700II characterization
	SS92d	44-1300	P	PIY and BR for multi-charge ions of Ne, Ar, Kr, Xe; $\Delta$ BR at edges
	WC&92	64-70	P	CIS spectra; Auger- $\beta$ ; near-threshold; ZEKE from 2-step processes
	BY&93	70-200	E	GOS (70-4000 eV impact) resonances; absolute
	PM&93	62-72	E	non-dipole ( $E_0=83$ eV) comp. to dipole ( $E_0=103$ eV); high efficiency magnetic spectrometer; no angular resolution
	PN93	60-140	P	absolute; comp. of atomic and $\text{Xe:C}_60$ inside cage; EXAFS
	C93	100-5000	T	X-sect; $\beta$ ; comp. of all rare gases; ang. cor. correct.; dipole breakdown
	T93	60-140	E	absolute; GOS ( $K^2$ ) at 1-2 keV impact
	AA&94	70-160	P	Auger branching ratios; 30% variation above 4d threshold, 2-step model invalid
	SS94	60-100	P	BR of multiple PI; Auger; comp. of 2e- ionization of Ne,Ar,Kr,Xe
	A95	65,67	P,R	resonant Auger; high resolution
	AB&95	100	E	Auger-photoelectron coinc.; ang. dist.; PCI effect in ang. dist. up to 30 eV above IP; EI senses PCI (1-step) even when PI fits 2-step model
	AO&95	75-240	P,T	PE branching ratio; expt.versus calculation; non-statistical in resonance region
	SA&95b	66,68	P	resonant Auger; very high resolution by line narrowing
	SK&95c	90-95	P	accurate natural linewidths as $f(n)$ ; comp. of Ar, Kr, Xe
	A96	40-500	T,R	absolute cross-sections; comp. to expt.; giant resonance
	AB&96	68-90	E	(e,2e) and (e,e',Auger) coinc.; $4d_{5/2}:4d_{3/2}$ BR; PCI; comp. to theory
	BS96	50-1000	P,R	absolute, partial cross-sect. comp. to total; $\beta$ 's
	HZ96	64-70	P,R	relative, partial & total ion yields; comp. of 3d TM element PA and PI.
	KA&96c	60-140	P	partial ion yields; comp. of Xe, Ba, Eu 4d
	LB&96	65.1	P	Auger resonant Raman; line narrowing; $\beta$ s at 40 meV res. (natural 106 meV)
	SI&96	40-120	P,T	partial ion yields; multiconfiguration Dirac-Fock calc.; 4d 6 np,nf 2e- transitions; larger 4f collapse in 2e- than 1e- states
	SK&96	64-71	P	high res.; 4 meV/eV E-scale comp.; natural widths decrease from 110(1) to 98(8) from 6p to 9p; comp. to SK&82
	AK&97b	65-67	P	resonant Auger; PCI studied; shake transitions
	BL97	65-67	P,R	resonant auger at 6p line; Auger resonant Raman; $\beta$ values
	LG&98	105-115	P	E-resolved (PE,PI) coinc; 4d 6 ef res.; 'FIRE' = Final Ion-charge Resolved Electron spectroscopy
	SM&98	70-80	P,T	interference effects; Auger, AI; angular distributions
	SS98a	60-90	P	charge state PIY; PE-PI coincidence
	WA&98	50-140	P	relative, ef resonance at similar position in $\text{Xe}, \text{Xe}^+, \text{Xe}^{++}$
	AH&99	65-190	P	Auger, high resolution; lifetime width varies (110-130 meV)through 4d $\rightarrow$ ef; PCI
	SL&99	60-200	P,T	spin-resolved Auger, PES; partial X-sect; 2 partial wave OK outside Cooper min
	AC&00a	50-150	T	RPAE, PI for $\text{Xe}^+\rightarrow\text{Xe}^{++}$ ; comp to expt
	AA&01	70-140	P,T	absolute; RPAE calc; $\text{Xe}^+, \text{Xe}^{++}$ excitation & ionization
	BA&01	105-127	P	thresold EY, ion coincidence
	II&01	50-150	P	absolute
	W01	70-130	P,R	review of atom and ion photoionization

Xe 4d . . .	BF&02	40-180	E	absolute, GOS, $\epsilon f$ shape resonance has minimum( $K^2 = 3\text{au}$ )/maximum( $K^2 = 6\text{au}$ )
	KA&02a	40-160	P	absolute, $\text{Xe}^0, \text{Xe}^+, \text{Xe}^{++}$ PIY; 4f collapse mapped; isonuclear identical; $\Sigma(\text{OOS}) \sim 10$ suggests little cross-shell correlation
	LS&02	64-76	P,T	TPEPICO; PCI; dynamics of Auger decay via $\text{Xe}^{++*}$
Xe 4p	LZB64	140-146	P	photographic
	C76	140-690	P	photographic, absolute, delayed 4p continuum
	SZ&92	140-150	P	threshold PES
	SW&99	140-150	P	gas-cluster-solid comparison; Rydberg – exciton conversion
	HM&02	138-152	P	relative, PIY, threshold e, ion coincidence; PCI effects
Xe 4s	WM69	150-305	P	photographic, Rydberg analysis IP (211.3)
Xe 3d	D68	670-790	P	absolute, continuum res.
	AI78	670-790	T	ab initio calculation, compared with experiment (D68, C76)
	WM78	50-1000	P,R	absolute total and partial X-sections
	YW83	670-720	P	solid-gas comparison, weak continuum res.
	SN&84	680-720	P	relative, collapse of f-continuum, compared to theory
	ZL84	650-740	T	time-dependent, local density with core-hole relax., comp. to expt (YW73)
	BK&87	650-1000	P	absolute total and partial X-sections
	TLP90	680-760	T	absolute; 3d-X-sect for $\text{Xe}^{n+}$ , $n=0,1,2$ ; evolution of delayed maximum
	SS92b	650-1250	P	total & partial ion yields, DES and Auger cascades in 3d/3p/3s
	C93	100-5000	T	X-sect; $\beta$ ; comp. of all rare gases; ang. cor. correct.; dipole breakdown
	AI&99	670-715	P,T	relative, TIY, 4f collapse; HF-calc; comp of Xe, Cs, Ba
	KH&00	670-725	P,T	relative, delayed onsets; relaxed HF calc
	SA&01	672-677	P	DES; angular distributions
	KM&07	660-720	P	absolute cross-section, natural lifetime (0.42(1) eV)
	CM12	680	P, R	review of lifetime-limited linewidths (many small mol. & atoms)
Xe 3p	SS03	880-1020	P	absolute cross-section
	KM&07	880-1020	P	absolute cross-section
Xe 2p	AA&80	4.78-4.83	P	Auger yield, large P.C.I. ( $>1\text{eV}$ shift at 3eV above threshold)
	AA&85	4.75-4.83	P	post-collision interaction effects on autoionisation
	KH&89	4.6-6.1	P	absolute; comp. to calc; 2p 6 nd white lines (collapse of 5d to inner-well)
	ZS&91	4.6-6.1	P,T	2e-excit in $L_1, L_2$ and $L_3$ , del-SCF; effects on EXAFS analysis evaluated
	DGT92	4.75-4.83	P	Rydberg, Z+1 comp.; LN double excit; compt. to KH&89
	KNY93	4.70-5.10	T	HF-MC; multi-electron effects at $L_3$ and $L_2$ thresholds in Kr 2p and Xe 2p; comp. to expt. (Tronc, unpub.)
	LM&94	4.78	P	(Auger-ion) coinc at 10 eV above IP
	AK&95b	4.7-6.2	P,T	absolute; multi-electron; LV satellites; MCDF calc
	MS&95b	4.78-4.79	P	X-ray emission at 2p 6 Ryd line; evolution from resonance Raman to XRF
	BA&96	4.75-4.83	P	partial ion yield; pre-edge ionization by $\sim 20$ eV
	HM&96	4.77-4.81	P	partial ion yields in coincidence with threshold electrons; PCI; isolation of non-PCI shifted Auger cascades
	AS&97	4.77-4.81	P	Auger resonant Raman; PCI effects
	IV&98	4.5-7.0	P	multi-electron excitation; three electron transitions
Xe 2s	DGT92	5.41-5.50	P	Rydberg, Z+1 comp.; LN double excit; compt. to KH&89
	MH&99	5.44-5.48	P	PIY, ERAMICO, PCI, multi-step Auger; modelled
Xe 1s	T85	34.6	T	0-803V above edge, relativistic calc., PCI small, no osc. (cf. MI80)
	YKD90	34.5-34.6	T	absolute; HF-MC; E,f calc; monopole redist.
	DBK91	34.5-40.0	P	absolute; comp. to theory (T85); relativistic effects on cont. decay
	DK92	34.0-36.0	P	absolute; KN double excitations
	HYP97	34.5-34.6	T	absolute; comp to DBK91; anomalous dispersion; inelastic X-ray scattering
Yb 4d	NY&90	60-220	P	total and partial ion yield; comp. across RE series, very weak!
Yb 3d	TL&85	1.51-1.54	P,T	electron yield ( $\text{Yb}_2\text{O}_3(s)$ ), comp to multiplet calc, full RE series; $f^{14}$
Yb 2p	AM&90	7.0-8.2	P	gas-sol. comp.; comp of 2p spectra of Ce, Er, Gd, Sm, Yb

Zn 3s	CM74a	115-180	P	photographic
Zn 3p	KC&97a	80-120	P,T	relative, dual plasma; Zn <sup>n+</sup> n=1-3 excitation; HF calculations
Zr 3p	GBP82	>330	T	inner-shell excitation contributions to total cross-section calculated

---

## MOLECULES

---

### Aluminum 2p (80 eV)

AlC <sub>3</sub> H <sub>9</sub>	NKM90	40-120	P	Al(CH <sub>3</sub> ) <sub>3</sub> , ion yield, PEPICO, PIPICO, DDI, selective fragm. at edge
	NK&91	40-120	P	ion yield, BR, PIPICO
Al <sub>2</sub> C <sub>3</sub> Cl <sub>3</sub> H <sub>9</sub>	NK&91	40-120	P	Al <sub>2</sub> (CH <sub>3</sub> ) <sub>3</sub> Cl <sub>3</sub> , ion yield, ion branching ratios, PIPICO

### Antimony 4d (35 eV)

Sb <sub>5</sub>	BC94	20-120	P,R	relative; comp. to atom, solid; giant resonances review
Sb <sub>n</sub>	BB&91	25-120	P	n=4, 7-16; clusters, size dependent giant res., comp. to GaSb(sol)

### Argon 2p,2s (250,310 eV)

Ar <sub>2</sub>	UF&08	262	P,T	PEPIPICO, interatomic coulomb decay (ICD); spin conserved processes faster than spin-flip processes; dipole forbidden processes observed
	SF&05	295	P	momentum imaging, PE-PE angular correlation
Ar <sub>n</sub>	RS&91	240-268	P	PIPICO, charge sep. in clusters
	RS&92a	248	P	PIPICO diss. of Ar clusters, KERS
	RH&93a	240-400	P	Ar clusters (to n~700); EXAFS, atom6sol
	RH&93d	240-400	P	Ar clusters (to n~700); EXAFS, atom6sol; Ar2p vs. 1s
	KJ&94	240-260	P	comp. of threshold (zeke) of Ar, Ar <sub>n</sub> ; PCI lineshape analysis
	BF&95b	243-248	P	partial ion yields; comp. of atoms & clusters
	RH&95	260	P,R	PEPIPICO; asymmetric charge separation
	KS&05	244-251	P	resonant Auger decay, comp. to Ar <sub>n</sub>
	BF&96	254	P	Ar2p PES, n=1-4000; atom, surf. bulk. shifts
	HR96	240-300	P,R	Ar clusters, 4s, EXAFS, comp. to BF&95b
	RK&96	240-265	P	TEY, AEW as f(size); ZEKE; PEPICO
	FB&03a	244-258	P	angle resolved ion yield,in-plne more bulk-like
	TF&03	244-252	P	TEY; resonant PES, BE as f(n), PEY
ArKr	UF&08	262	P,T	PEPIPICO, interatomic coulomb decay (ICD); spin conserved processes faster than spin-flip processes; dipole forbidden processes observed

### Argon 1s (3.2 keV)

Ar <sub>n</sub>	RH&93c	3.1-3.8	P	comp. of gas, cluster and solid; EXAFS & XANES
	RH&93d	3.1-3.8	P	comp. of gas, cluster and solid; EXAFS & XANES; Ar2p vs. 1s
	KB&97	3.18-3.38	P	XAFS as f(size); 12-2900 ; fcc structure > 200; icosahderal <200

### Arsenic 2p (1330,1360 eV)

AsCl <sub>3</sub>	GDT97	1.31-1.39	P,T	relative; TIY, MS-X $\alpha$ ; pot. barr.; AsCl <sub>3</sub> , PCl <sub>3</sub> , GeCl <sub>4</sub> , SnCl <sub>4</sub> comp.
-------------------	-------	-----------	-----	---

### Arsenic 1s (11.7 keV)

AsF <sub>3</sub>	MB&79	11.8-11.9	P	pot. bar. effects, comp. to AsF <sub>5</sub> -doped polyacetylene
	MB&84	11.8-11.9	T	non-relativistic HF, comp. to expt (MB&79)
AsF <sub>5</sub>	MB&79	11.8-11.9	P	pot. bar. effects, comp. to AsF <sub>5</sub> -doped polyacetylene
	MB&84	11.8-11.9	T	non-relativistic HF, comp. to expt (MB&79)
AsGa	BF&93	11.6-12.3	P	GaAs; EXAFS; in situ monitor of CVD; fluorescence detection

### Barium 4d (90 eV)

Ba:C <sub>60</sub>	PN&93	80-180	P	absolute; comp. of atomic and BaC <sub>60</sub> - inside cage; EXAFS
--------------------	-------	--------	---	--

### Beryllium 1s (110 eV)

BeH <sub>2</sub>	CC&81	110-115	T	ab initio calc.
BeF <sub>2</sub>	CC84	122	T	delta SCF, B1s->5σ* 121.6eV, T=1.53eV, dissociative

### Bismuth 5d (25 eV)

BiC <sub>3</sub> H <sub>9</sub>	NS&90	16-42	P	Bi(Me) <sub>3</sub> , ZEKE, PI yield, BR, comp. of methyl-metal fragmentation (Bi, Ga, Zn, Ge, Sn, Pb)
---------------------------------	-------	-------	---	--

### As 1s (11.8 keV)

AsBr <sub>3</sub>	H31	11.86	P	1 <sup>st</sup> chemical state XAS s; photographic; As, AsBr <sub>3</sub> , AsCl <sub>3</sub> , AsH <sub>3</sub> As <sub>2</sub> O <sub>3</sub>
AsCl <sub>3</sub>	H31	11.86	P	1 <sup>st</sup> chemical state XAS s; photographic; As, AsBr <sub>3</sub> , AsCl <sub>3</sub> , AsH <sub>3</sub> As <sub>2</sub> O <sub>3</sub>
AsH <sub>3</sub>	H31	11.86	P	1 <sup>st</sup> chemical state XAS s; photographic; As, AsBr <sub>3</sub> , AsCl <sub>3</sub> , AsH <sub>3</sub> As <sub>2</sub> O <sub>3</sub>
As <sub>2</sub> O <sub>3</sub>	H31	11.86	P	1 <sup>st</sup> chemical state XAS s; photographic; As, AsBr <sub>3</sub> , AsCl <sub>3</sub> , AsH <sub>3</sub> As <sub>2</sub> O <sub>3</sub>

### Boron 1s (190 eV)

BB <sub>3</sub>	II&80	170-280	P	absolute
	II&82	190-280	P,T	absolute, discrete shape res., ab initio calc.
BClF <sub>2</sub>	HD&92	190-220	P	partial IY; yield spectra distinguish mixed (BCl <sub>x</sub> F <sub>3-x</sub> )
BCl <sub>2</sub> F	HD&92	190-220	P	partial IY; yield spectra distinguish mixed (BCl <sub>x</sub> F <sub>3-x</sub> )
BCl <sub>3</sub>	FB70	190-210	P	pressure dependence, pot. bar. effects
	HB71	192-212	P	strong line at 192.44 eV
	NB71	190-210	T	semi-empirical calc.
	BK74	190-210	P	pot. bar. effects
	II&80	190-280	P	absolute
	II&82	190-280	P,T	absolute, discrete shape res., ab initio calc.
	UC&94b	190-208	P	absolute, resonance Auger; spectator & participant at π*, σ*
	UT&00	195-199	P,T	TIY, relative, resonant Auger probe of Jahn-Teller coupling
<b>BF<sub>3</sub></b>	F68	190-210	P	pot. bar. effects, comp. to B, BN, B <sub>2</sub> O <sub>3</sub> - solids
	FB70	190-210	P	pot. bar. effects
	HB71	192-212	P	absolute, pot. bar. effects
	NB71	190-210	T	semi-empirical calc.
	CP&72	192-210	T	ab initio calc., pot. bar. effects
	D72	190-210	P,R	pot. bar. effects
	ZV72	190-215	P	pot. bar. effects
	BK74	190-210	P	pot. bar. effects
	R75	185-212	T	alternate assignment of ZV72
	II&80	190-280	P	absolute, pot. bar. effects

BF <sub>3</sub> ...	SDD81	190-225	T	MSM X- $\alpha$ calc., shape res., comp. to experiment(HB72)
	II&82	190-280	P,T	absolute, cont. shape res., ab initio calc.
	GSS83	192-212	T	ab initio, comp. to expt (HB71), cove-hole induced reorganisation
	SM&83	194-214	T	ab initio (EICVOM); comp. to KBF <sub>4</sub> (s), CF <sub>4</sub> ; expt (HB71, II&82)
	CF&84a	190-215	E	comp. of 2.5 and 15° spectra, $\sigma^*$ (e) enhanced
	KI&84	190-225	P	relative, DES enhanced valence PES at discrete res.
	SSH84a	205	T	$\sigma^*$ -res./bond length relationship
	VA&85	190-230	P,R	comp. to N <sub>2</sub> , NO <sub>3</sub> <sup>-</sup> , shape resonances
	KYK86	190-225	P,T	comp to II&82 BF <sub>4</sub> <sup>-</sup> ; Ni(CN) <sub>4</sub> <sup>2-</sup> Ni1s; Fe(CN) <sub>6</sub> Fe,N1s; edg. geom.
	T86	150-200	T	X $\alpha$ ; comp of BF <sub>3</sub> , B(OH) <sub>3</sub> , C(OH) <sub>3</sub> <sup>+</sup> XANES, R & symmetry effects
	HJ&87	190-220	P	partial ion yields, strong variation of $\sigma^*/\pi^*$ with channel, QMS
	NAV88a	190-220	P	comp. to KNO <sub>3</sub> , NaNO <sub>3</sub> ; $\delta(\pi-\sigma)$ versus R
	NAV88b	190-220	P	comp. to KNO <sub>3</sub> , NaNO <sub>3</sub> ; $\delta(\pi-\sigma)$ versus R
	PV&90	190-210	P	comp. to NO <sub>2</sub> <sup>-</sup> , NO <sub>3</sub> <sup>-</sup> ; $\delta(\pi-\sigma)$ versus R
	EA&91	180-230	E,T	comp. to BF <sub>4</sub> <sup>-</sup> , EHT calc; (np- $\pi^*$ ) distinguishes trigonal/non geom.
	NAV91	190-220	P	comp. of planar co-ordinated anions, $\pi$ - $\sigma$ bond length correlation
	U91	196,206	P,R	PE & Auger study of decay of a <sub>1</sub> , e states
	K92	190-220	R	survey of numerical XANES
	UC&92	196,206	P	resonant Auger-ion coincidence; dissociation dynamics
	U93	196,206	P	resonant Auger; spectator is 3x participator
	UC&94a	190-220	P	resonant Auger; 2a <sup>"</sup> mostly spect.; part. uses B-char. bonding orbitals
	SM&95	170-225	P	PEPIPICO; state dependent fragmentation mechanisms
	UO&95b	190-215	P	TIY, resonant Auger-ion coinc; dramatic changes with AI energy
	UO&96	195-216	P	(Auger,ion) coinc.; ion KE; yield as f(AI,Auger state); ion $\beta$ 's; X-sections for F <sup>+</sup> ; fragmentation mechanisms
	SM&97	192	P,T	resonance Auger - nuclear motion coupled; Jahn-Teller model - Auger is coherent 2nd order quantum process; wave packet analysis
	TKU98	194-198	P,T	2a <sub>2</sub> <sup>"</sup> resonant Auger; nuclear motion - core hole decay interference; detuning effect observed; energy domain - dynamic Jahn Teller
	U98	192	P,R	Auger-ion coincidence; molecular distortion
	MF&02	195	P	resonant Auger Raman; mapping potential energy surfaces
BF <sub>4</sub> <sup>-</sup>	HS&81	190-210	P,T	ABF <sub>4</sub> solid compounds (A=K,Na,NH <sub>4</sub> ) comp. to BF <sub>3</sub> , CF <sub>4</sub>
	SM&83	190-215	P,T	solid state, res. structure, comp. to BF <sub>3</sub> and CF <sub>4</sub> .
BHO	EH99	160-240	E,T	absolute; transient from H <sub>2</sub> S+B+SiO <sub>2</sub> ; comp of HBO, HBS, H <sub>3</sub> B <sub>3</sub> O <sub>3</sub>
	H00	160-250	E,R	transient ISEELS; comp of HBO,HBS, H <sub>2</sub> S
	HE&01	160-240	E	absolute; transient ISEELS
BHS	EH99	160-240	E,T	absolute; transient from H <sub>2</sub> S+B+SiO <sub>2</sub> ; comp of HBO, HBS, H <sub>3</sub> B <sub>3</sub> O <sub>3</sub>
	H00	160-250	E,R	transient ISEELS; comp of HBO,HBS, H <sub>2</sub> S
	HE&01	160-240	E	absolute; transient ISEELS
H <sub>3</sub> O <sub>3</sub>	T86	150-200	T	X $\alpha$ ; comp of BF <sub>3</sub> , B(OH) <sub>3</sub> , C(OH) <sub>3</sub> <sup>+</sup> XANES; $\delta(R)$ & sym. eff.
B <sub>2</sub> H <sub>6</sub>	ZV72	185-210	P,R	relative intensities
B <sub>3</sub> H <sub>3</sub> O <sub>3</sub>	EH99	185-210	E,T	absolute; from H <sub>2</sub> O+B; comp of HBO, HBS, H <sub>3</sub> B <sub>3</sub> O <sub>3</sub>
B <sub>3</sub> H <sub>6</sub> N <sub>3</sub>	DG&86	185-235	E	(borazine), comp. to Bz & cyclohexane, aromatic, split $\sigma^*$ res.
	PVN91	188-212	E	comp. of benzene, borazine and BN(s); shape resonances at edge
	SC95	192	T	ADC local/delocal calc; Jahn-Teller localisation; comp. to N 1s, C <sub>3</sub> H <sub>3</sub> <sup>+</sup>
	PV&03	188-204	P	TEY, resonant Auger, 30 meV fwhm, vibrational fine structure
B <sub>4</sub> C <sub>6</sub> H <sub>14</sub>	HW&93	180-240	E,T	2,3-diethylcarborane, absolute, EHMO, MNDO; ref. for CVD of BC
B <sub>5</sub> H <sub>9</sub>	HW&93	180-240	E,T	pentaborane, absolute, EHMO, MNDO; ref. for CVD of BC
	LD&92a	180-280	E,T	EXELFS, MNDO geometry
B <sub>5</sub> C <sub>12</sub> H <sub>18</sub> P	HLD91	160-220	E	Ph <sub>2</sub> PB <sub>5</sub> H <sub>8</sub>
B <sub>5</sub> C <sub>19</sub> FeH <sub>17</sub> O <sub>2</sub> P	HLD91	160-220	E	Cp(CO) <sub>2</sub> FeB <sub>5</sub> H <sub>2</sub> P(Ph) <sub>2</sub>
B <sub>9</sub> C <sub>2</sub> H <sub>11</sub>	HW&93	180-270	E,T	nido-1,2-dicarbaundecaborane, absolute, EHMO, decomp. of Ni(M) <sub>2</sub>

<b>B<sub>10</sub>C<sub>2</sub>H<sub>12</sub></b>	G91	190-193	T	o-carborane, ab initio, Z+1; comp. to expt. (Anderson, unpublished)
	HW&93	180-240	E,T	absolute, EHMO, MNDO; ref. for CVD of BC
	HR96	185-210	P,R	absolute, comp. of ortho, meta, para isomers
	HR&96	180-220	P	TIY, PIY, PEPICO; comp. of ortho, meta, para isomers
	HU&97	185-220	E,P,T	absolute; ab initio; EELS, TIY comp. for o, m, p-isomers; ioniz. eff.
	RH&09	180-220	P	ionic fragmentation of clos-carborane
<b>B<sub>10</sub>C<sub>2</sub>H<sub>12</sub></b>	HU&97	185-220	E,P,T	m-carborane, absolute; ab initio; EELS, TIY comp. for isomers; ioniz. eff.
<b>B<sub>10</sub>C<sub>2</sub>H<sub>12</sub></b>	HU&97	185-220	E,P,T	p-carborane, absolute; ab initio; EELS, TIY comp. for isomers; ioniz. eff.
<b>B<sub>10</sub>H<sub>14</sub></b>	HW&93	180-240	E,T	decaborane, absolute, EHMO, MNDO; ref. for CVD of BC
	LD&92a	180-640	E,T	EXELFS, comparison to solid decaborane, MNDO geometry
B <sub>18</sub> C <sub>4</sub> H <sub>22</sub> Ni	HLD91	160-220	E	Ni(B <sub>9</sub> C <sub>2</sub> H <sub>11</sub> ) <sub>2</sub> , Ni bollyl complex (Cp-analog)

Bromine 3d (75 eV)

BrCClH <sub>2</sub>	SR&94	68-110	P	TIY; PEPICO; PEPI3CO; selective frag.; Br(CH <sub>2</sub> ) <sub>n</sub> Cl, n=1-3
	MS&98b	90	P	ES-AEPICO, PE, site-selective fragmentation & kinetics
BrCF <sub>3</sub>	JC&97	68-80	P	relative; PES, PA comp.; ligand field and spin-orbit splitting; same ligand field paramaters in excitation and ioniz.
BrCH <sub>3</sub>	HB78a	50-300	E	CH <sub>3</sub> Br, cont. res.
	MN87	68-79	P	TPES, DES σ*(C-Br); PIPICO, partial dissociation prior to decay
	N88	63-79	P,R	σ*(C-Br); PIPICO, partial dissociation prior to decay
	NE&88	68-79	P	σ*(C-Br); PIPICO, partial dissociation prior to decay
	NML88	68-80	P,R	partial ion, PIPICO & ZEKE yields; double ionisation via ISE; review
	NM&88	68-79	P	σ*(C-Br); PIPICO, partial dissociation prior to decay
	NM&90	50-170	P	decay of core states, PIPICO yield spectra
	JC&97	68-80	P	relative; PES, PA comp.,ligand field and spin-orbit splitting; same ligand field paramaters in excitation and ioniz.
	OC&97a	10-450	E,P	absolute; high res. (0.1 eV); dipole breakdown, PES, (e,e+ion)
BrCN	OBI95	60-460	E,T	absolute; 0.1-1 eV fwhm; ligand field splitting
BrC <sub>2</sub> ClH <sub>4</sub>	SR&94	68-110	P	TIY; PEPICO; PEPI3CO; selective frag.; Br(CH <sub>2</sub> ) <sub>n</sub> Cl, n=1-3
BrC <sub>2</sub> F <sub>4</sub> I	NM&90	60-140	P	Auger, AI and ion yield (PIPICO); selective fragmentation
BrC <sub>2</sub> H <sub>3</sub>	SBK88	60-100	E	v vinyl bromide, high res.
	MLL89	68-110	P	mass spectra, ion yields, selective fragmentation
BrC <sub>2</sub> H <sub>5</sub>	MLL89	68-110	P	PIPICO spectra, ion yields, selective fragmentation
BrC <sub>3</sub> ClH <sub>6</sub>	SR&94	68-110	P	TIY; PEPICO; PEPI3CO; selective frag.; Br(CH <sub>2</sub> ) <sub>n</sub> Cl, n=1-3
BrC <sub>6</sub> H <sub>5</sub>	HP&78	68-80	E	comp. with carbon 1s pre-edge structure
BrD	JC&97	68-80	P	relative; PES, PA comp.; ligand field and spin-orbit splitting; same ligand field paramaters in excitation and ioniz.
BrH	SC&84	69-80	E	75 meV fwhm, Ryd. IP [3d <sub>5/2</sub> =77.12(3), 3d <sub>3/2</sub> =78.23(3)]
	BI&85	60-100	E	absolute, photoionization and fragmentation, similar to CH <sub>3</sub> Br
	KL86	60-100	T	atomic d-->f res., distinguishes atomic/molecular shape res.
	MN86	68-78	P	ionic dissociation at σ* prior to core hole decay
	MN87	68-79	P	TPES, DES σ*(H-Br); PIPICO, partial dissociation prior to decay
	NB87	68-80	P,R	σ*(H-Br); dissociation prior to decay; review
	N88	63-79	P,R	σ*(H-Br); PIPICO, electron and ion spectroscopy
	NM&88	68-79	P	σ*(H-Br); PIPICO, partial dissociation prior to decay
	LLM90	68-80	P	total ion yield, comp. to PIPICO yields, ultra-fast decay
	SH&91	68-80	P,T	anisotropic H <sup>+</sup> , ang. dist., KER etc from MRD-CI calc of HBr <sup>2+</sup>
	LB&93	69-74	P	0.12 eV resonant Auger; ultrafast decay; hi. res. of MN86
	LB&94a	74-78	P	ligand field split. eliminated & linewidth reduced by res. Auger detection
	LB&94c	73-77	P	EELS reinterpreted in terms of ligand field splitting; comp. to PES

BrH ...	PD&95	69-79	P	10 meV fwhm; 95 mV nat.; analysed with PES (JEL 67 (94) 299); 5-line pattern of S-O plus ligand field splitting
	NM96	70-79	P,R	ultrafast decay; electronic-nuclear motion coupling; fragmentation
	HB+97	74-78	P	TIY, resonant Auger; ultrafast decay; ultra-high resolution (10 meV); Auger resonant Raman
	JC&97	68-80	P	relative; PES, PA comp.; ligand field and spin-orbit splitting; same ligand field parameters in excitation and ioniz.
	PH&02	68-77	P	high res.; angle resolved (ion coinc.); symmetry-based re-assignments
	MM12	68-72	P,R	ultra-fast decay (HBr-Br3d; DCl, HCl-Cl2p; H2S - S2p, O2-O1s)
Br <sub>2</sub>	SC&84	66-80	E	75 meV fwhm, strong res. 9.1 eV below IP
	IH&96	20-140	E,P	absolute; abs. ion yield, PIPICO yields; dipole breakdown scheme
	JC&97	68-80	P	relative; PES, PA comp.; ligand field and spin-orbit splitting; same ligand field parameters in excitation and ionisation
Br <sub>4</sub> C	BS&02A	50-450	P,T	relative, TIY, PIY, compared to SiBr <sub>4</sub> , GeBr <sub>4</sub> , Me <sub>3</sub> SiBr (BL&98)
Br <sub>4</sub> Si	BL&98	50-450	P,T	relative, TIY, PIY
<b>Bromine 3p (190,196 eV)</b>				
C <sub>2</sub> H <sub>3</sub> Br	SBK88	60-100	E	v vinyl bromide, high res., width of 3p <sub>3/2</sub> >3p <sub>1/2</sub> due to C-K
<b>Bromine 2s (1790 eV)</b>				
Br <sub>4</sub> Si	BM&89a	1.75-1.90	P	SiBr <sub>4</sub> ; broad line; no pre-edge feature
<b>Bromine 1s (13.5 keV)</b>				
AsBr <sub>3</sub>	H31	13.4-13.5	P	1 <sup>st</sup> chemical state XAS ; photographic; AsBr <sub>3</sub> , Br <sub>2</sub> , HBr
BBBr <sub>3</sub>	FA98	13.4-14.4	P	relative; EXAFS; MSxα calc; 0.1 pm accuracy claimed; compare to ED
BrC <sub>6</sub> H <sub>5</sub>	OT&86	13.4-13.5	P	Bz-Br; comp of Br <sub>2</sub> , Bz-Br and Br-polyacetylene
	O96	13.4-13.5	P,R	XAFS review; comp. to Br-polyacetylene
BrH	H31	13.4-13.5	P	1 <sup>st</sup> chemical state XAS ; photographic; AsBr <sub>3</sub> , Br <sub>2</sub> , HBr
	C37	13.5	P	50 eV about edge, gas-solid comp.
	S40	13.5	P	50 eV about edge
	AC&93	13.4-13.9	P,T	EXAFS and KM double excitation
BrI	C37	13.5	P	50 eV about edge, gas-solid comp.
Br <sub>2</sub>	H31	13.4-13.5	P	1 <sup>st</sup> chemical state XAS ; photographic; AsBr <sub>3</sub> , Br <sub>2</sub> , HBr
	S36	13.5	P	20 eV about edge
	C37	13.5	P	50 eV about edge, gas-solid comp.
	S40	13.5	P	50 eV about edge
	KE75	13.4-14.6	P	extended fine structure (EXAFS), comp. to theory
	CEK76	13.4-14.6	P	extended fine structure (EXAFS)
	OT&86	13.4-13.5	P	Bz-Br; comp of Br <sub>2</sub> , Bz-Br and Br-polyacetylene
	FE&86	13.4-14.7	P	near edge and EXAFS, comp. to theory, Br <sub>2</sub> on graphite
	K92	13.4-13.6	R	survey of numerical XANES
	TH&92a	13.4-14.6	T,P	MS calc. of xfs; amplitude red. factor; comp. of Br <sub>2</sub> , GeCl <sub>4</sub> , SF <sub>6</sub>
	AC&93	13.4-13.9	P,T	EXAFS and KM double excitation
	FD95	13.4-14.6	P,T	GNXAS analysis; KL jumps corrected; good error analysis
	O96	13.4-13.5	P,R	XAFS review; comp. to Br-polyacetylene
	YK&96	13.4-14.6	P,T	T-dependent XAFS; cumulant analysis; Feff 6.0; force constants and anharmonic potentials derived
Br <sub>4</sub> C	FA98	13.4-14.4	P	relative; EXAFS; MS-Xα calc; 0.1 pm accuracy claimed; compare to ED
	CEK76	13.4-14.6	P	extended fine structure (EXAFS)

Calcium 2p (350 eV)CaBr<sub>2</sub> KR&02a 346-357 P, T partial electron yield from 2D (hv, e) maps, relative; atomic multipletCarbon 1s (290 eV)

<b>B<sub>4</sub>C<sub>6</sub>H<sub>14</sub></b>	HW&93	280-316	E,T	2,3-diethylcarborane, absolute, EHMO, MNDO; ref. for CVD of BC
<b>B<sub>5</sub>C<sub>12</sub>H<sub>18</sub>P</b>	HLD91	280-316	E	Ph <sub>2</sub> PB <sub>5</sub> H <sub>8</sub>
<b>B<sub>5</sub>C<sub>19</sub>FeH<sub>17</sub>O<sub>2</sub>P</b>	HLD91	280-316	E	Cp(CO) <sub>2</sub> FeB <sub>5</sub> H <sub>2</sub> P(Ph) <sub>2</sub>
B <sub>9</sub> C <sub>2</sub> H <sub>11</sub>	HW&93	280-316	E,T	nido-1,2-dicarbaundecaborane, absolute, EHMO, decomp. of Ni(M) <sub>2</sub>
<b>B<sub>10</sub>C<sub>2</sub>H<sub>12</sub></b>	HW&93	280-316	E,T	o-carborane, absolute, EHMO, MNDO; ref. for CVD of BC
	HR96	280-305	P,R	absolute, comp. of ortho, meta, para isomers
	HR&96	280-305	P	TIY, PIY, PEPIPICO; comp. of ortho, meta, para isomers
	HU&97	280-305	E,P,T	absolute; ab initio; EELS, TIY comp. for o, m, p-isomers; ioniz. eff.
	RH&09	280-305	P	ionic fragmentation of clos-carborane
<b>B<sub>10</sub>C<sub>2</sub>H<sub>12</sub></b>	HU&97	280-305	E,P,T	m-carborane, absolute; ab initio; EELS, TIY comp. of isomers; ioniz. eff.
<b>B<sub>10</sub>C<sub>2</sub>H<sub>12</sub></b>	HU&97	280-305	E,P,T	p-carborane, absolute; ab initio; EELS, TIY comp. of isomers; ioniz. eff.
B <sub>18</sub> C <sub>4</sub> H <sub>22</sub> Ni	HLD91	280-316	E	Ni(B <sub>9</sub> H <sub>11</sub> C <sub>2</sub> ) <sub>2</sub> , Ni bollyl complex (Cp-analog)
BrCD <sub>3</sub>	HB79c	285-290	E	vibrational structure, isotope shifts
BrCH <sub>3</sub>	HB78a	50-350	E	vibrational structure
	HB79c	284-293	E	vibrational structure, isotope shift
	OC&97a	10-450	E,P	absolute; dipole breakdown from comparison of PES, (e,e+ion)
BrCN	OBI95	60-460	E,T	absolute; 0.1-1 eV fwhm; DFT calculation
BrC <sub>2</sub> H <sub>3</sub>	BMT88	280-310	E	comp. to ETS
	SKB88	275-320	E	high res., comp. to vinyl halides
BrC <sub>4</sub> H <sub>43</sub> N <sub>2</sub>	BO&10	283-300	P,T	2-Br-pyrimidine; hi-res; comp of halogenated pyrimidines
BrC <sub>4</sub> H <sub>43</sub> N <sub>2</sub>	BO&10	283-300	P,T	5-Br-pyrimidine; hi-res; comp of halogenated pyrimidines
<b>BrC<sub>5</sub>MnO<sub>5</sub></b>	HR89	280-320	E	Mn(CO) <sub>5</sub> Br, absolute, $\pi^*$ intensity as measure of d $\pi$ -p $\pi$ backbonding
	RH89a	275-330	E	comp. to CO, Mn(CO) <sub>10</sub> & M(CO)s; E(ref); f( $\pi^*$ ) $\alpha$ backbond
	H90a	280-325	E,R	absolute; comp. to TM-COs; relaxation and $\delta$ (R) for $\sigma^*(CO)$
	HWR90a	280-325	E	absolute; comp. to TM-COs; f( $\pi^*$ ) vs. extent of backbonding
	SLD95	287	T	absolute, DF-LCAO; OS for C1s, O1s $\rightarrow \pi^*$ ; orbital mapping
BrC <sub>6</sub> H <sub>5</sub>	HP&78	283-295	E	XPS-EELS chemical shifts comp.
Br <sub>2</sub> C <sub>12</sub> H <sub>8</sub>	WC&05	284-308	E,T	o,o-dibromo-biphenyl, quantitative, GSCF <sub>3</sub> , ring-ring-interactions
Br <sub>4</sub> C	BS&02A	50-450	P,T	relative, TIY, PIY, compared to SiBr <sub>4</sub> , GeBr <sub>4</sub> , Me <sub>3</sub> SiBr (BL&98)
CClF <sub>3</sub>	CS90	292-301	P	high res. (50 meV); sharp $\sigma^*(C-Cl)$ , broad $\sigma^*(C-F)$ ; comp of CCl <sub>x</sub> F <sub>4-x</sub>
	WMT92	295-291	T	ETS vs. ISEELS, SE=6.4 eV; prediction of TVs
	ZIB92	280-330	E	absolute, high res. (70 meV), pot. bar., comp. of CCl <sub>x</sub> F <sub>4-x</sub> , x=1-4
	YL94	285-330	E	absolute GOS; comp. of CF <sub>4-n</sub> Cl <sub>n</sub> (n=0-4); $\sigma^*(C-Cl)$ GOS changes
	SS&95	290-325	P	PIPICO; start = selective ion gate; PIPICO yields; comp of Cl2p, C1s, F1s edges; only selective at Cl 2p edge
	L99b	200-230	E	REVIEW, GOS, compare CF <sub>4-n</sub> Cl <sub>n</sub> (n=0-4)
CClH <sub>3</sub>	HB78a	180-350	E	vibrational structure
	HB78b	286-292	E	comp. through CH <sub>x</sub> Cl <sub>4-x</sub> series, pot. bar. Development
	HB79c	284-293	E	vibrational structure
	WMT92	295-291	T	ETS vs. ISEELS, SE=6.4 eV; prediction of TVs
	ZIB92	280-330	E	absolute, high res. (70 meV), pot. bar., comp. of CCl <sub>x</sub> F <sub>4-x</sub> , x=1-4
	CP&07	280-350	P	relative, TIY, PIY +ve, -ve; state-selective frag.
CClF <sub>2</sub> H	L99b	200-230	E	REVIEW, GOS, compare CF <sub>4-n</sub> Cl <sub>n</sub> (n=0-4)
CCl <sub>2</sub> FH	L99b	200-230	E	REVIEW, GOS, compare CF <sub>4-n</sub> Cl <sub>n</sub> (n=0-4)
CCl <sub>2</sub> F <sub>2</sub>	CS90	291-299	P	$\sigma^*(C-Cl)$ , $\sigma^*(C-F)$ slit; comp of CCl <sub>x</sub> F <sub>4-x</sub>
	ZIB92	280-330	E	absolute, high res. (70 meV), pot. bar., comp. of CCl <sub>x</sub> F <sub>4-x</sub> , x=1-4
	BSS93b	50-1500	P	partial ion yields at coarse resolution

CCl <sub>2</sub> F <sub>2</sub> ...	SBS94a	44-120	P	partial ion yields; site-selective frag. at C 1s, Cl 2p, F 1s
	SSB94	44-120	P	partial ion-pair yields; site-selective frag.
	YL94	285-330	E	absolute GOS; comp. of CF <sub>4-n</sub> Cl <sub>n</sub> (n=0-4); $\sigma^*(C-Cl)$ GOS changes
	L99b	200-230	E	REVIEW, GOS, compare CF <sub>4-n</sub> Cl <sub>n</sub> (n=0-4)
CCl <sub>2</sub> H <sub>2</sub>	HB78b	286-295	E	pot. bar. effects, extended fine structure (EXAFS)
	WMT92	295-291	T	ETS vs. ISEELS, SE=6.4 eV; prediction of TVs
CCl <sub>2</sub> O	HUR92	280-340	E	phosgene; absolute; EHT calc., comp to terethaloylchloride
	RY&92	280-320	E	comp. of small mol. analogs with PET polymer
CCl <sub>3</sub> F	ZIB92	280-330	E	absolute, high res. (70 meV), pot. bar.
	YL94	285-330	E	absolute GOS; comp. of CF <sub>4-n</sub> Cl <sub>n</sub> (n=0-4); $\sigma^*(C-Cl)$ GOS changes
	SS97	290,310	P	PIPICO branching ratios; site-specific fragmentation; comp. to CF <sub>x</sub> Cl <sub>4-x</sub>
	SS98b	280-320	P	PIY, comp of C 1s, F1s, Cl 2p
	L99b	200-230	E	REVIEW, GOS, compare CF <sub>4-n</sub> Cl <sub>n</sub> (n=0-4)
CCl <sub>3</sub> H	HB78b	286-295	E	pot. bar. effects, extended fine structure (EXAFS)
	WMT92	295-291	T	ETS vs. ISEELS, SE=6.4 eV; prediction of TVs
	ZIB92	280-330	E	absolute, high res. (70 meV), pot. bar., comp. of CCl <sub>x</sub> F <sub>4-x</sub> , x=1-4
	L99b	200-230	E	REVIEW, GOS, compare CF <sub>4-n</sub> Cl <sub>n</sub> (n=0-4)
CCl <sub>4</sub>	HB78b	290-600	E	pot. bar. effects, extended fine structure (EXAFS)
	CKS80	280-310	P	photographic, laser bombardment X-ray light source
	TD84	280-295	T	multiple scattering calc., comp. to expt (HB78b)
	SSS86	285-295	T	SCF calc; assignments of HB79c questioned
	WMT92	295-291	T	ETS vs. ISEELS, SE=6.4 eV; TV preds; comp. of CCl <sub>x</sub> F <sub>4-x</sub> , x=1-4
	ZIB92	280-330	E	absolute, high res. (70 meV), pot. bar.
	BC&93	0-400	E	absolute; atomic ca. 25% too high; (e,e+ion) PIMS; dipole breakdown
	YL94	285-330	E	absolute GOS; comp. of CF <sub>4-n</sub> Cl <sub>n</sub> (n=0-4); $\sigma^*(C-Cl)$ GOS changes
	L99b	200-230	E	REVIEW, GOS, compare CF <sub>4-n</sub> Cl <sub>n</sub> (n=0-4)
	SC&02	288-296	P	absolute; high res.; weak Ryd.; $\Gamma \sim 72$ meV; comp. of CX <sub>4</sub> , X=H,Cl,F
CCuO	YA&97	287	T	Cu-(CO); STEX; $\pi^*$ OS comp. of CO, CuCO, Cu <sub>17</sub> CO, Cu <sub>50</sub> Co; initial and final state rules
CCu <sub>17</sub> O	YA&97	287	T	Cu-(CO); STEX; $\pi^*$ OS comp. of CO, CuCO, Cu <sub>17</sub> CO, Cu <sub>50</sub> Co; initial and final state rules
	PA&96	280-340	T	absolute, STEX; comp. of CO, Cu <sub>17</sub> CO, Cu <sub>50</sub> Co; models of CO/Cu(100)
CCu <sub>50</sub> O	YA&97	287	T	Cu-(CO); STEX; $\pi^*$ OS comp. of CO, CuCO, Cu <sub>17</sub> CO, Cu <sub>50</sub> Co; initial and final state rules
	PA&96	280-340	T	absolute, STEX; comp. of CO, Cu <sub>17</sub> CO, Cu <sub>50</sub> Co; models of CO/Cu(100)
CDHO <sub>2</sub>	GM&06	280-340	P	(DCOOH) , TIY, PIY, fragmentation, PEPIPICO, compare 4 isotopomers
CDHO <sub>2</sub>	GM&06	280-340	P	(HCOOD) , TIY, PIY, fragmentation, PEPIPICO, compare 4 isotopomers
CD <sub>2</sub> O	RD&92	285-312	P	high res.; Franck-Condon analysis 6 geometry; E <sub>el</sub> as f(isotope)
	PP&00	286	T	MC-SCF Z+1 calc; vibrational structure, XPS better than NEXAFS, comp. to expt (RD&92)
CD <sub>2</sub> O <sub>2</sub>	GM&06	280-340	P	(DCOOD) , TIY, PIY, fragmentation, PEPIPICO, compare 4 isotopomers
CD <sub>4</sub>	HPB77	285-293	E	vib'n'l struct; isotope intensity effects (J-T vibronic coupling)
	HM&91b	287-294	P	ZEKE, 0.15 eV fwhm; comp. of CH <sub>4</sub> , CD <sub>4</sub> ; PCI modifies ZEKE; FC anal. of C <sub>K</sub> <sup>+</sup> possible ( $\Delta\Gamma = -0.052(7)$ Å; hole relax. > internucl. rep.
	RDK93	286-291	P	high res (60 meV); I <sup>D</sup> /I <sup>H</sup> (3s) = 0.57(5); B-O not H-T vibronic coupling; comp. of CH <sub>4</sub> /CD <sub>4</sub> ; C <sub>2</sub> H <sub>6</sub> /C <sub>2</sub> D <sub>6</sub> ; C <sub>3</sub> H <sub>8</sub> /C <sub>3</sub> D <sub>8</sub>
	ST&93	286-291	P,T	high res (60 meV); CH <sub>4</sub> /CD <sub>4</sub> comp; 3s/3p (D/H) is 0.65; 0.8 in EELS (HPB77) attributed to 1s 6 3s quadrupole contribution
	DRK94	286-291	P,R	SX700 high res. studies; vibrational structure in small mols.
	RK&00b	286-292	P	TIY, Auger-ion coincidence; 3p vs. C 1s <sup>-1</sup>
	KR&02b	260,350	P, T	ERAMICO, 2-step model of fragmentation

CD <sub>4</sub> ...	RG&02	286-289	P	(Auger, ion) coinc. participant decay leads to dissociation, EREICO
	SR&02	286-292	P	DES vs PES; ERAMICO, vibration-dissociation correlation
CD <sub>4</sub> O	AJ&97a	278-293	P	CD <sub>3</sub> OD; relative, 45 meV fwhm; vibrational struct; comp to CH <sub>3</sub> OH
<b>CFH<sub>3</sub></b>	BBB78	282-310	P	absolute, CH <sub>x</sub> F <sub>4-x</sub>
	HB78a	284-295	E	vibrational structure, comp. through CH <sub>3</sub> X series
	HB79c	284-293	E	vibrational structure
	SSH84a	295	T	$\sigma^*$ -res./bond length relationship
	RS&89	290-330	T	MS-X $\alpha$ calc. of f & $\beta$ for (CF <sub>x</sub> H <sub>4-x</sub> , x=0-4); only CH <sub>4</sub> resonant
	LAL91	285-305	T	CNDO, systematic calc. of $\sigma^*$ energies; ISEELS, ETS for param. det.
	S92	280-320	E,R	comp. of CH <sub>3</sub> X, X=H, CH <sub>3</sub> , NH <sub>2</sub> , OH, F; $\sigma^*(X-H)$
	KU+95	287-294	P,T	60 meV fwhm; ab initio $\Delta$ SCF-CI; resonant Auger; confirms $\sigma^*/3s$ but mixed; Rydberg structure very similar to CH <sub>4</sub> ; reassigned peaks
	US&96	285-305	P,T	high res (60 meV); comp. of CH <sub>x</sub> F <sub>4-x</sub> (0<x<4); Auger and AI decay; SCF calculation; Rydberg vs. valence
	AM97	284-295	T	electronegativity correlations used for assignments; comp. to BBB78
<b>CFHO</b>	IH87	275-325	E	HCOF, absolute, comp. to (HCOX, X=NH <sub>2</sub> , OH), $\pi^*$ mapping
	RI&88	275-336	E	absolute, per-fluoro effect
	S92	280-320	E,R	comp. of CH <sub>x</sub> F <sub>2-x</sub> O, $\sigma^*(C-F)$ development
	SLD95	287	T	absolute, DF-LCAO; OS for C1s, O1s $\rightarrow \pi^*$ ; orbital mapping
	HC96	290	T	DFT; singlet-triplet (0.90 eV)
CF <sub>2</sub> H <sub>2</sub>	BBB78	282-310	P	absolute, pot. bar. effects
	SSH84a	295	T	$\sigma^*$ -res./bond length relationship
	RS&89	290-330	T	MS-X $\alpha$ ; C1s X-sect. & $\beta$ for (CF <sub>x</sub> H <sub>4-x</sub> , x=0-4); only CH <sub>4</sub> resonant
	US&96	285-305	P,T	high res (60 meV); comp. of CH <sub>x</sub> F <sub>4-x</sub> (0<x<4); Auger and AI decay; SCF calculation; Rydberg vs. valence
	AM97	284-295	T	electronegativity correlations used for assignments; comp. to BBB78
<b>CF<sub>2</sub>O</b>	RI&88	275-325	E	carbonyl fluoride, C-F $\sigma^*$ res., absolute, perfluoro effect
	S92	280-320	E,R	comp. of CH <sub>x</sub> F <sub>2-x</sub> O, $\sigma^*(C-F)$ development
	SLD95	287	T	absolute, DF-LCAO; OS for C1s, O1s $\rightarrow \pi^*$ ; orbital mapping
	HC96	290	T	DFT; singlet-triplet (1.04 eV)
<b>CF<sub>3</sub>H</b>	BBB78	282-310	P	absolute, pot. bar. effects
	SSH84a	295	T	$\sigma^*$ -res./bond length relationship
	HN86	275-330	E	absolute
	RS&89	290-330	T	MS-X $\alpha$ ; C1s X-sect. & $\beta$ for (CF <sub>x</sub> H <sub>4-x</sub> , x=0-4); only CH <sub>4</sub> resonant
	LAL91	285-305	T	CNDO, systematic calc. of $\sigma^*$ energies; ISEELS, ETS for param. det.
	US&96	285-305	P,T	high res (60 meV); comp. of CH <sub>x</sub> F <sub>4-x</sub> (0<x<4); Auger and AI decay; SCF calculation; Rydberg vs. valence
	AM97	284-295	T	electronegativity correlations used for assignments; comp. to BBB78
<b>CF<sub>3</sub>NO</b>	HIR89	280-340	E	absolute, weak bond effect

<b>CF<sub>4</sub></b>	WB74d	290-335	E	res. at thr., pot. barr. effects, unusual fine structure
	BBB78	280-460	P	absolute, pot. bar. effects, extended fine structure (EXAFS)
	TKR79	296-302	E	<70meV FWHM res., unassigned fine structure
	B81	280-340	P	XANES-structure relationship
	BH81	290-330	E,R	wide range
	HS&81	290-305	T	X- $\alpha$ , comp. to BBB78; BF <sub>4</sub> <sup>-</sup> (B1s)
	AP&82	280-345	T	ab initio, cont. X-sect, comp. to (BBB 78), cont. res. predicted
	SM&83	296-316	T	ab initio (EICVOM), comp. to (WB74d, TKR79), pre-edge res.; Ryd.
	SSH84a	295	T	$\sigma^*$ -res./bond length relationship
	TD84	280-295	T	multiple scattering calc., comp. to expt (WB74d)
	TL&84	300-350	P	absolute, Auger and PES cross-sections, asymmetry parameters
	PV&85	280-310	T	1s62p(t <sub>2</sub> ) & 1s6ε3p pred; corr. with LiF, K <sub>2</sub> BeF <sub>4</sub> & KBF <sub>4</sub> (A1s)
	HI86	300-1000	E	extended fine structure, comp. to BBB78
	SA&86b	250-780	P	absolute, comp. to CH <sub>4</sub> ; transfer of OS (cont'd discrete)
	SDD86	300-330	T	MS-Xα, β, cross-section, comp. to (WB74d, TKR79, TL&84)
	HI86	300-1000	E	EXELFS, comp. to photabsorption (BBB78)
	LCS87	200-700	E	EXELFS; q-independent; Teo & Lee phases inadequate; new background subtraction; Bethe ridge
	HFM87	280-320	E	comp. to other fluorocarbons; $\sigma^*(C-F)$ 'giant shape res.'
	SAV87	280-320	P	absolute; thr. integrated OS comp. to CH <sub>4</sub> , CO <sub>2</sub>
	LM&89	290-345	P	total ion yield, TOF mass spec at sel. E; no sel. frag.; comp. to SiF <sub>4</sub>
	RS&89	290-330	T	MS-Xα; X-sect, β for (CF <sub>x</sub> H <sub>4-x</sub> ,x=0-4); CH <sub>4</sub> res.; comp. to [TL&84]
	ZC&89	200-700	E	absolute, comp. of sum rule and atomic X-sect. normalisation
	CS90	295-305	P	50 mV fwhm; matches TKR79; no assgn.; comp. of CCl <sub>2+x</sub> F <sub>4-x</sub> , x=0-2
	H90a	290-320	E,R	absolute, pot. bar. effect on I{ $\sigma^*(C-F)$ } through CF <sub>x</sub> series
	HW&90	300-700	E	EXELFS, comp. to PA (BBB78)
	LAL91	285-305	T	CNDO, systematic calc. of $\sigma^*$ energies; ISEELS, ETS for param. det.
	ZIB92	280-330	E	absolute, high res. (70 meV), pot. bar., comp. of CCl <sub>x</sub> F <sub>4-x</sub> , x=1-4
	HM94	270-410	E,R	absolute; improved osc. str. conversion; this bibliography!!
	SBS94b	44-1500	P	partial and total ion yields; PEPIPICO; site selective fragmentation
	YL94	285-330	E	absolute GOS; comp. of CF <sub>4-n</sub> Cl <sub>n</sub> (n=0-4); $\sigma^*(C-Cl)$ GOS changes
	IK&95a	294-390	P	absolute; Beers' law; careful corr. of artefacts; x2 diff. from IM&88
	SBS95	294-317	P	PEPIPICO and KERD's; (C,F) site differences probed
	US&96	285-305	P,T	high res (60 meV); comp. of CH <sub>x</sub> F <sub>4-x</sub> (0<x<4); Auger and AI decay; SCF calculation; Rydberg vs. valence
	AM97	284-295	T	electronegativity correlations used for assignments; comp. to BBB78
	NK&97	295-303	P	resonant Auger; high res.; Jahn-Teller split $\sigma^*(t_2)$ ; mostly spectator; questions participator/total ratio as measure of valence/Ryd. Character vibronic theory; JT (t <sub>2</sub> ) and quasi-JT; Ryd-val interference; comp. to US&96; vibronic Fano; Ryd. anti-resonant versus prompt at 299.5 eV
	ITK99	295-302	P,T	relative; TIY, threshold EY, TPEPIPICO; kinematics; branching ratios
	TF&99	295-305	P	TIY, ion-auger coinc; J-T vibronic in core hole decay; 2-step dissociation
	US&99b	295-302	P,T	absolute; high res.; Γ~74 meV; comp. of CX <sub>4</sub> , X=H,Cl,F
	SC&02	288-296	P	TIY, resonant 2D Auger maps. Ultra-fast dynamics, Jahn-Teller (1s, 3p) t <sub>2</sub>
	PG&12	295-302	P	resonant (Auger,ion) coincidence
	IIS12b	299	P	dissociation dynamics (Auger-photoion coincidence; (2 time scales)
	IL&17	298.4	P	CF <sub>3</sub> OF, low-lying $\sigma^*(F-O)$
<b>CF<sub>4</sub>O</b>	IM&87	290-330	E	PEPICO, PIPICO, site-selective fragmentation
CF <sub>8</sub> S	IS&05	285-320	P	cont. res., vibrational structure
CHN	HB79a	280-320	E	cont. res., vibrational structure, Z+1 analogy
	HB79b	280-320	E	$\sigma^*$ -res./bond length relationship
	SSH84a	300	T	$\sigma^*$ shape res.; position & shape as f(R); approx. cyl. well & ab initio
	SG&89	290-330	T	

CHN . . .	LAL91	285-305	T	CNDO, systematic calc. of $\sigma^*$ energies; ISEELS, ETS for param. det.
	ZZ&92	285-300	T	$\Delta$ SCF; explicit core hole; localisation; rules for E(MO) for 2nd row
CH <sub>2</sub>	CG&80	283-300	T	ab initio calc.
CH <sub>2</sub> O	HB80b	280-320	E	formaldehyde; vibrational structure, cont. res., Z+1 analogy
	SSH84a	300	T	$\sigma^*$ -res./bond length relationship
	RI&88	270-330	E	absolute, comp. to H <sub>x</sub> F <sub>2-x</sub> CO, perfluoro effect
	SBT88	285-293	T	absolute; ab initio; low-lying double excitation; comp to HB80b
	SG&89	290-330	T	$\sigma^*$ shape res.; position & shape as f(R); approx. cyl. well & ab initio
	LAL91	285-305	T	CNDO, systematic calc. of $\sigma^*$ energies; ISEELS, ETS for param. det.
	RD&92	285-312	P	high res.; Franck-Condon analysis 6 geometry; E <sub>el</sub> as f(isotope)
	S92	280-320	E,R	comp. of CH <sub>x</sub> F <sub>2-x</sub> O, $\sigma^*(C-F)$ development
	KS&93	295-350	P	absolute; partial PI X-sect.; $\beta$ ; shape-resonance pos.
	NB95	284-292	T	coupled cluster abi initio; S-T splittings of Rydberg states
	SLD95	287	T	absolute, DF-LCAO; OS for C1s, O1s $\rightarrow \pi^*$ ; orbital mapping
	HC96	286	T	DFT; singlet-triplet (0.76 eV)
	SB&96	290-350	T,R	absolute, partial PI; $\beta$ s
	SCT96	295-320	T	core-valence double ionisation; $^1\pi$ , $^3\pi$ states; comp. of CO, H <sub>2</sub> CO, N <sub>2</sub>
	YA&96	280-320	T	STEX; comp. to expt. and other theory; R <sub>2</sub> CO species
	TPA98	280-320	T	absolute; DFT vs. STEX, compares CO and R <sub>2</sub> CO, R = H, Me
	YA&97	287	T	$\pi^*$ OS for CO bound to hydrocarbons; test of initial and final state sum rules; comp to expt.
	PP&00	286	T	MC-SCF Z+1 calc; vibrational structure, XPS better than NEXAFS, comp. to expt (RD&92)
	TG&00	285-290	T	ab initio; bound ( $1s^{-1}$ , $\pi^{-1}$ , $\pi^2$ ) state predicted
	TMG01	285-292	T	absolute; AC2, MRCI; comp. to RD&92
	TM&01	284-292	T	relative, Green's function methods; vibrations; comp. to expt. (RD&92)
	JC&03	285-287	P	PEY 75 meV resolution, vibrations, resonant Auger and valence PES at $\pi^*$
	CT06	284-296	T	ADF-DFT, compared to experiment, agree within 0.3 eV
CH <sub>2</sub> O <sub>2</sub>	IH87	275-325	E	(formic acid), absolute, $\pi^*$ mapping, $\sigma^*(C-O)$
	IH88	275-325	E	absolute; comp. to sol. (dimer?), spectr. add'n in methyl formate
	LAL91	285-305	T	CNDO, systematic calc. of $\sigma^*$ energies; ISEELS, ETS for param. det.
	S92	280-325	E,R	comp. of HCO <sub>2</sub> H, HCO <sub>2</sub> CH <sub>3</sub> and PMMA nEXAFS
	GM&06	280-340	P	TIY, PIY, fragmentation, PEPIPICO, comparison of 4 isotopomers
	GSL09	285-315	P	PIY, dication and re-arrangement ions differ from singly charged fragments
				cont. res.
CH <sub>3</sub> I	HB78a	50-350	E	vibrational structure
	HB79c	284-293	E	
	OCB98	5-480	E	absolute; (e,2e); (e,e+ion); ion yields, dipole induced breakdown
CH <sub>3</sub> NO	IH86	275-325	E	HCONH <sub>2</sub> formamide, comp. to (HCOX, X=F,OH)
CH <sub>3</sub> NO <sub>2</sub>	VA&92	280-750	P	absolute; analysed as (CH <sub>3</sub> <sup>+</sup> , NO <sub>2</sub> <sup>-</sup> ); bond length corr.
CH <sub>3</sub> NS <sub>2</sub>	TV93	285-295	T	NH <sub>3</sub> CS <sub>2</sub> ; ab initio-SCF-EICVOM; pre-edge res. ( $\pi^*$ , $\sigma^*_{O-O}$ , $\sigma^*_{S-S}$ )
CH <sub>3</sub> O <sub>3</sub>	T86	290-310	T	C(OH) <sub>3</sub> <sup>+</sup> ; X $\alpha$ calc; comp of BF <sub>3</sub> , B(OH) <sub>3</sub> , C(OH) <sub>3</sub> <sup>+</sup> , $\delta(R)$ – symmetry
CH <sub>4</sub>	LBZ64	30-620	P	absolute
	C69	284-292	P	photographic
	BKL73	285-295	T	ab initio calc., isotope intensity effect prediction (see HPB77)
	DK73	285-295	T	ab initio calc., one-centre expansion
	WB74b	283-323	E	weak cont. features
	WB74g	286-292	E	Z+1 analogy
	WB74h	286-292	E	Z+1 analogy
	DK75	285-295	T	ab initio calc.
	R75	285-320	T	alternate assignment of WB74g
	S75b	285-320	T	Z+1 analogy calc., comp. to experiment (WB74b)
	BW&76	0.2-2.5	E	Compton profile

(CH <sub>4</sub> cont' d)	DC76	285-295	T	ab initio calc.
	EH&76	280-300	P	photoelectric yield
	TK&76	287-289	E	<70meV FWHM res., vibrational structure
	HPB77	285-293	E	vibrational structure, isotope intensity effects
	BBB78	282-310	P	absolute
	TKR79	287-291	E	vibrational structure, <70meV FWHM res.
	A80	285-300	P	relative, (see SYD82)
	AVZ82b	532-540	P	comp. to NH <sub>3</sub> ,H <sub>2</sub> O,Ne isoelectronic series (WB74b data)
	SYD82	285-300	T	ab initio, absolute, comp. to expt (A80)
	MRR84a	275-290	E	1s->3p res. in elastic scattering, E=283.75eV
	MRR84b	280-286	E	angular dependence of C1s->3p res. in elastic scattering, f-wave
	HB&84	280-320	E	comp. of WB74b data to C <sub>2</sub> H <sub>6</sub> (HB77) - no σ*(C-C) res.
	SSH84a	305	T	σ*-res./bond length relationship
	TD84	280-295	T	multiple scattering calc., comp. to expt (WB74b)
	GK86	288	T	3s,3p singlet, triplet energies (.39/.13 eV split)
	SA&86b	250-780	P	absolute, comp. to CF <sub>4</sub> ; transfer of OS (cont'discrete in CF <sub>4</sub> )
	SS86a	240-390	P	total (e <sup>-</sup> ,ion) yield (w-value), 3% modulation by edge structure, PCI
	HFM87	280-320	E	comp. to other fluorocarbons; σ*(C-F) 'giant shape res.'
	HI87	275-325	E	π*(CH <sub>3</sub> ), comp. to other alkanes
	SAV87	280-320	P	absolute; thr. integrated OS comp. to CF <sub>4</sub> , CO <sub>2</sub>
	RS&89	290-330	T	MS-Xα; C1s X-sect. & β for (CF <sub>x</sub> H <sub>4-x</sub> ,x=0-4); only CH <sub>4</sub> res.!
	MR&90	280-320	P	ion desorption (H <sup>+</sup> from ice); comp. to TEY; gas (WB74b)
	RC&90	280-320	P	comp. of gas, solid; ion yields, H <sup>+</sup> ultrafast diss.
	HM&91b	287-294	P	ZEKE, 0.15 ev fwhm; comp. of CH <sub>4</sub> , CD <sub>4</sub> ; PCI modifies ZEKE; FC analysis of C <sub>K</sub> <sup>+</sup> (ΔΓ=-0.052(7)A; hole relax. > internucl. rep.
	LAL91	285-305	T	CNDO, systematic calc. of σ* energies; ISEELS, ETS for param. det.
	KNP92	285-290	T	SCF-CI with (Z+1); comp. to expt. [WB74b]; small dev. in triplet states assoc. with (Z+1) errors
	KP92a	287-291	T	absolute, MR-CI; comp. to expt. [TKR79]
	S92	280-320	E,R	comp. of CH <sub>3</sub> X, X=H, CH <sub>3</sub> , NH <sub>2</sub> , OH, F; σ*(X-H)
	RDK93	286-291	P	high res (60 meV); I <sup>D</sup> /I <sup>H</sup> (3s) = 0.57(5); B-O not H-T vibronic coupling; comp. of CH <sub>4</sub> /CD <sub>4</sub> ; C <sub>2</sub> H <sub>6</sub> /C <sub>2</sub> D <sub>6</sub> ; C <sub>3</sub> H <sub>8</sub> /C <sub>3</sub> D <sub>8</sub>
	ST&93	286-291	P,T	high res (60 meV); ab initio; CH <sub>4</sub> /CD <sub>4</sub> comp; 3s/3p (D/H) is 0.65; comp of H <sub>2</sub> O, NH <sub>3</sub> , CH <sub>4</sub> - all σ* dissoc.
	DRK94	281-291	P,R	SX700 high res. studies; vibrational structure in small mols.
	UO&95a	286-291	P,T	60 mV fwhm; resonant Auger used to detect Ryd-val. mixing; no Jahn-Teller; predicts C-H val. states in continuum (cf SSH84a)
	K96	286-291	P,R	sym. resolved; TIY, 3p Jahn-Teller distortion → non-symmetric ang. dist.
	KI&96	280-320	P	absolute; high res. XAS and XPs; partial PI X-sect. (satellites); ang. dist.; conjugate shake-up; continuum peaks (303,311) identified as doubly excited states; conclude σ*(C-H) (a <sub>1</sub> ,t <sub>2</sub> ) are mixed with Rydbergs
	US&96	285-305	P,T	high res (60 meV); comp. of CH <sub>x</sub> F <sub>4-x</sub> (0<x<4); Auger and AI decay; GSCF3 calculation; Rydberg vs. valence
	AM97	284-295	T	electronegativity correlations used for assignments; comp. to BBB78
	K01	286-290	P,T	symmetry resolved; high res.; Jahn-Teller
	SC&02	288-296	P	absolute; high res.; Γ~88 meV; comp. of CX <sub>4</sub> , X=H,Cl,F
	UG05	286-292	P,T	high-res, 40 meV; comparison of small alkanes; Ryd-val mix; GSCF3
	JV&06	286-291	P	luminescence yield, strong variation on 3s/2p, 100 meV fwhm
	JV&07	286-291	P	luminescence yield, strong variation on 3s/2p, 100 meV fwhm
	HV&20	287-292	P	TEY, 116meV, VerSoX end-station test
	RB&23	286-291	P	ion yield versus TEY, soft X-ray-induced dimerization of methane
(CH <sub>4</sub> ) <sub>n</sub>	KB&97	284-296	P	NEXAFS as f(cluster size); gas-solid evolution

<b>CH<sub>4</sub>N<sub>2</sub>O</b>	UH&95b	284-300	E	urea, comparison to polymers
<b>CH<sub>4</sub>O</b>	WB74b	282-325	E	(CH <sub>3</sub> OH - methanol)
	SSH84a	295	T	σ*-res./bond length relationship
	IH88	280-325	E	absolute OS, used to test spectral additivity in methyl formate
	H89	280-320	E,R	review of electron-beam core excitation spectroscopies (Aussois)
	LAL91	285-305	T	CNDO, systematic calc. of σ* energies; ISEELS, ETS for param. det.
	BC&92	280-340	E	absolute
	S92	280-320	E,R	comp. of CH <sub>3</sub> X, X=H, CH <sub>3</sub> NH <sub>2</sub> , OH, F; σ*(X-H)
	AJ&97a	278-293	P	relative, 45 meV fwhm; vibrational struct; comp to CD <sub>3</sub> OD
	HP&99	287-298	P	relative, TIY, PIY, PEPICO yields, site specific fragmentation
	SO&02	285-298	P	relative, anion PIY, OH <sup>-</sup> only in discrete C1s states
	IH07	284-302	T	relative, Gaussian augmented plane wave (GAPW) - DFT; (-5 to +3 eV errors on 14 small molecules, methanol dimer
<b>CH<sub>4</sub>O<sub>3</sub>S</b>	HH14	280-330	E	(methane sulfonic acid), references for PFSA (Nafion)
<b>CH<sub>4</sub>S</b>	DTH90	275-325	E	CH <sub>3</sub> SH; absolute, comp. to other RSH, RSR'; σ*(C-S)
	TV93	285-295	T	ab initio-SCF-EICVOM; pre-edge res. (π*, σ* <sub>O-O</sub> , σ* <sub>s-s</sub> ); comp to DTH90
<b>CH<sub>5</sub>N</b>	WB74b	280-320	E	(CH <sub>3</sub> NH <sub>2</sub> - methylamine) res. at thr.
	SSH84a	295	T	σ*-res./bond length relationship
	SB85b	285-335	E	σ* res. at thr., comp. to (CH <sub>3</sub> ) <sub>x</sub> NH <sub>3-x</sub> , x=0-3
	LAL91	285-305	T	CNDO, systematic calc. of σ* energies; ISEELS, ETS for param. det.
	S92	280-320	E,R	comp. of CH <sub>3</sub> X, X=H, CH <sub>3</sub> NH <sub>2</sub> , OH, F; σ*(X-H)
<b>CNiO</b>	OD93	287-300	T	ab initio SCF-CI; comp. of CO, NiCO; comp. to expt. (CSB89), NEXAFS of CO/Ni (PC&78); intensity ratios predicted; f(π*)=0.24; no reduction in f(π*) relative to free CO (.239 6 .234)
<b>CO</b>	SLD95	287	T	absolute, DF-LCAO; OS for C1s, O1s → π*; orbital mapping
	WSB70	280-310	E	ionic fragmentation (C <sup>+</sup> , CO <sub>2</sub> <sup>+</sup> yields)
	NM&71	281-298	P	photographic
	WS72	284-314	E	absolute, ionic fragmentation
	WBW73	280-325	E	cont. res., Z+1 analogy
	DSD76	290-360	T	MS X-α calc., shape res. photoelectron βs
	TK&76	287-288	E	vibrational structure
	GMK77	287-288	T	ab initio calc. of vibrational structure
	KLW77a	200-500	E	absolute, cont. res.
	KLW77b	200-500	E	absolute, ionic fragmentation, post-collision interaction effects
	KMR77	284-300	E	negative-ion K-shell-excited res.
	KM&77	280-320	T	ab initio calc., vibn'l struct; comp. to expt (NM&71, WBW73)
	IKN78	280-320	T	ab initio calc., comp. to experiment (WBW73), two-electron transitions
	PC&78	290-320	T	ab initio calc., comp. to experiment (KLW77a), cont. shape res.
	DD79	290-350	T	X-α (MSM) calc., cont. shape res.
	KDC79	287-288	T	ab initio calc. of vibrational structure, comp. to experiment (TK&76)
	KMN79	285-310	T	ab initio calc., comp. to experiment (KLW77a), oscillator strengths
	TKR79	287-297	E	<70meV FWHM res., vibrational structure, Z+1 analogy
	ZT&79	284-290	E	-ve ion K-shell-excited res. obsv'd in ionic frag. yields
	DS&80	290-320	T	X-α (MSM) calc., shape res. Auger electron ang. dist.
	HB80a	280-320	E	vibrational structure, cont. res., comp. to theory
	W80	295-310	E	cont. shape res., ionic fragmentation
	BH81	280-320	E,R	re. absorption vs. ion yields, PCI effEffects, comp. to N <sub>2</sub> calibration (π*=287.40eV)
	BD&82	285-290	E,R	total ion yield and fragmentation (PIMS), comp. to KLW776
	ES&83a	284-302	P	comparison of core and valence cont. shapes
	GN&83	280-320	P,T	ab initio (Z+1) basis calc. of (1s,π*) energy, comp. to expt (HB80a)
	KK83	285-289	T	dipole forbidden transitions
	SK&83	280-300	E	

(CO cont' d)				
	TS&83	270-320	P	absolute, cont. X-sect., Auger yield, $\beta$ value, shape res.
	UT83	280-290	E	$^3\pi$ state observed in ELS (Eo=400eV) and Auger-ELS (e,2e)
	ZMP83	280-500	E	appearance pot.s, $\pi^*$ at 287.3
	AA84	285-310	T	ab initio, CI, all 1-e & 2-e transitions, oscillator strength
	CF&84b	287	P	DES, $\pi^*$ AI; comp. to Cr(CO) <sub>6</sub> , CO/Cu(100); $^1\pi \rightarrow ^3\pi$ before AI on surf.?
	EC&84	280-340	P	ion yield, ion KE, comp. to DES, CO/Cu and Mn,Co,Fe carbonyls
	ES84	285-300	P	partial and total ion yields
	JH&84	283-293	P	EY; sol./gas/chemisorbed Ni(111) comp., (-0.3eV chemisorb. shift); M->C=O backbonding, 0.2eV FWHM, vibrl. struct.
	SB84	287.40(2)	E	calibration standard ( $\pi^* v=0$ )
	SK&84a	286-302	E	apparatus, 55meV FWHM; $^3\pi$ (410eV impact), Ryd. IP=296.07(4); vibnl struct. in 2e- excit. (300-302eV) ( $^3\pi \rightarrow ^1\pi = 1.45$ eV)
	SK&84b	270-320	P	absolute, Auger (AI) X-sect.; comp. to KLW77a, calc.
	SSH84a	295	T	$\sigma^*$ -res./bond length relationship
	TL&84	280-320	P	Auger on $\pi^*$ , cont; PES X-sect. & $\beta$ s; absolute, comp. to KLW77a
	UH84	280-315	E	conjugate shakeup enhancement; comp. of Auger, (e,2e) and EELS
	BS85	285-295	T	polarisation-propogators, allowed, forbidden, double excitations, absolute, comp. to HB80a
	CF&85	286-289	T	calc. of vibrational structure in $\pi^*$ , comp. to TKR79
	RL&85	280-320	P	comp. of multilayer PSID and ISEELS; comp. of CO, N <sub>2</sub> , NO, N <sub>2</sub> O
	UT85	275-315	E	autoionization and Auger decay by (e,2e)
	BH&86	285-320	P	$\beta$ s change at $\pi^*$ but not $\sigma^*$ res.
	HI86	280-530	E	weak EXAFS
	HK86	283-290	E	5-40 eV constant final energy scans, $^3\pi \rightarrow ^1\pi$ ratio, $\sigma^*$ negative ion res. at 14 eV excitation
	KS&86	287	T	DV-X $\alpha$ , 1s--> $\pi^*$ , comp. to IPES, NiCO, sensitive to R(Ni-C)
	RS&86	300-400	P	partial X-sections, $\beta$ s for main line & sat.(S <sub>1</sub> , S <sub>2</sub> ); S <sub>1</sub> (308 eV) displaced $\sigma^*(C-O)$ ; S <sub>2</sub> (315 eV) - no shape res., diff. $\beta$
	AWS87	303-308	T	2e- excited states (1s <sup>-1</sup> , val <sup>-1</sup> , $\pi^{*2}$ )
	E87	285-340	P	IYs; (e,ion) coinc.; ion KE, comp. to TM COs & chemisorbed CO
	FR&87	300-400	P	XPS satellite part. X-sect.; S1 - displaced res.; S2 - no $\sigma^*$
	K87	287-295	T	ab initio, CI, absolute dipole, comp. to expt
	MC&87	280-330	E	absolute, test of EELS6PA conversion
	H89	280-320	E,R	review of electron-beam core excitation spectroscopies (Aussois)
	HKA88	280-300	E	thr. excited Auger, PCI, negative ion res.
	HL&88	260-360	P	absolute, total & part. IY; PIPICO, ion breakdown patterns
	MF&88	280-320	P	ZEKE; XPS-sat & EELS/PA, higher Ryd., 2e & shake-up, PCI
	NE&88	287,305	P	PIPICO, comp. to valence & O1s double ionisation
	CSB89	280-335	E	comp. to Ni(CO) <sub>4</sub> ; vibrations resolved on $\pi^*$
	SG&89	290-330	T	$\sigma^*$ shape res.; pos. & shape as f(R); approx. cyl. well; ab initio
	SY&89	280-320	P	comp to EELS, lower discrete/cont.; cont. flatter; O1s 2nd order
	BS90	296-400	P	satellite line X-sect; comp. to atomic and N <sub>2</sub>
	DX&90	285-310	P	85 meV fwhm; vibn struct. in 2-e- transitions
	H90a	280-325	E.R	absolute; comp. to TM-COs; relaxation and $\delta(R)$ for $\sigma^*(CO)$
	HWR90a	280-325	E	absolute; comp. to TM-COs; f( $\pi^*$ ) vs. extent of backbonding
	SBM90	292-322	T	RCHF calc, improved agreement with experiment [LT&84]
	BH91	280-320	E,R	re. absorption vs. ion yields, PCI effFects, comp. to N <sub>2</sub>
	FA91	287-290	T	ab initio; XAS and XRF; comp. to expt. (HB80a)
	L91	295-320	T	$\beta$ -parameter; comp. to DS&80
	LAL91	285-305	T	CNDO, systematic calc. of $\sigma^*$ energies; ISEELS, ETS for param. det.

(CO cont' d)	MC&91	285-304	P	150 meV fwhm; isotope effect on $\pi^*$ , Ryd vib'n; comp to N <sub>2</sub> ; vibr'ns in 2e; ECM breakdown in intensities
SBM91	305-400	T	RCHF; SD & SI satellite X-sections; comp. to ext.	
DM&92	286-289	P	high res. (55 meV)	
H92b	286-292	E	comp of ${}^3\pi$ - ${}^1\pi$ split. in CO and Fe(CO) <sub>5</sub>	
MH&92b	285-310	P	ZEKE-PES; 140mV fwhm; ion state vibn. (ad.); 2e-; comp. to AWS87	
RF&92	286-289	P	high res. (<50 meV); instrument description	
RS&92a	280-330	P	TEY, TIY; comp. of CO <sup>+</sup> and (CO) <sub>2</sub> <sup>+</sup> from (CO) <sub>n</sub> , n to 8; cont. incr. in CO <sup>+</sup> ; ms; PIPICO	
SK&92a	298-322	P	cross-sect. & $\beta$ from PES; (1s <sup>-1</sup> ) comp. to total Auger; 2e- excit. seen in 1e-X-sect.; CANNOT use CIS top distinguish 1e- vs. 2e-	
TWT92	287-288	P	140 meV, accurate v=0/v=1 intensities	
YM&92	286-289	P	50 meV resolution	
YS92	285-315	P	symmetry resolved PI (0, 90° ion yield); high res. (51 meV)	
ZZ&92	285-300	T	$\Delta$ SCF; explicit core hole; localisation; rules for E(MO) for 2nd row	
BL93	285-320	T	PI cross-section, multichannel CI	
HH&93	285-320	P	$\beta$ -values for C <sup>+</sup> and Auger; $\beta>1$ at 305 ( $\sigma^*$ ) in both; $\pi$ - $\sigma$ interactions decrease molecular alignment	
OD93	287-300	T	ab initio SCF-CI; comp. of CO, NiCO; comp. to expt. (CSB89), NEXAFS of CO/Ni (PC&78); intensity ratios predicted; f( $\pi^*$ )=0.24	
RK&93	300-320	P	vibrationally resolved partial PI X-section; $\sigma^*$ resonance affects vibrational populations; vibrations in shake-up signal	
SH&93	280-320	P,T	symmetry resolved spectra using ion ang. dist.	
BSS94	280-320	P,T	$\beta = -0.8 (\pi^*), +0.5 (\sigma^*)$ for C <sup>+</sup> , O <sup>+</sup> ; relaxed core HF calc; effect of C 1s shake-up on $\beta$	
DK94	286,287.4	E	autoioniz. decay of ${}^3\pi$ (Eo=315 eV); PCI shifts (95 mV <sup>-1</sup> $\pi$ ; 115 mV <sup>-3</sup> $\pi$ )	
DRK94	286-291	P,R	SX700 high res. studies; vibrational structure in small mols.	
FKH94	284-288	E,T	angle and Eo study of ${}^3\pi$ ; ab initio CI potential curves; ${}^1\pi$ and ${}^3\pi$ differ	
FE&94	285-290	E,T	triplet $\pi^*$ ; INDO calc; correlation of S-T split. and f( ${}^1\pi^*$ )	
HH&94	285-320	P	Auger anisotropy at $\sigma^*$	
NR&94	287.4	P,T	DES; v of CO <sup>+</sup> (val) depends on v of (C1s <sup>-1</sup> , $\pi^*$ ); comp. to N <sub>2</sub> , O <sub>2</sub>	
RH&94	296-320	P,T	ZEKE and partial X-sec. for satellites; comp. of C1s and O 1s	
S94	635,823	T	doubly K-excited & K-ionized states predicted; $\Delta$ SCF with opt. geom.	
YND94	292-320	T	absolute; ab initio; Z+1; multiple excitations; comp. to (TKR75)	
BM95	287,305	P	angle-dependent Auger (0,54.7°), $\beta$ ; initial state alignment produces anisotropic Auger; effect stronger at $\pi^*$ than $\sigma^*$	
CC&95	286-295	P	SGM at SRBC performance test; high resolution	
EK&95a	286-290	P	PIY; selective fragmentation at Rydberg states	
HA&95	299,326	P	(e,ion) PEPICO; PE ang. dist. with parallel and perp. excit.; f-wave char. of $\sigma^*$ SR only seen in parallel	
HW&95	330	P	ang.dist. of shake-up; participator Auger dominates	
KK&95	298-325	P	absolute; partial X-sect; high res.; shape res. in main & satellite channels; vibrationally resolved XPS	
NB95	285-295	T	coupled cluster abi initio; S-T splittings of Rydberg states	
OA&95	287	P,T	vibrationally-resolved AI; vib.-lifetime interference shift detected; nat. linewidths: C1 $\sigma^*$ =86(10) mV; C1s <sup>-1</sup> =97(10) mV	
SAA95	287-288	P	high res. (<50 meV); resonant Auger; (vibrational-lifetime) interference; comp. to OA&95	
SA&95	321	P	photoelectron asymmetry; fixed-in-space; forward-backward asymmetry	
SH&95	285-320	P	total and partial ion yields; e-ion coincidence	
SLD95	287	T	absolute, DF-LCAO; OS for C1s, O1s $\rightarrow \pi^*$ ; orbital mapping	
SS95	287-296	P,R	PEPICO; ang. dist.; KERD at $\pi^*$ , Ryd.	

(CO cont' d)	EK&96	286-294	P	partial ion yields; KERDs; frag. mechanisms; enhanced v=4 of $\pi^*$ in both QMS, TOF; comp. to SH&95, HL&88; KE discrimination in QMS
HC96	286-288	T		accurate excitation calc. by DFT; singlet-triplet split. pred. (1.28 eV)
KK&96b	288-340	P		absolute; autoionization of double excited states
L96b	286-296	P,R		high res. absorption; isotope effects
NM96	280-320	P,R		PIPICO, partial ion cross-sections (from HL&88); coincidence expts
PA&96	280-340	T		absolute, STEX; comp. of CO, Cu <sub>17</sub> CO, Cu <sub>50</sub> Co; models of CO/Cu(100)
SB&96	295-395	T,R		absolute, partial cross-sections; comp. to expt.
SCT96	295-320	T		core-valence double ionisation; $^1\pi$ , $^3\pi$ states; comp. of CO, H <sub>2</sub> CO, N <sub>2</sub>
SH&96b	287-287	P		(C <sup>+</sup> , O <sup>+</sup> ) angular and KE distributions; $\beta$ s; vibn=ly resolved (0.1 eV fwhm); $\beta(\pi^*) < 1$ ; long-lived low-KE components allow rotation prior to decay
SST96	285-315	T		constant chemical potential LDA; $\pi^*$ , $\sigma^*$ res. rel. position; comp. of $\pi$ - $\sigma$ sep. in CO, C <sub>2</sub> H <sub>2</sub> , C <sub>2</sub> H <sub>4</sub> , N <sub>2</sub> , O <sub>2</sub>
SO&96	293-296	P		vibrationally selected resonant Auger at 3p state; spectator dominant; v-dependent angular effects
WW&96	287.4,312	P		Auger-ion coinc., at $\pi^*$ , $\sigma^*$ ; (C,O <sup>+</sup> ) NOT detected, contrary to HL&88
YA&96	280-320	T		STEX; comp. to expt. and other theory; R <sub>2</sub> CO species
AK&97	285-289	P		angle-resolved ion yields; ion $\beta$ s
AMK97	285-287	T		absolute, DWA, cross-section for $^3\pi$ , $^1\pi$
BL97a	285-320	T		PI cross-sections; multichannel CI
BS97	287-295	T		MC-CI; absorption, AI, RIXS; interference effects
CC&97	287.4	P,T		resonant photoemission, frequency detuning; magic angle; (val) <sup>-1</sup> and resonant interference ; PE branching ratios as f(E) from interreference
GA97	280-340	T		absolute; STEX; resonant elastic scatt.; vib'n $\alpha$ detuning in REXS
HG&97	321,326	P		mass & angle resolved PEPICO; TOF e-,ion; forward/backward asymmetry due to multiple scattering; agrees with DSD76
JA&97b	286-297	P		relative; 12500 resolving power; 25 meV fwhm instrumental
NG&97	287-296	P,R		resonant X-ray emission (RIXS); ang. dep. at 3s, 3p, Ryd; v-dependent
PN&97	287-289	P,T		relative; high-res.; vibrationally resolved AI decay; ab initio calcs; vibrational-lifetime interference
SA97	287	P,R		Auger resonant Raman; interference controlled by detuning
SG&97a	287-292	P,T		resonant X-ray emission; screening shifts; ang. dep.; lifetime-vibrational interference; ab initio RIXS calc'n
SG&97b	286-289	P,T		lifetime-vibrational interference in RIXS, LVI important for lineshapes; self-absorption corrections
SG&97c	286-288	P		Auger resonant Raman; vib'nl struct. $\alpha$ detuning; t-v interference
SG&97d	293-296	P,T		resonant Auger of Rydberg; intermediate state relaxes
SL&97	296-350	P		PCI affects Auger decay, B-state vibrationally resolved
YA&97	287	T		$\pi^*$ OS for CO bound to hydrocarbons; test of initial and final state sum rules; comp to expt.
ZZL97	285-310	T		MS-SCF; comp. to DV-X $\alpha$ using Z+1 and g.s. approaches
GTM98	287	P,T		Auger resonant Raman; time domain; detuning effects
OS&98	287	P		AI; vib'n-resolved; lifetime-vib'n interference; Morse potential no good
S98	285-315	P,T		fixed-in-space molecule; symmetry resolved PA and PI; Angular distribution.; partial wave decomposition at $\sigma^*$
SA&98a	300-340	P		fixed-in-space molecule; symmetry repsolved PA and PI; Angular distribution.; forward scattering effect
SA&98b	305,330	PT		$\sigma^*$ shape resonance affects vibrations in XPS; num. simulation indicates F-C works with distorted intermediate state; Auger ang. dist. anisotropic
TPA98	280-320	T		absolute; DFT vs. STEX, compares CO with R <sub>2</sub> CO, R=H, Me, Ph
YNH98	290-340	T		absolute; many e-; comp. to expt (BL93, SBM91); multiplets too high
AD&99	285-287	E		resonant ion autoionization; $^3\pi$ , $^1\pi$ ratio = 8 at threshold; comp to AMK97

(CO cont' d)	BW&99	287, 350	P	PEPICO; Auger-ion coinc; 2-step ( $C^+, O^+$ ) at $\pi^*$ ; wall coll. & KERD
	HH&99	290-300	P	Ryd states; angle unresolved resonant Auger; $\beta_s$ , screening energies
	KB&99	287.4	P	resonant AI; participator/spectator; very high resolution
	P99	292-316	T	inelastic scattering; double excit; quasi-atomic; comp. to KK&96b
	PV&99	287-296	P	$\pi^*$ (79(5) and Ryd (3s 92(5), 3p 108(20)) lifetime widths
	SS&99	287-292	P	resonant Auger at $\pi$ , 2s, 3p; 3s valence-like; strict spectator OK for 3p
	CR&00	290-315	P,T	fixed-in-space ang. dist; theory; double excitation; shape resonance
	FK&00	287	P	vibrationally resolved resonant Auger
	H00	285-289	E,R	triplet non-dipole, vibrational structure
	MA&00	290-315	P,T	fixed-in-space ang. dist; theory
	PP&00	287.4	T	MC-SCF Z+1 calc; vibrational structure, XPS better than NEXAFS
	PR00	280-330	P,T	relative; molecule solid comparison; only Rydberg changes
	SH&00	287-288	P	TIY, PIY, PIPICO; lifetime-vibration effects; comp. of CO & N <sub>2</sub>
	YH&00	286-289	P	TEY; resolution test of CSRF-SGM
	CPA01	280-320	T	STEX with screening; comp. to expt. (HB80)
	I01	300-330	P,T	absolute, fixed-in-space photoelectron ang. dist.; shape resonances
	KML01	285-900	T	electron impact GOS, singlet-triplet ration as f(E <sub>0</sub> )
	KS01	296-1000	E	electron impact excited Auger-ion coincidence; comp to CO <sup>++</sup> PE curves
	WJ&01	306	P,T	COLTRIMS detailed ionization analysis; shape resonance dynamics
	SH&01	285-310	P	anionic photofragmentation
	FK&02	285-289	P	DES; resonant Auger reveals v=3, v=4 vibrational structure better
	GC&02	299-320	T	fixed-in-space ang. dist.; comp to expt.
	HS&02	295-299	P	anion yield at threshold, high-res – vibn'l effects; PCI
	JW&02	306	P, T	fixed-in-space PES; COLTRIMS; circular dichroism at shape resonance, MS , RPAE calc
	K02	284-298	P,T,R	symmetry resolved, high resolution; review
	MR&02	296-330	P	fixed-in-space ang. dist.; shape resonance; comp. to (SA&98a, MA&00)
	AH&04	298-312	P, T	fixed-in-space ang. dist.; vibrational effect on shape resonance
	GM&04	275-325	P	TIY, PIPICO, PEPIPICO, absolute, partial ion & ion pair yields
	MTU04	296-310	P	vibrationally resolved PI X-sections – bond length dependence of SR
	C05	287	T	DFT, small molecue BE and excitation energies
	YHA05	305	P, R	ion angular dist; fixed-molecule PAD spectra, review, small mol.
	BF&07	285-320	P	fixed-in-space, Auger-PI coincidence & ang. dist. ; apparatus ; ab initio calc. of ion distributions agree well with exp't
	HK&07	280-320	P	relative, O <sup>-</sup> yield, ang. dist. from imaging time-of-flight; tracks absorption
	IH07	284-302	T	relative, Gaussian augmented plane wave (GAPW) - DFT; (-5 to +3 eV errors on 14 small molecules, comp. to TPA98
	CC11	200-600	E	EELS in TEM; in situ catalysis
	AK&12	340-440	P,T	molecular-frame photoelectron angular distributions; XPD calculation
	CM12	287.4	P, R	review of lifetime-limited linewidths (many small mol. Atoms)
	MC14	275-285	E	in-situ catalysis tracking (CO oxidation) in a E-TEM
	BF15	670	P,T	double core hole (DCH) PES&Auger; compare CO, CO <sub>2</sub> , N <sub>2</sub> , N <sub>2</sub> O
	PN&15	856	P	2-site double core hole IP (ts-DCH), SR, not FEL, coincidences
	TKU15	855	T	(XH <sub>m</sub> -YH <sub>n</sub> ) X,Y = C,N,O,F; m,n = 0-3 – 2-site double core hole IPs
COPd	SLD95	287	T	absolute, DF-LCAO; OS for C1s, O1s → $\pi^*$ ; orbital mapping
COPt	SLD95	287	T	absolute, DF-LCAO; OS for C1s, O1s → $\pi^*$ ; orbital mapping
<b>COS</b>	WB74e	282-328	E	pot. bar. effects
	TKR79	288-289	E	<70meV FWHM res., vibrational structure
	SSH84a	295	T	$\sigma^*$ -res./bond length relationship, anomalus
	TL&84	280-320	P	Auger on $\pi^*$ , Auger, PES cross-sections, $\beta_s$ , absolute
	HK87	285-297	E	singlet-triplet ( $\pi$ ) = 1.13 eV, $\sigma^*(C-S)$ = 0.3 eV
	HI88b	280-530	E	near edge and EXELFS; comp to calc (unpublished)

(COS cont'd)	NE&88	305	P	PIPICO, ion kinetic energies, comp. to valence, O1s ionization
	NH&88	285-325	R	comp. of ETS, all edges, CO <sub>2</sub> , CS <sub>2</sub> re localization of $\sigma^*$ , decay
	MH&89	275-340	E,T	absolute, ab initio, comp. of CO <sub>2</sub> , COS & CS <sub>2</sub> - all edges
	SY&89	280-320	P	comp to EELS, lower discrete/cont.; cont. flatter, O1s 2nd order
	EK&95c	288	P	PEPIPICO, lineshape distribution for ion pairs
	AK&97a	288	P,T	Renner-Teller split $\pi^*$ state of CO <sub>2</sub> , COS, CS <sub>2</sub> ; ion yield polarization
	EK&97a	287-297	P	TIY, PEPICO; $\beta$ ; high res.; PEPICO
	EK&97b	286-296	P	TIY, PEPICO; fragmentation mechanisms
	EK&97c	286-296	P	TIY, PIY; PE3PICO; fragmentation mechanisms
	MB&98	287-290	P	resonant Auger; vibrational resolved; Renner-Teller; lifetime-vib'n interfer.
	MG&99	280-300	P,T	TIY, STEX, resonant emission; atomic like ultra-fast decay of $\sigma^*$
	FCB00	50-360	E	absolute; good match to atomic (Henke); aum rule analysis
	K02	284-298	P,TR	symmetry resolved, high resolution; review
	KM&03	288	T	GOS and incident energy (Jubilee) resonances calculated
	GA&05a	298-335	P, T	PAD, comp of S2p, C1s, O1s at selected energies, MS-X $\alpha$
	GA&05b	298-335	P, T	AR-PEPICO, comp of S2p, C1s, O1s at selected energies, MS-X $\alpha$
<b>CO<sub>2</sub></b>	WB74a	285-328	E	cont. res., Z+1 analogy
	SB76	285-330	T	geometry corrected, Z+1 analogy calc., E( $^1\pi^-$ $^3\pi$ )=1.15eV
	BDW79	.05-2.5	E	generalized oscillator strengths, Bethe surface
	HBW79	291	E	ionic fragmentation
	TK&79	289-291	E	<70meV FWHM res.
	PC&81a	295-335	T	ab initio calc.; comp. to experiment (WB74e), cont. shape res.
	B82a	291	E,R	ionic frag. of discrete autoionizing states, review (HBW79 data)
	LM82b	295-325	T	ab initio, comp. to experiment (WB74a), cont. shape res.
	NP&82	278-281	P	K-emission spectrum (e- excited), C1s <sup>-1</sup> width = 0.07(2) eV
	KK83	285-289	T	ab initio (Z+1) basis calc. of (1s, $\pi^*$ ) energy, comp. to expt (WB74a)
	SK&83	280-300	E	dipole forbidden transitions
	ZMP83	280-500	E	appearance pot.s, $\pi^*$ at 291.3
	SA&84	280-520	P	absolute, 0.2eV FWHM, comp. to WB74a, Z+1 analogy
	SK&84b	295-340	P	absolute, Auger (AI) yield, comp. to expt. [WB74a], calc. [LM82b]
	SSH84a	295	T	$\sigma^*$ -res./bond length relationship, anomalous
	TL&84	280-320	P	Auger on $\pi^*$ , Auger, PES cross-sections, $\beta$ s, absolute
	DH&86	295-325	T	critical of LM82b calc.
	HI86	280-530	E	weak EXAFS
	SKR86	287-294	E	high res. (65meV), E( $^1\pi^-$ $^3\pi$ )=1.48eV, comp. to theory (SB76)
	HK87	288-299	E	singlet-triplet ( $\pi^*$ ) = 1.42 eV
	MC&87	280-330	E	absolute OS, test of EELS6OOS conversion
	PL&87	290-330	T	shape-resonance bond length refutation
	SAV87	10-1000	P,T	absolute; comp. to X- $\alpha$ ; thr. inte. OS comp. to CH <sub>4</sub> , CF <sub>4</sub>
	NH&88	285-325	R	comp. of ETS, all edges, CO <sub>2</sub> , CS <sub>2</sub> re localization of $\sigma^*$ , decay
	MH&89	275-340	E,T	absolute, ab initio, comp. of CO <sub>2</sub> , COS & CS <sub>2</sub> - all edges
	SG&89	290-330	T	$\sigma^*$ shape res.; pos. & shape as f(R); approx. cyl. well & ab initio
	SY&89	280-320	P	comp to EELS, lower discrete/cont; cont. flatter, O1s 2nd order
	CT91	291	E	(e,e); DES comp. to Auger, theory [Phys. Rev. B 41 (90) 10510]
	LAL91	285-305	T	CNDO, systematic calc. of $\sigma^*$ energies; ISEELS, ETS for param. det.
	MC&91	292-297	P	50 meV; vibrations in Ryd. states
	BBS91	260-380	E,T	GOS ( $\pi^*$ ); ab initio $\Delta$ SCF calc of GOS
	FA91	290-294	T	ab initio, calc of E,f for XRF, XAS; comp. to expt. (WB74)
	DJ&92	295-320	P	ZEKE, (ZEKE, ion,ion) yield; comp. to cluster (CO <sub>2</sub> ) <sub>n</sub>
	SK&92a	298-340	P	cross-sect. & $\beta$ from PES; (1s <sup>-1</sup> ) comp. to total Auger; 2e- excit. seen in 1e-X-sect.; CANNOT use CIS top distinguish 1e- vs. 2e-
	S92	288-326	E,T,R	MS-X $\alpha$ ; comp. to WB74

(CO <sub>2</sub> cont' d)	BD93	288-292	E	near threshold (0°) excit.; σ* res. in I( <sup>1</sup> π/ <sup>3</sup> π); δE( <sup>1</sup> - <sup>3</sup> )=1.46(4) eV
	MB93	290.7	T	ab initio CI; GOS comp. to expt. [BBS91]; OOS=0.164
	ML&93	285-320	P	ionic fragmentation mechanisms; comp. of CO <sub>2</sub> , N <sub>2</sub> O, Fe(CO <sub>2</sub> (NO) <sub>2</sub>
	L94	290,303	P,T	resonant AI and X-ray emission; comp. to HF calc.
	NBE94	284-340	P	DES, Auger lineshapes; through edge; unified (excite-decay) model
	BSS95	288-330	P	total and partial ion yields, βs; PIPICO; O-C-O angle = 124° in π*
	HC&95	288-302	P	TIY, PIY; thr. e, ion,ion coinc.; site-specific fragment. (not in O1s)
	SK&95b	298-360	P	partial PE X-sect; βs for main & satellite lines; coupling prevents use of main lines to identify SR; strong conjugate shake-up
	SS95	291-296	P,R	PEPICO; ang. dist.; KERD at π*, Ryd.
	AK&96a	288-300	P	ion ang. dist. symmetry resolved for Rydbergs; vibronic coupling
	FCM96	291	T	GOS extrapolation to K <sup>2</sup> =0; comp. to BBS91
	HC&96	300	P	triple coincidence (C+,O+,O+) PIPICO
	K96b	292-298	P,R	symmetry resolved; 3sσ <sub>g</sub> shows anisotropy assoc. with bending; vibronic coupling in antisym. mode; strong effect on 3p,3d; no axial recoil approx.
	RJ96	280-330	P	O yield; compared to cation and TIY; O <sup>-</sup> from primary process
	YA&96	280-320	T	STEX; comp. to expt. and other theory; R <sub>2</sub> CO species
	AK&97a	291	P,T	Renner-Teller split π* state of CO <sub>2</sub> , COS, CS <sub>2</sub> ; ion yield polarization
	NG&97	291	P,R	resonant X-ray emission (RIXS)
	YA&97	287	T	π* OS; test of initial and final state sum rules; comp to expt.
	PV&99	290-296	P	Ryd (3s100(10), 3p 90(10), 4p (80(20)) lifetime widths
	ET&00	280-296	E,T	methods; GOS at π*, Ryd; MC-GMS calc
	H00	282-330	E,T,R	dipole, non-dipole spectra; π* GOS; parallel detection evaluation
	KBB00	289-292	P,T	high res.; resonant Auger; Renner-Teller; participator decay to A state; potential energy curves derived
	MS&00	290-298	P	E-PEPICO; bending mode affects ionic frag; more (O <sup>+</sup> ,CO) on low-E side
	SO&01	290.7	P	sub-natural linewidths by resonant Auger
	TE&01b	280-340	E,T	GOS at π*, Ryd; MC-GMS calc
	AM&02	288-325	P	fixed-in-space PE ang. dist.; f,p,h waves similar intensity at σ*
	HR&02	285-320	P,T	threshold yield; shake-up satellites; time domain analysis
	K02	284-298	P,TR	symmetry resolved, high resolution; review
	MC&02	290-292	P	Auger-ion imaging; bent-linear changes fragmentation, ES-AEPICO
	N02	290-292	T	symmetry-resolved Renner-Teller, A <sub>1</sub> , B <sub>1</sub> potentials and spectra; vibrational structure; comp to YN&02
	OS&02	288-312	P	relative, Anion, cation PIY; only O <sup>-</sup> at (C1s <sup>-1</sup> ,π*); O <sup>-</sup> , C <sup>-</sup> at O1s edge
	RB02	292	T	GOS computed with vibronic contributions
	SM&02	291	P, T	COLTRIMS, ion-ion correlation, geometry deformation in (1s <sup>-1</sup> , π*)
	YN&02	290-292	P	symmetry-resolved Renner-Teller; separation of A <sub>1</sub> , B <sub>1</sub> signals
	SF&03	285-335	P,T	fixed-in-space ang. dist.; RCHF calc agree with measurements
	KM&03	290	T	GOS and incident energy (Jubilee) resonances calculated
	MB&93	290-300	T	GOS calculation
	RF04	290	P	PIPIPICO (-ve, +ve) at π*; mechanism via (CO <sup>++</sup> ,O <sup>-</sup> )
	BRB05	292-296	T	GOS; oscillations from Young-type interference; comp to ET&00
	YHA05	315	P,R	ion angular dist; fixed-molecule PAD spectra, review
	TA&07	300-325	P,T	PE ang. dist., expt'l dipole matrix elements, shape resonance @ 315 eV
	CC11	200-600	E	EELS in TEM; in situ catalysis
	SS&12	320	P	Auger-ion-ion coincidence, [Auger, metastable CO <sub>2</sub> <sup>2+</sup> ] coinc.
	MC14	275-285	E	in-situ catalysis tracking (CO oxidation) in a E-TEM
	TK&14	320	P,T	(CO <sup>+</sup> , O <sup>+</sup> ) ang. dist in coinc with PE; bend angle geometric effect
	BF15	664	P,T	double core hole (DCH) PES&Auger; compare CO, CO <sub>2</sub> , N <sub>2</sub> , N <sub>2</sub> O
(CO <sub>2</sub> ) <sub>n</sub>	DJ&92	295-320	P	ZEKE, (ZEKE, ion,ion) yield; threshold ion-pairs with atomic ions are quenched in cluster; fast charge transfer; participator val. Auger

CO <sub>3</sub> H <sub>2</sub>	TV93	285-295	T	H <sub>2</sub> CO <sub>3</sub> ; ab initio-SCF-EICVOM; pre-edge res. ( $\pi^*$ , $\sigma^*_{\text{o-o}}$ , $\sigma^*_{\text{s-s}}$ )
CS <sub>2</sub>	WB74e	280-325	E	pot. bar. effects
	SSH84a	295	T	anomalous $\sigma^*$ -res./bond length relationship
	H87	270-310	P	relative yields of CS <sub>2</sub> <sup>+</sup> , CS <sup>+</sup> , CS <sub>2</sub> <sup>2+</sup> ; ion state decay, quadrupole MS
	HK87	284-297	E	singlet-triplet ( $\pi^*$ ) = 0.9 eV, $\sigma^* = 0.8$ eV
NH&88	285-325	R		comp. of ETS, all edges, CO <sub>2</sub> , CS <sub>2</sub> re localization of $\sigma^*$ , decay
MH&89	275-340	E,T		absolute, ab initio, comp. of CO <sub>2</sub> , COS & CS <sub>2</sub> - all edges
AK&97a	286	P,T		Renner-Teller split $\pi^*$ state of CO <sub>2</sub> , COS, CS <sub>2</sub> ; ion yield polarization
KE&98	280-320	P		TIY, angle-resolved PEPICO; $\beta = -0.65$ for S <sup>+</sup> at $\pi^*$ ; doubly excited states; anisotropy as f(KE); 80 meV fwhm
	FE&99	283-320	P	TIY; ionic frag; branching ratios; state selective fragmentation
	YE&99	283-320	P	TIY; ionic frag; branching ratios; state selective fragmentation
C <sub>2</sub>	K02	284-298	P,TR	symmetry resolved, high resolution; review
C <sub>2</sub> <sup>-</sup>	KM&03	286	T	GOS and incident energy (Jubilee) resonances calculated
C <sub>2</sub> ClH <sub>3</sub>	ET&07	280-310	E,T	absolute, OOS, , non-dipole, triplet states
C <sub>2</sub> ClH <sub>5</sub>	TR&07	280-310	E,T	absolute, OOS, GOS to 30 a.u. <sup>-1</sup> , MP-CI calc
	SG&89	290-330	T	$\sigma^*$ shape res.; pos. & shape as f(R); approx. cyl. well & ab initio
	SH&23	275-305	P	di-carbon anion, 1s $\sigma_u \rightarrow 3s\sigma_g$ , broad, 279.5 vert, <b>278.2</b> adiabatic
	BMT88	280-310	E	comp. to ETS
	SKB88	275-320	E	high res., comp. to vinyl halides
	HB78b	284-300	E	ethyl chloride; test of spectral additivity
	FL02	284-299	E	absolute, GOS profiles compared of C 1s, Cl 2p & valence
CCl <sub>2</sub> F <sub>2</sub>	H18	275-320	E	Freon152, absolute
CClF <sub>3</sub>	H14	280-330	E	trifluoro-chloroethylene, absolute
C <sub>2</sub> Cl <sub>2</sub> H <sub>2</sub>	CT&12	283-291	P, T	iso-dichloroethylene, PEY, resonant Auger, ADC Green's fn. calc.
C <sub>2</sub> Cl <sub>2</sub> H <sub>4</sub>	H92a	280-340	E	1,2-dichloroethene, absolute, comp. to NEXAFS (W. Walter)
C <sub>2</sub> Cl <sub>3</sub> H	WH90	275-340	E	trichloroethylene
C <sub>2</sub> DH	KI&97	282-292	P,T	high res. (20 meV); isotopomer comp.; vibronic coupling at $\pi^*$ ; bending modes excited; ab initio calc.
C <sub>2</sub> D <sub>2</sub>	MC&91	284-291	P	50 meV fwhm; $\pi^*$ & Ryd vibns; comp of C <sub>2</sub> H <sub>x</sub> , C <sub>2</sub> D <sub>x</sub> (isotope eff.)
	KI&97	282-292	P,T	high res. (20 meV); isotopomer comp.; vibronic coupling at $\pi^*$ ; bending modes excited; ab initio calc.
C <sub>2</sub> D <sub>2</sub> H <sub>2</sub>	KI&95b	283-291	P	CD <sub>2</sub> CH <sub>2</sub> ; absolute; ethene isotopomers 40 meV fwhm; vib'n'l isotope study; non-TS modes => symmetry breaking → core hole localization
	KG&97	283-287	T	vibronic coupling; symmetry breaking and core hole localization; comparison of isotopomers (C <sub>2</sub> D <sub>4</sub> , C <sub>2</sub> H <sub>4</sub> , CH <sub>2</sub> CD <sub>2</sub> , cis-CHDCHD)
C <sub>2</sub> D <sub>2</sub> H <sub>2</sub>	KI&95b	283-291	P	cis-CHDCHD; absolute; 40 meV fwhm; isotopomers; hole localiz.
	KG&97	283-287	T	vibronic coupling; symmetry breaking and core hole localization; comparison of isotopomers (C <sub>2</sub> D <sub>4</sub> , C <sub>2</sub> H <sub>4</sub> , CH <sub>2</sub> CD <sub>2</sub> , cis-CHDCHD)
C <sub>2</sub> D <sub>4</sub>	CS90	284-287	P	$\pi^*$ vib'n'l isotope effect; symmetry breaking; localised core hole
	MS&89	284-287	P	$\pi^*$ vib'n'l isotope effect; symmetry breaking; localised core hole
	MS&90	284-287	P	$\pi^*$ vib'n'l isotope effect; symmetry breaking; localised core hole
	MC&91	286-291	P	50 meV fwhm; $\pi^*$ & Ryd vibns; comp of C <sub>2</sub> H <sub>x</sub> & C <sub>2</sub> D <sub>x</sub> (isotope eff.)
	RA&92	284-286	P	high. res. (<90meV); vib'n'l; comp. to C <sub>2</sub> H <sub>4</sub>
	KI&95b	283-291	P	40 meV fwhm; $\pi^*$ vib'n's in isotopomers; hole localiz.
	KG&97	283-287	T	vibronic coupling; symmetry breaking and core hole localization; comparison of isotopomers (C <sub>2</sub> D <sub>4</sub> , C <sub>2</sub> H <sub>4</sub> , CH <sub>2</sub> CD <sub>2</sub> , cis-CHDCHD)
C <sub>2</sub> D <sub>6</sub>	MC&91	287-291	P	50 meV fwhm; $\pi^*$ & Ryd vibns; comp of C <sub>2</sub> H <sub>x</sub> & C <sub>2</sub> D <sub>x</sub> (isotope eff.)
	RDK93	286-291	P	high res (60 meV); comp. of CH <sub>4</sub> /CD <sub>4</sub> ; C <sub>2</sub> H <sub>6</sub> /C <sub>2</sub> D <sub>6</sub> ; C <sub>3</sub> H <sub>8</sub> /C <sub>3</sub> D <sub>8</sub>

<b>C<sub>2</sub>FH<sub>3</sub></b>	BB&85	280-296	P	parent ion yields, distorted cont./discrete intensities; QMS
	MC&87	275-325	E	absolute, comp. to C <sub>2</sub> H <sub>x</sub> F <sub>4-x</sub> , development of pot. bar.
	HFM87	280-320	E	comp. to other fluorocarbons; σ*(C-F) 'giant shape res.'
	BMT88	280-310	E	comp. to ETS
	RI&88	275-325	E	perfluoro effect, σ*(C-F)
	SKB88	275-320	E	high res., comp. to vinyl halides
C <sub>2</sub> FeN <sub>2</sub> O <sub>4</sub>	SL&92	280-300	P	Fe(CO) <sub>2</sub> (NO); PEPICO; stewise fragmentation; non-selective
	ML&93	285-320	P	ionic fragmentation mechanisms; comp. of CO <sub>2</sub> , N <sub>2</sub> O, Fe(CO <sub>2</sub> (NO)) <sub>2</sub>
	L95	320	P,R	PEPICO dissoc.; review of coinc. studies of DI dynamics
	NM96	320	P,R	PEPICO; review of fragmentation
<b>C<sub>2</sub>F<sub>2</sub>H<sub>2</sub></b>	BB&85	280-296	P	1,1-CH <sub>2</sub> =CF <sub>2</sub> , parent IY; distorted cont./discrete intens; QMS
	HC&87b	288-325	P	thr. e-, TOF-MS, claims selective fragmentation
	HFM87	280-320	E	comp. to other fluorocarbons; σ*(C-F) 'giant shape res.'
	MC&87	275-325	E	absolute, comp. to C <sub>2</sub> H <sub>x</sub> F <sub>4-x</sub> , C-F σ* res., pot. bar.
	RI&88	275-325	E	perfluoro effect, σ*(C-F)
	JS&90	285-306	P	ZEKE, PE-PI coinc.; sel. frag.; comp. of CF <sub>2</sub> CH <sub>2</sub> , CF <sub>3</sub> CH <sub>3</sub>
	HB&91	285-310	P	ZEKE, TEY, TIY; TOF-MS; site-selective frag.; "memory-eff."
	OY&05	283-308	P	absolute, PIY, KE distributions of CFH <sub>2</sub> <sup>+</sup> , CH <sub>2</sub> <sup>+</sup> , vibrational effects
<b>C<sub>2</sub>F<sub>2</sub>H<sub>2</sub></b>	MC&87	275-325	E	1,2-CHF=CHF; absolute, comp. to C <sub>2</sub> H <sub>x</sub> F <sub>4-x</sub> , C-F σ* res., pot. bar.
<b>C<sub>2</sub>F<sub>3</sub>H</b>	BB&85	280-296	P	parent ion yields, distorted cont./discrete intensities; QMS
	HFM87	280-320	E	comp. to other fluorocarbons; σ*(C-F) 'giant shape res.'
	MC&87	275-325	E	absolute, comp. to C <sub>2</sub> H <sub>x</sub> F <sub>4-x</sub> , C <sub>2</sub> H <sub>x</sub> F <sub>4-x</sub> , pot. bar.
	RI&88	275-325	E	perfluoro effect, σ*(C-F)
<b>C<sub>2</sub>F<sub>3</sub>HO<sub>2</sub></b>	RI&88	280-330	E	CF <sub>3</sub> COOH, comp. to other acids
<b>C<sub>2</sub>F<sub>3</sub>H<sub>3</sub></b>	MS&84	280-309	P	CH <sub>3</sub> CF <sub>3</sub> ; thr. e <sup>-</sup> , total & partial yield, site sel. frag.
	BB&85	280-296	P	parent ion yields, distorted cont./discrete intensities; QMS
	H90a	284-316	E	absolute; comp. of C <sub>2</sub> H <sub>6</sub> , CH <sub>3</sub> CF <sub>3</sub> , C <sub>2</sub> F <sub>6</sub> ; partial pot. barr.
	JS&90	285-306	P	ZEKE, PE-PI coinc.; sel. frag.; comp. of CF <sub>2</sub> CH <sub>2</sub> , CF <sub>3</sub> CH <sub>3</sub>
	HB&91	285-310	P	ZEKE, TEY, TIY; TOF-MS; site-selective frag.; "memory-eff."
	SSL91	290-300	T	site-selective frag. at CF <sub>3</sub> ; but stat. redist. int. energy in M <sup>2+</sup>
C <sub>2</sub> F <sub>3</sub> H <sub>4</sub> N	HC&87b	278-305	P	CF <sub>3</sub> CH <sub>2</sub> NH <sub>2</sub> , thr. e-, TOF-MS, claims selective fragmentation
<b>C<sub>2</sub>F<sub>3</sub>N</b>	HS90	280-340	E	CF <sub>3</sub> CN, absolute; comp. to other triply bonded species
<b>C<sub>2</sub>F<sub>3</sub>H<sub>3</sub>O<sub>3</sub>S</b>	HH14	280-320	E	(Methyl trifluoromethanesulfonate), absolute, comp to Nafion
<b>C<sub>2</sub>F<sub>4</sub></b>	BB&85	280-296	P	parent ion yields, distorted cont./discrete intensities; QMS
	HFM87	280-320	E	comp. to other fluorocarbons; σ*(C-F) 'giant shape res.'
	MC&87	275-325	E	absolute, comp. to C <sub>2</sub> H <sub>x</sub> F <sub>4-x</sub> , C-F σ* res.
	RI&88	275-325	E	perfluoro effect, σ*(C-F)
	H90a	290-320	E,R	absolute, pot. bar. effect on I{σ*(C-F)} through CF <sub>x</sub> series
	LAL91	285-305	T	CNDO, systematic calc. of σ* energies; ISEELS, ETS for param. det.
<b>C<sub>2</sub>F<sub>2</sub>H<sub>4</sub></b>	H19	275-325	E	1,2di-fluoro-ethne, absolute, compare to
<b>C<sub>2</sub>F<sub>6</sub></b>	HFM87	280-320	E	comp. to other fluorocarbons; σ*(C-F) 'giant shape res.'
	IM&88	275-325	E	C-F σ* res.
	H90a	284-320	E	absolute; comp. of C <sub>2</sub> H <sub>6</sub> , CH <sub>3</sub> CF <sub>3</sub> , C <sub>2</sub> F <sub>6</sub> and CF <sub>x</sub> ; pot. barr.
	AC&95	290-315	T	STEX ab initio; absolute; growth of poly (CF <sub>2</sub> ) <sub>n</sub> by C <sub>2n</sub> F <sub>4n+2</sub> , n=1-5
<b>C<sub>2</sub>F<sub>6</sub>O<sub>2</sub></b>	H86b	285-335	E,R	orbital mapping
	IM&87	285-335	E	CF <sub>3</sub> -O-O-CF <sub>3</sub> , long O-O bond = low σ*
	HM&89	275-350	P	absolute; total, partial ion yields; PIPICO, diss. IY; sel. frag.
<b>C<sub>2</sub>H<sub>2</sub></b>	EH&76	280-300	P	photoelectric yield
	HB77	280-340	E	cont. res.
	IKN78	280-330	T	ab initio calc., comp. to experiment (WBW73)
	TKR79	285-291	E	<70meV FWHM res., vibrational structure
	BB&80	285-320	T	ab initio calc. with CI, shake-up states

(C <sub>2</sub> H <sub>2</sub> cont'd)	HB81a	280-315	E	absence of plural scattering (pressure study)
	B81	280-355	P	cont. res. at 310 eV (vs 309 EELS), related to bond length
	B82b	280-355	P	cont. res. at 310 eV (vs 309 EELS), related to bond length
	ML&82	290-330	T	moment theory, shape of cont. res., comp. to expt. (HB77)
	SSH84a	295	T	$\sigma^*$ -res./bond length relationship
	HK87	283-293	E	Eo=120 eV, no triplets resolved, $\pi^*$ broader, Rydbergs modified
	AR&89	280-320	P,E,T	curve fit of HB77; comp. to NEXAFS; theor. (SW) lineshape; multi e- $\sigma^*$ shape res.; position & shape as f(R); approx. cyl. well & ab initio
	SG&89	290-330	T	binary (e,2e), EMS; 5 eV fwhm; BE is 0.5(2) eV higher than XPS
	ACS90	290	E	absolute; L <sup>2</sup> , delocal. hole; C <sub>2</sub> H <sub>x</sub> (x=2,4,6); $\sigma^*(C-H)/\sigma^*(C-C)$ reversal
	FSL91	290-390	T	CNDO, systematic calc. of $\sigma^*$ energies; ISEELS, ETS for param. det.
	LAL91	285-305	T	50 meV fwhm; $\pi^*$ & Ryd vibns; comp of C <sub>2</sub> H <sub>2</sub> &C <sub>2</sub> D <sub>2</sub> (isotope effect)
	MC&91	284-291	P	comp. of gas,sol, monolayer (Ag); Ryd. lost in cond. phase; IP shift
	RA&92	280-302	P	comp. of C <sub>2</sub> H <sub>x</sub> , x=2,4,6; $\sigma^*(C-C)$
	S92	280-330	E,R	<sup>3</sup> $\pi^*$ ; INDO calc; correl. of $\Delta(1,3)$ and $\pi^*$ osc. str.
	FE&94	284-286	E,T	absolute; improved method for X-section detection; this bibliography!!
	HM94	270-350	E,R	GOS for <sup>1</sup> $\pi^*$ ; relax., corr. & core-hole local. considered; OOS=0.147
	MB&94a	280-292	E,T	NB95 coupled cluster abi initio; S-T splittings of Rydberg states
	NB95	284-292	T	STS95 local density; Hedin-Lundquist potential needed to match expt.
	STS95	284-310	T	HC96 DFT calc.; <sup>3</sup> $\pi^{-1}\pi$ split = 0.50 eV
	HC96	285-286	T	SST96 constant chemical potential LDA; $\pi^*$ , $\sigma^*$ res. rel. position; comp. of $\pi$ - $\sigma$
	SST96	285-315	T	sep. in CO, C <sub>2</sub> H <sub>2</sub> , C <sub>2</sub> H <sub>4</sub> , N <sub>2</sub> , O <sub>2</sub>
	KI&97	282-292	P,T	high res. (20 meV); isotopomer comp.; vibronic coupling at $\pi^*$ ; bending modes excited; ab initio calc.
	KK&97a	280-350	P	main line cross-sections; comp. to absorption; weak peak at C <sub>2</sub> H <sub>2</sub> abs. max;
	KK&97b	290-360	P,T	comp. of C <sub>2</sub> H <sub>x</sub> , x=2,4,6; disputing existence of shape resonances
	KK&97c	298, 338	P,T	absolute; C 1s <sub>1</sub> main line & satellite X-sections; broad 310 eV peak assigned to shake-up NOT $\sigma^*$ ; smooth main line $\beta$ at 310 eV 6 no $\sigma^*$
	KN&97b	280-340	P	XPS, g-u splitting = 0.05(1) eV; vibrational and 2 state fit
	TPA98	280-320	T	resonance Auger, well-resolved Rydberg spectrum; angle resolved; $\pi^*, \sigma^*$
	GG&99	284-292	P,T	anisotropic; double excitation
	KK&99	290-360	P	absolute; DFT vs. STEX, comparison of C <sub>2</sub> H <sub>2x</sub> , x=1,2,3; comp. to C <sub>2</sub> H <sub>2</sub> /Cu
	TB&99	297-348	P,T	core hole localization in C <sub>2</sub> H <sub>2x</sub> ; symmetry broken X-ray emission; HF calc; localization increases with increasing bond length
	HC&00	280-340	T	absolute; main line partial cross-sections; disputes shape resonance in C <sub>2</sub> H <sub>6</sub>
	LL00	290-360	T	$\sigma_g$ & $\sigma_u$ partial X-sections; resonance in ratio of X-sect.; disputes KK&97b
	HJ&02	278-330	E,T	shape resonances from MS (Feff8) in C <sub>2</sub> H <sub>2x</sub> ; ang. dep; IPs good to 0.5 eV
	K02	284-298	P,TR	absolute; partial channel; $\beta$ ; comp. to KK&97a; $\sigma^*$ overlaps 2-electron symmetry resolved, high resolution; review
	PS&02	284-320	P	PIY, fragmentation mechanisms; Ryders versus shape resonances
	MGK03	286-292	P	angle-resolve phtoion-yield, symmetry resolved Rydbergs.
	ZTC03	280-320	T	MS-cluster calc, C-H resonances in near continuum, $\delta(R)$ for $\sigma^*_{C-C}$ in C <sub>2</sub> H <sub>x</sub>
	K04	287-292	P,T	symmetry resolved Ryd states; g-u splitting, Ryd-val. Exchange
	MTU04	298-356	P	vibrationally & $\sigma_g/\sigma_u$ resolved PI X-sections; SR only in $\sigma_g$ ; R-dep
	MG&05	287-292	P	angle resolved ion yield, polarization study, Ryd-valence mixing, retarding potential used to resolve overlapping states of same symmetry
	MP&05	284-286	T	GOS for excitation from 300-800 eV, 0-40 au <sup>-2</sup> , <sup>3</sup> $\pi^*$ , <sup>1</sup> $\pi^*$
	SF&05	270,286,540	P	momentum imaging, (H <sup>+</sup> , H <sup>+</sup> , C <sub>2</sub> <sup>+</sup> ) newton diagram at C1s <sup>-1</sup> , $\pi^*$
	AH&07	311	P	PE ang. Dist. In 3 ion pair channels; core hole localization
	IH07	284-302	T	relative, Gaussian augmented plane wave (GAPW) - DFT; (-5 to +3 eV errors on 14 small molecules

(C <sub>2</sub> H <sub>2</sub> cont'd)	S09	286, 288	P	(C <sup>+</sup> ,H <sup>+</sup> ) PIPICO KER profiles, symmetry breaking, vibrational effects
	PN&15	597,654	P	1-site, 2-site double core hole IP (ts-DCH), SR, not FEL, coincidences
C <sub>2</sub> H <sub>2</sub> O <sub>2</sub> S <sub>4</sub>	TV93	285-295	T	(OHCS <sub>2</sub> ) <sub>2</sub> ; ab initio-SCF-EICVOM; pre-edge res. ( $\pi^*$ , $\sigma^*_{O-O}$ , $\sigma^*_{S-S}$ )
C <sub>2</sub> H <sub>3</sub> I	BMT88	280-310	E	comp. to ETS
	SBK88	275-320	E	high res., comp. to vinyl halides
<b>C<sub>2</sub>H<sub>3</sub>N</b>	HTM89	275-325	E,P	(CH <sub>3</sub> CN), comp. to solid, $\sigma^*$ res./bond length
	HM&89	275-350	P	absolute; total, partial ion yields; PIPICO, diss. IY; sel. frag.
	S92	280-320	E,R	comp. of gas, sol. monolayer(Pt)
	PS&01	280-315	T	STEX, comp. to expt.; extensive series of C-N compounds
<b>C<sub>2</sub>H<sub>3</sub>N</b>	HTM89	275-340	E	(CH <sub>3</sub> NC), comp to CH <sub>3</sub> CN, vibrational ELS
<b>C<sub>2</sub>H<sub>3</sub>NS</b>	HTM89	275-340	E	(CH <sub>3</sub> SCN), comp to CH <sub>3</sub> NCS, vibrational ELS
<b>C<sub>2</sub>H<sub>3</sub>NS</b>	HTM89	275-340	E	(CH <sub>3</sub> NCS), comp to CH <sub>3</sub> SCN, vibrational ELS
<b>C<sub>2</sub>H<sub>4</sub></b>	EH&76	280-300	P	(ethylene) photoelectric yield
	HB77	280-340	E	vibrational structure, cont. res.
	TKR79	284-291	E	<70meV FWHM res., vibrational structure
	BB&80	285-320	T	ab initio calc. with CI, shake-up states
	B81	280-355	P	cont. res. at 306 eV (vs 302 EELS(HB77)), related to bond length
	B82b	280-355	P	cont. res. at 306 eV (vs 302 EELS(HB77)), related to bond length
	SSH84a	295	T	$\sigma^*$ -res./bond length relationship
	HR87	280-300	E	use of core excitation (HB77) to interpret Auger satellites (DES)
	MC&87	275-325	E	absolute, comp. to C <sub>2</sub> H <sub>x</sub> F <sub>4-x</sub>
	SS87b	269-324	P	8% modulation of W-value (energy/ion pair); Ryd., cont. struct; weak $\pi^*$ , prominent $\sigma^*$ , PCI
	BMT88	280-310	E	comp. to ETS
	H89	280-320	E,R	review of electron-beam core excitation spectroscopies (Aussois)
	MF&88	280-320	P	ZEKE; XPS-sat & EELS/PA, higher Ryd., 2e & shake-up, PCI
	RI&88	275-325	E	absolute, perfluoro effect, $\sigma^*(C-F)$
	SBK88	275-320	E	high res., comp. to vinyl halides
	AR&89	280-320	P,E,T	curve fit of HB77; comp. to NEXAFS; theor. (SW) lineshape
	MS&89	284-887	P	30 meV fwhm, vib'n's; comp. to C <sub>2</sub> D <sub>4</sub> , sym. breakdown, local. hole
	PF&89	280-360	P	partial X-sect., $\sigma^*$ at 302 eV
	CS90	284-287	P	$\pi^*$ vib'nl isotope effect; symmetry breaking; localised core hole
	HS&90	284-292	P	0.15 eV fwhm; vib'ns of Rydbergs discussed
	MS&90	284-287	P	$\pi^*$ vib'nl isotope effect; symmetry breaking; localised core hole
	FSL91	290-390	T	absolute; L <sup>2</sup> , delocal. hole; C <sub>2</sub> H <sub>x</sub> (x=2,4,6); $\sigma^*(C-H)/\sigma^*(C-C)$ reversal
	GK&91	283-291	P,T	40 meV fwhm; ( <sup>1</sup> B <sub>1u</sub> , <sup>1</sup> B <sub>2g</sub> ) vibronic coupling; 0.02 eV sep.; dynamic hole localisation by vibronic-coupled symmetry breaking
	LAL91	285-305	T	CNDO, systematic calc. of $\sigma^*$ energies; ISEELS, ETS for param. det.
	MC&91	284-291	P	50 meV fwhm; $\pi^*$ & Ryd vibns; comp of C <sub>2</sub> H <sub>x</sub> & C <sub>2</sub> D <sub>x</sub> (isotope eff.)
	TF&91	280-300	T	MS (cluster); calc. of pol. dep. on Cu(100); C-H res. (288 eV) with $\sigma$ -pol.; comp. to expt. (SSH84a)
	RA&92	284-286	P	high. res. (<90meV); vib'n'l; comp. to C <sub>2</sub> D <sub>4</sub> ; M-C <sub>2</sub> H <sub>4</sub> bond mod. vib.
	S92	280-330	E,R	comp. of C <sub>2</sub> H <sub>x</sub> , x=2,4,6; $\sigma^*(C-C)$
	KS&93	290-350	P	absolute; partial PI, $\beta$ ; no conjugate shake-up; shape res. pos. @ 295.5 eV, below absorption SR
	LA93	282-292	T	1-particle Green's function; comp. of C <sub>2</sub> H <sub>4</sub> , C <sub>4</sub> H <sub>6</sub> , C <sub>6</sub> H <sub>8</sub> ; comp. to GK&91 (solid); claims relaxation shifts dominate; $\pi^*$ split small.
	FE&94	284-287	E,T	<sup>3</sup> $\pi^*$ ; INDO calc; correl. of $\Delta(1,3)$ and $\pi^*$ osc. str.
	MB&94b	285	T	vibrational structure; comp. to expt.
	C95	285	T	core hole localisation via vibronic coupling; lifetime effects
	GA95	284-290	T	delocalization in polyenes; comp. of H-(CH=CH) <sub>n</sub> -H, n=1-5

(C <sub>2</sub> H <sub>4</sub> cont'd)	KI&95b	283-291	P	40 meV fwhm; $\pi^*$ vibn's in isotopomers; hole localiz.
	NB95	284-292	T	coupled cluster abi initio; S-T splittings of Rydberg states
	GYA96	285	T	X-ray emission as f(conjugation); $\pi$ -exciton effects; H(C <sub>2</sub> H <sub>2</sub> ) <sub>n</sub> H, n=1,10
	HC96	285	T	DFT calc.; $^3\pi^-1\pi$ split = 0.43 eV
	SB&96	290-350	T,R	absolute, partial cross-sections; comp. to expt.
	SST96	285-315	T	constant chemical potential LDA; $\pi^*$ , $\sigma^*$ res. rel. position; comp. of $\pi$ - $\sigma$ sep. in CO, C <sub>2</sub> H <sub>2</sub> , C <sub>2</sub> H <sub>4</sub> , N <sub>2</sub> , O <sub>2</sub>
	YA96	290-315	T	STEX; shake-up spectra related to NEXAFS; H(C <sub>2</sub> H <sub>2</sub> ) <sub>n</sub> H, n=1-5
	AJ&97a	284-292	P	relative, 35 meV; Rydberg vibrational structure
	KG&97	283-287	T	vibronic coupling; symmetry breaking and core hole localization; comparison of isotopomers (C <sub>2</sub> D <sub>4</sub> , C <sub>2</sub> H <sub>4</sub> ,CH <sub>2</sub> CD <sub>2</sub> , cis-CHDCHD)
	KK&97a	280-350	P	main line cross-sections; comp. to absorption; weak peak at C <sub>2</sub> H <sub>4</sub> abs. max; comp. of C <sub>2</sub> H <sub>x</sub> , x=2,4,6; disputing existence of shape resonances
	KK&98c	284-350	P	absorption; PES; C1s <sup>-1</sup> & satellite partials; disputes shape resonance
	TPA98	280-320	T	absolute; DFT vs. STEX, comparison of C <sub>2</sub> H <sub>2x</sub> , x=1,2,3
	GG&99	284-292	P,T	core hole localization in C <sub>2</sub> H <sub>2x</sub> ; symmetry broken X-ray emission; HF calc; localization increases with increasing bond length
	KK&99	290-360	P	absolute; main line partial cross-sections; disputes shape resonance in C <sub>2</sub> H <sub>6</sub>
	SW&98	280-320	P	TIY; vibr'nlly resolved PES; SR perturbs at 304; disputes KK&97a
	NG99	284-286	T	ab initio-CI; vibrations; non-TS modes; localized core hole; symmetry breaking needed to fit experiment
	SF&99	283-292	P, T	reonant Auger at $\pi^*$ and Rydbergs; CI calc; vibronic core hole localization
	FS&00	2858	T	resonant Auger; vibronic core hole localization
	HC&00	280-340	T	shape resonances from MS (Feff8) in C <sub>2</sub> H <sub>2x</sub> ; ang. dep; IPs good to 0.5 eV
	RB00	285-289	T	absolute; GMS-ab initio; GOS for $\pi^*$ , Ryd
	HJ&02	278-322	E,T	absolute GOS; calculated strong quadrupole $\pi^*$ not observed
	K02	284-298	P,TR	symmetry resolved, high resolution; review
	PS&02	284-320	P	PIY, fragmentation mechanisms; Ryders versus shape resonances
	ZTC03	280-320	T	MS-cluster calc, C-H resonances in near continuum, $\delta(R)$ for $\sigma^*_{C-C}$ in C <sub>2</sub> H <sub>x</sub>
	IH07	284-302	T	relative, Gaussian augmented plane wave (GAPW) - DFT; (-5 to +3 eV errors on 14 small molecules
	PN&15	595,652	P	1-site, 2-site double core hole IP (ts-DCH), SR, not FEL, coincidences
	TP&24	275-295	T	Auger & XAS, compare to C <sub>2</sub> H <sub>4</sub> <sup>+</sup>
C <sub>2</sub> H <sub>4</sub> <sup>+</sup>	TP&24	275-295	T	Auger & XAS, compare to C <sub>2</sub> H <sub>4</sub>
(C <sub>2</sub> H <sub>4</sub> ) <sub>n</sub>	RS&92b	280-320	P	clustered ethylene; comp. of partial, total yield channels
	HR96	282-296	P,R	clustered ethylene; comp. of partial, total yield channels
C <sub>2</sub> H <sub>4</sub> O	HB80b	280-320	E	(CH <sub>3</sub> CHO - acetaldehyde) cont. res.
	SSH84a	295	T	$\sigma^*$ -res./bond length relationship
	YA&96	280-320	T	STEX; comp. to expt. and other theory; R <sub>2</sub> CO species
	YA&97	287	T	$\pi^*$ OS; test of initial and final state sum rules; comp to expt.
	TJ&99	284-300	P	relative; TIY; participator decay; 2 states in $\pi^*$
C <sub>2</sub> H <sub>4</sub> O	SB91a	280-410	P	ethylene oxide; high res.; Ryd. vib'n'l resolved; comp to C <sub>3</sub> H <sub>6</sub>
C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	ES84	270-310	P	(CH <sub>3</sub> COOH, acetic acid), partial & total ion yields, mass spectra
	RI&88	270-330	E	C-F $\sigma^*$ res., absolute, perfluoro effect
	S92	280-325	E,R	comp. of HCO <sub>2</sub> H, HCO <sub>2</sub> CH <sub>3</sub> and PMMA NEXAFS
	PB&07	283-312	P	relative, TIY, PEPEPICO; PE3PICO; mechanistic discussion
	DF&08	280-320	E,T	valence-Rydberg mixed states; vibrational structure; ab initio, Z+1
C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	IH88	275-325	E	HCOOCH <sub>3</sub> , methyl formate, absolute, spectral aditivity tested
	JT94b	275-316	E,T	ISEELS as f(resolution); DES by (e,2e); strong participator
C <sub>2</sub> H <sub>5</sub> NO <sub>2</sub>	PC&98	285-315	T	glycine; STEX; comp. of NEXAFS and circ. Dichroism of amino acids
	GC&03	283-310	E,T	absolute, comp Gly, Gly-Gly; tri-gly; peptide bonds; GSCF3
	CG&04	284-306	E	absolute, comp Gly, Gly-gly, gas-solid, peptide bond exp. spectrum

$\text{C}_2\text{H}_5\text{NO}_2$ (cont'd)	IK&14	330	P	fragmentation of ionized glycine
	MG&16	284-310	P,T	comp Gly, Gly-gly
$\text{C}_2\text{H}_5\text{N}_3\text{O}_2$	UA&99	280-340	E	biuret; $(\text{NH}_2(\text{CO})\text{NH}(\text{CO})\text{NH}_2)_2$ ; absolute; polymer model
	LC&07	280-320	E,T	comp.of di-carbonyls; charge shifts for fingerprinting, GSCF3
$\text{C}_2\text{H}_6$	EH&76	280-300	P	photoelectric yield
	HB77	280-340	E	comp. to $\text{CH}_4$ & EH&76 $\text{C}_2\text{H}_6$ data
	HB&84	280-320	E	comp. to $\text{CH}_4$ (WB74b), (HB77) data, $\sigma^*(\text{C-C})$ res. at thr.
	SSH84a	295	T	$\sigma^*$ -res./bond length relationship
	HI87	275-325	E	$\pi^*(\text{CH}_3)$ , comp. to other alkanes
	HR87	280-300	E	use of core excitation (HB77) to interpret Auger satellites (DES)
	IM&88	275-325	E	absolute OS, comp. to $\text{C}_2\text{F}_6$
	AR&89	280-320	P,E,T	curve fit of HB77; comp. to NEXAFS; theor. asymmetric $\sigma^*$ lineshape
	SG&89	290-330	T	$\sigma^*$ shape res.; pos. & shape as f(R); approx. cyl. well & ab initio
	H90a	284-316	E,R	absolute; comp. of $\text{C}_2\text{H}_6$ , $\text{CH}_3\text{CF}_3$ , $\text{C}_2\text{F}_6$ ; partial pot. barr.
	FSL91	290-390	T	absolute; $\text{L}^2$ , delocal. hole; $\text{C}_2\text{H}_x$ ( $x=2,4,6$ ); $\sigma^*(\text{C-H})/\sigma^*(\text{C-C})$ reversal
	LAL91	285-305	T	CNDO, systematic calc. of $\sigma^*$ energies; ISEELS, ETS for param. det.
	MC&91	284-291	P	50 meV fwhm; $\pi^*$ & Ryd vibns; comp of $\text{C}_2\text{H}_x$ & $\text{C}_2\text{D}_x$ (isotope eff)
	S92	280-320	T,R	MS-X $\alpha$ ; comp. of propane, ethane
	RDK93	286-291	P	high res (60 meV); comp. of $\text{CH}_4/\text{CD}_4$ ; $\text{C}_2\text{H}_6/\text{C}_2\text{D}_6$ ; $\text{C}_3\text{H}_8/\text{C}_3\text{D}_8$
	KK&97a	280-350	P	main line cross-sections; comp. to absorption; no peak at claimed position of $\sigma^*$ in abs. (but main line cross-section does not reach); comp. of $\text{C}_2\text{H}_x$ , $x=2,4,6$ ; disputing existence of shape resonances
	TPA98	280-320	T	absolute; DFT vs. STEX, comparison of $\text{C}_2\text{H}_{2x}$ , $x=1,2,3$
	GG&99	284-292	P,T	core hole localization in $\text{C}_2\text{H}_{2x}$ ; symmetry broken X-ray emission; HF calc; localization increases with increasing bond length
	KK&99	290-360	P	absolute; main line partial cross-sections; disputes shape resonance in $\text{C}_2\text{H}_6$
	RK&99	250-560	P	absolute; true absorption; vibn'l resolved PES; $\text{C}1\text{s}^{-1}$ , Sat., X-sect
	HC&00	280-340	T	shape resonances from MS (Feff8) in $\text{C}_2\text{H}_{2x}$ ; ang. dep; IPs good to 0.5 eV
	ZTC03	280-320	T	MS-cluster calc, C-H resonances in near continuum, $\delta(\text{R})$ for $\sigma^*_{\text{C-C}}$ in $\text{C}_2\text{H}_x$
	UG05	286-292	P,T	high-res, 40 meV; comparison of small alkanes; Ryd-val mix; GSCF3
	PN&15	592,652	P	1-site, 2-site double core hole IP (ts-DCH), SR, not FEL, coincidences
	TKU15	590	T	$(\text{XH}_m\text{-YH}_n)$ X,Y = C,N,O,F; m,n = 0-3 – 2-site double core hole IPs
$\text{C}_2\text{H}_5\text{NO}_2$	CG&04	282-304	E	(glycine), comp. of Gly, Gly-gly, Gly <sub>3</sub> , gas-solid
$\text{C}_2\text{H}_6\text{O}$	WB74b	285-325	E	$(\text{CH}_3\text{OCH}_3$ - dimethyl ether)
	SSH84a	295	T	$\sigma^*$ -res./bond length relationship
	SY&89	280-320	P	comp to EELS, lower discrete/cont.; cont. flatter, O1s 2nd order
	LAL91	285-305	T	CNDO, systematic calc. of $\sigma^*$ energies; ISEELS, ETS for param. det.
$\text{C}_2\text{H}_6\text{O}$	SY&89	280-320	P	$(\text{C}_2\text{H}_5\text{OH})$ , lower discrete/cont. ratio, cont. flatter, O1s 2nd order
$\text{C}_2\text{H}_6\text{O}_2$	EUH98	280-320	E	ethylene glycol; $(\text{CH}_2\text{OH}-\text{CH}_2\text{OH})$ ; absolute; comp to PEO
$\text{C}_2\text{H}_6\text{O}_3$	HW&91	280-340	E	$(\text{CH}_3\text{O})_2\text{C=O}$ ; absolute; comp. to phenyl carbonate
$\text{C}_2\text{H}_6\text{OS}$	TB&88	280-320	E	$(\text{CH}_3)_2\text{S=O}$ , DMSO, comp. to S1s
$\text{C}_2\text{H}_6\text{O}_3\text{S}$	HH14	280-320	E	$(\text{CH}_3)\text{SO}_3\text{CH}_3$ , absolute, comp. to PFSA (Nafion) spectra
$\text{C}_2\text{H}_7\text{N}$	SB85b	285-335	E	$\sigma^*$ res. at thr., comp. to $(\text{CH}_3)_x\text{NH}_{3-x}$ , $x=0-3$
$\text{C}_2\text{H}_8\text{O}_2$	IH07	284-302	T	methanol dimer; relative, Gaussian augmented plane wave (GAPW) - DFT; (-5 to +3 eV errors on 14 small molecules
$\text{C}_2\text{N}_2$	HB79b	280-320	E	cont. res.
	SSH84a	295	T	$\sigma^*$ -res./bond length relationship
	SG&89	290-330	T	$\sigma^*$ shape res.; pos. & shape as f(R); approx. cyl. well & ab initio
$\text{C}_3\text{D}_8$	RDK93	286-291	P	high res (60 meV); comp. of $\text{CH}_4/\text{CD}_4$ ; $\text{C}_2\text{H}_6/\text{C}_2\text{D}_6$ ; $\text{C}_3\text{H}_8/\text{C}_3\text{D}_8$
$\text{C}_3\text{F}_3\text{H}$	HS90	280-340	E	$\text{CF}_3\text{C}\text{:CH}$ , absolute; comp. to other triply bonded species
$\text{C}_3\text{F}_3\text{H}_3\text{O}$	HC&87b	280-310	P	$\text{CF}_3\text{COCH}_3$ , thr. e-, TOF-MS, claims selective fragmentation
$\text{C}_3\text{F}_6\text{O}$	RI&88	280-325	E	(perfluoroacetone), C-F $\sigma^*$ res., absolute, perfluoro effect

<b>C<sub>3</sub>F<sub>6</sub></b>	IM&88	275-325	E	perfluoro-cyclopropane, C <sub>x</sub> F <sub>2n</sub> series, σ*(C-F) dominated
<b>C<sub>3</sub>F<sub>8</sub></b>	HFM87	280-320	E	comp. to other fluorocarbons; σ*(C-F) 'giant shape res.'
	IM&88	275-325	E	perfluoropropane, C <sub>x</sub> F <sub>2n+2</sub> series, σ*(C-F) dominated
<b>C<sub>3</sub>H<sub>2</sub>O<sub>2</sub></b>	IH88	275-325	E	(propionic acid), comp. to solid, absolute
<b>C<sub>3</sub>H<sub>3</sub>N<sub>2</sub>O<sub>2</sub></b>	IH&11	330	P	(uracil), site-selective fragmentation after C 1s ionization, PEPICO
<b>C<sub>3</sub>H<sub>2</sub>N<sub>2</sub>OBr</b>	IH&10	330	P	(Br-uracil), site-selective fragmentation after C 1s ionization, PEPICO
	IH&11	330	P	(Br-uracil), site-selective fragmentation after C 1s ionization, PEPICO
<b>C<sub>3</sub>H<sub>3</sub></b>	SC95	288	T	c-C <sub>3</sub> H <sub>3</sub> <sup>+</sup> ; ADC local/delocal calc; Jahn-Teller localis.; comp. to B <sub>3</sub> H <sub>3</sub> N <sub>6</sub>
<b>C<sub>3</sub>H<sub>3</sub>N</b>	MB&94b	280-320	P,T	C <sub>2</sub> H <sub>3</sub> CN - acrylonitrile; <100 mV fwhm; ab initio; vibrational structure; comp. of C <sub>2</sub> H <sub>4</sub> , C <sub>3</sub> H <sub>3</sub> N, C <sub>4</sub> H <sub>6</sub> , C <sub>4</sub> H <sub>8</sub>
	HA&97	282-307	E,T	relative; 0.25 eV fwhm; Z+1 calc'n; π* interactions; comp. of CH <sub>2</sub> =CHCN, C <sub>2</sub> H <sub>2</sub> (CN) <sub>2</sub> , CH <sub>2</sub> =CHCH <sub>2</sub> CN
	DS&05	282-318	E,T	assignments revised;
<b>C<sub>3</sub>H<sub>3</sub>N<sub>3</sub></b>	AGH93	280-320	E	s-triazine; absolute; comp. to solid
	PS&01	280-315	T	STEX, extensive series of C-N compounds
	VG&08	284-330	P,T	relative, transmission, double ion cell, DEMON calc, comp of 5 aza-rings
<b>C<sub>3</sub>H<sub>3</sub>N<sub>3</sub>O<sub>2</sub></b>	BC&19	290-295	P,T	2-nitroimidazole, NEXAFS, XPS, PIY; HF, DFT, MCSCF, TDDFT calc
<b>C<sub>3</sub>H<sub>4</sub></b>	SB85a	280-320	E	CH <sub>2</sub> =C=CH <sub>2</sub> (allene), 0.11eV FWHM, unusual cont. structure
	LAL91	285-305	T	CNDO, systematic calc. of σ* energies; ISEELS, ETS for param. det.
	S92	275-325	T,R	MS-Xα; comp. to allene on Ag(110)
<b>C<sub>3</sub>H<sub>4</sub></b>	HI88a	275-325	E	CH <sub>3</sub> C::CH, propyne, absolute, reference for perfluoro effect
	HS90	280-340	E	absolute; comp. to other triply bonded species
	S92	280-320	E,T,R	MS-Xα; comp to 2,4-hexadiyne
<b>C<sub>3</sub>H<sub>4</sub>N<sub>2</sub></b>	AGH93	280-320	E,P	imidazole; absolute; gas-EELS; comp. to sol.-NEXAFS
	CPA01	280-310	T	STEX with screening; comp. to expt. (AGH93)
<b>C<sub>3</sub>H<sub>4</sub>N<sub>2</sub></b>	DH&98	280-330	E,T	pyrazole, relative, 0.2 eV fwhm, Z+1 HONDO, pyrrole vs. pyrazole
<b>C<sub>3</sub>H<sub>4</sub>O</b>	IH88	275-325	E	(propionic alcohol), comp. to solid, absolute, group analysis
<b>C<sub>3</sub>H<sub>4</sub>O</b>	SB92	280-320	E	ethylene oxide; high. res.; comp. to cyclopropane
<b>C<sub>3</sub>H<sub>4</sub>O</b>	DF&03	280-320	E	CH <sub>2</sub> =CH-CHO, acrolein; π* delocalisation; ab initio GAMES
<b>C<sub>3</sub>H<sub>4</sub>O<sub>2</sub></b>	IH88	275-325	E	(acrylic acid), comp. to solid, absolute, group analysis
<b>C<sub>3</sub>ClH<sub>5</sub>O</b>	LDN07	283-298	P	epichlorohydrin – CH <sub>3</sub> (CH-O-CH <sub>2</sub> ); PIY, PEPICO, site selective
<b>C<sub>3</sub>H<sub>6</sub></b>	H86b	280-320	E,R	(cyclopropane), comp. to propane
	HN&86	275-325	E	comp. to other cyclics
	LAL91	285-305	T	CNDO, systematic calc. of σ* energies; ISEELS, ETS for param. det.
	SB91a	280-410	P	high res.; Ryd. vib'nl resolved; comp to C <sub>2</sub> H <sub>4</sub> O
	S92	280-320	E,T,R	MS-Xα; comp. of cyclic-C <sub>n</sub> alkanes
	SB92	280-320	E	ethylene oxide; high. res.; comp. to cyclopropane
	FL96	282-294	T	absolute; ASCF-CI; comp. to XPS shake-up and expt. [S92]; n-C <sub>n</sub> H <sub>2n</sub> , n=3,4,5,6 compared
<b>C<sub>3</sub>H<sub>6</sub></b>	HS90	280-340	E	propene; absolute; comp. to calc. (S92)
	S92	280-320	T,R	MS-Xα; site-selected calc.
	PN&15	645	P	2-site double core hole IP (ts-DCH), SR, not FEL, coincidences
<b>C<sub>3</sub>H<sub>6</sub>NO<sub>2</sub>S</b>	PC&98	285-315	T	cysteine; (D,L) STEX; comp. of NEXAFS, circ. Dichr. of amino acids
<b>C<sub>3</sub>H<sub>6</sub>N<sub>2</sub>O<sub>2</sub></b>	LC&07	280-320	E,T	malonamide; comp.of di-carbonyls; charge shifts for fingerprinting, GSCF3
<b>C<sub>3</sub>H<sub>6</sub>O</b>	IH88	275-325	E	(acrylic alcohol), comp. to solid, absolute, group analysis
<b>C<sub>3</sub>H<sub>6</sub>O</b>	WB74c	282-328	E	((CH <sub>3</sub> ) <sub>2</sub> CO - acetone)
	HB80b	280-320	E	cont. res.
	ES&83a	275-312	P	photoionization mass spectrometry, site-selective fragmentation
	ES84	275-312	P	partial & total IY; mass spectra, site-selective fragmentation
	ES&84	275-315	P	photoionization mass spectrometry, site-selective fragmentation
	SSH84a	295	T	σ*-res./bond length relationship
	RI&88	270-330	E	absolute, comp. to (CF <sub>3</sub> ) <sub>2</sub> C=O re perfluro effect

C <sub>3</sub> H <sub>6</sub> O (cont'd)	SY&89	280-320	P	comp to EELS, lower discrete/cont.; cont. flatter, O1s 2nd order
	TPA98	280-320	T	absolute; DFT vs. STEX, compares CO and R <sub>2</sub> CO, R = H, Me
	TJ&99a	284-297	P,T	absolute; resonant Auger; STEX calc.
	TJ&99b	284-300	P	relative, TIY
	SS00	280-320	P	TIY, PIY; weak site or state selective fragmentation
C <sub>3</sub> H <sub>6</sub> O	YA&96	280-320	T	propaldehyde; absolute; STEX; R <sub>2</sub> CO comparison
	YA&97	287	T	$\pi^*$ OS; test of initial and final state sum rules; comp to expt.
	TJ&99b	284-300	P	relative, TIY
C <sub>3</sub> H <sub>6</sub> O	PL&07	285-295	P, T	methyloxirane CH <sub>3</sub> -[CHOCH <sub>2</sub> ]; TIY; XPS, calc; resonant Auger
C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	IH88	275-325	E	(propionic acid), comp. to solid, absolute, group analysis
C <sub>3</sub> H <sub>6</sub> O <sub>3</sub>	HW&91	275-325	E	(CH <sub>3</sub> O) <sub>2</sub> C=O, methyl carbonate; absolute, comp. to PEELS
C <sub>3</sub> H <sub>6</sub> O <sub>3</sub>	LC&07	280-320	E,T	(dimethoxymethanone)comp.of di-carbonyls; charge shifts for fingerprinting, GSCF3
C <sub>3</sub> H <sub>6</sub> O <sub>3</sub>	H01	280-320	E	lactic acid; Me(CHOH(COOH); absolute
C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub>	GH01	280-320	E	alanine; absolute; comp of amino acids
	CG&04	282-304	E	comp. of alanine, benzene, phenylalanine - additivity
	GT&11	270-330	P, T	gas, crystal, adsorbate comparison; conformers
	GW09	288-296	T	DFT (B3LYP/TZVP) comp to, C <sub>6</sub> H <sub>6</sub> , C <sub>8</sub> H <sub>10</sub> O <sub>2</sub> , C <sub>8</sub> H <sub>11</sub> N, C <sub>9</sub> H <sub>11</sub> NO <sub>2</sub>
C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub>	UH&95a	280-320	E,T	NH <sub>2</sub> CO <sub>2</sub> Et, urethane; absolute; comp. to model polyurethane polymers
	UH&95b	280-320	E,T	NH <sub>2</sub> CO <sub>2</sub> Et, urethane; absolute; EHMO; dist. urethane & ureas
C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub>	PC&98	285-315	T	alanine; (D-,L-) STEX; comp. of NEXAFS, circ. Dichroism of amino acids
	PV&04	280-310	P	TIY, PIY, CD asymmetry <1e-3; <1e-2 for fixed-in-space
C <sub>3</sub> H <sub>7</sub> NO <sub>3</sub>	PC&98	285-315	T	serine; (D-,L-) STEX; comp. of NEXAFS, circ. Dichro. of amino acids
	PV&04	280-310	P	TIY, PIY, CD asymmetry <1e-3; <1e-2 for fixed-in-space
C <sub>3</sub> H <sub>8</sub>	SS85	260-360	P	(propane), 5% modulated W (energy/ion pair); roughly matches abs; PCI
	H86b	280-320	E,R	, comp. of n-alkanes
	HI87	275-325	E	comp. of saturated alkanes
	SO&87	285-310	T	X $\alpha$ -SW, molecular orientation
	LAL91	285-305	T	CNDO, systematic calc. of $\sigma^*$ energies; ISEELS, ETS for param. det.
	S92	280-320	T,R	MS-X $\alpha$ ; comp. of propane, ethane
	RDK93	286-291	P	high res (60 meV); comp. of CH <sub>4</sub> /CD <sub>4</sub> ; C <sub>2</sub> H <sub>6</sub> /C <sub>2</sub> D <sub>6</sub> ; C <sub>3</sub> H <sub>8</sub> /C <sub>3</sub> D <sub>8</sub>
	VF&98	285-320	T	comp. to HI87, X $\alpha$ -SW; long-chain alkanes; $\sigma^*$ along C-C bonds
	WBW99	280-320	T	ab initio $\Delta$ SCF; comp to solid & clusters; conformational dep; Ryd persist in condensed phase
	UG05	286-292	P,T	high-res, 40 meV; comparison of small alkanes; Ryd-val mix; GSCF3
C <sub>3</sub> H <sub>8</sub> O	IH88	275-325	E	(n-propanol), absolute, group analysis
	TH&98	285-295	P	threshold e-; TIY; TPEPICO; triple coinc; isomer study
C <sub>3</sub> H <sub>8</sub> O	TH&98	285-295	P	(isoproponol); threshold e-; TIY; TPEPICO; triple coinc; isomer study
C <sub>3</sub> H <sub>8</sub> O <sub>2</sub>	LB764	30-620	P	(CH <sub>2</sub> (OCH <sub>3</sub> ) <sub>2</sub> - methylal), absolute
C <sub>3</sub> H <sub>8</sub> O <sub>2</sub>	EUH98	280-320	E	1,2-propane diol; absolute; comp to PPO
C <sub>3</sub> H <sub>9</sub> P	SB85c	280-330	E	(Me) <sub>3</sub> P
	HH&98	284-304	E	absolute; comp. to (t-Bu) <sub>2</sub> PCl
C <sub>3</sub> H <sub>9</sub> N	SB85b	285-335	E	(Me) <sub>3</sub> N, $\sigma^*$ res. at thr., comp. to (CH <sub>3</sub> ) <sub>x</sub> NH <sub>3-x</sub> , x=0-3
C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub>	UH&95b	280-330	E	NH <sub>2</sub> -CO <sub>2</sub> Et, absolute; modelling of polyurethane PEELS
C <sub>4</sub> ClH <sub>3</sub> N	BO&10	283-300	P,T	2-Cl-pyrimidine; hi-res; comp of halogenated pyrimidines
C <sub>4</sub> ClH <sub>3</sub> N	BO&10	283-300	P,T	5-Cl-pyrimidine; hi-res; comp of halogenated pyrimidines
C <sub>4</sub> F <sub>3</sub> H <sub>9</sub> O <sub>3</sub> SSi	UH94a	280-330	E	Me <sub>3</sub> SiOSO <sub>2</sub> CF <sub>3</sub> ; comp of Si-O-X species; inductive, resonance effects
C <sub>4</sub> F <sub>3</sub> H <sub>5</sub> O <sub>2</sub>	PN&15	597,654	P,T	ethyl trifluoroacetate, 1-site, 2-site double core hole IP (ts-DCH), SR, not FEL, coincidences (2 PE, 2 AE); IPs of all 4 sites; compare to XPS
C <sub>4</sub> F <sub>6</sub>	MC&87	275-325	E	perfluorobutadiene, absolute
	RI&88	275-325	E	absolute, comp. to C <sub>4</sub> H <sub>6</sub> re perfluoro effect
C <sub>4</sub> F <sub>6</sub>	RI&88	275-325	E	perfluorobutyne, CF <sub>3</sub> C:::CCF <sub>3</sub> , comp. to C <sub>4</sub> H <sub>6</sub> , perfluoro effect

<b>C<sub>4</sub>F<sub>6</sub>H<sub>2</sub></b>	IO&12	297	P	cis-cyclic-C <sub>4</sub> F <sub>6</sub> H <sub>2</sub> , resonant Auger - ion coincidence, site specific frag.
<b>C<sub>4</sub>F<sub>8</sub></b>	HB&84	280-325	E	(CF <sub>3</sub> CFCFCF <sub>3</sub> ) - strong $\sigma^*$ (C-F) res.
	SSH84b	290-300	T	test of bond length determination from $\sigma^*$ res.
	RI&88	280-340	E	reassigned HB&84
	LAL91	285-305	T	CNDO, systematic calc. of $\sigma^*$ energies; ISEELS, ETS for param. det.
<b>C<sub>4</sub>F<sub>8</sub></b>	IM&88	275-325	E	perfluoro-cyclobutane, C <sub>x</sub> F <sub>2x</sub> series, $\sigma^*$ (C-F) dominated
<b>C<sub>4</sub>F<sub>10</sub></b>	HFM87	280-320	E	comp. to other fluorocarbons; $\sigma^*$ (C-F)'giant shape res.'
	IM&88	275-325	E	perfluorobutane, absolute, comp to C <sub>x</sub> F <sub>x+2</sub>
	AC&95	290-315	T	STEX ab initio; absolute; growth of poly-(CF <sub>2</sub> ) <sub>n</sub> by C <sub>2n</sub> F <sub>4n+2</sub> , n=1-5
<b>C<sub>4</sub>GeH<sub>12</sub></b>	BS&02B	50-450	P, T	GeMe <sub>4</sub> ; PEPIPICO, PIPICO, partial ion yields; EICVOM calc
<b>C<sub>4</sub>H<sub>2</sub>N<sub>2</sub></b>	HA&97	282-307	E,T	trans-dicyanoethylene; relative; 0.25 eV fwhm; Z+1 calc'n; $\pi^*$ interactions; comp. of CH <sub>2</sub> =CHCN, C <sub>2</sub> H <sub>2</sub> (CN) <sub>2</sub> , CH <sub>2</sub> =CHCH <sub>2</sub> CN
<b>C<sub>4</sub>H<sub>4</sub>N<sub>2</sub></b>	HD&99	280-315	E,T	(pyrazine); 0.2 eV fwhm; Z+1 calc; comp to pyridine; s-triazine
	PS&01	280-315	T	STEX, extensive series of C-N compounds
	VG&08	284-330	P,T	relative, transmission, double ion cell, DEMON calc, comp of 5 aza-rings (pyrimidine), STEX, extensive series of C-N compounds
<b>C<sub>4</sub>H<sub>4</sub>N<sub>2</sub></b>	PS&01	280-315	T	, TIY vs. vis-UV fluorescencence yield; state selective decay
	VC&06	280-320	P	2 hi-res; comp with 5- and 5- halogenated pyrimidines
	BO&10	283-300	P,T	relative, transmission, double ion cell, DEMON calc, comp of 5 aza-rings
	VG&08	284-330	P,T	(pyridazine), STEX, extensive series of C-N compounds
<b>C<sub>4</sub>H<sub>4</sub>N<sub>2</sub></b>	PS&01	280-315	T	relative, transmission, double ion cell, DEMON calc,
	VG&08	284-330	P,T	comp of 5 aza-rings
<b>C<sub>4</sub>H<sub>5</sub>N<sub>3</sub>O</b>	FP&10	283-298	P,T	(uracil), tautomerism
<b>C<sub>4</sub>H<sub>6</sub>N<sub>2</sub>O<sub>2</sub></b>	IH&10	330	P	(thymine), site-selective fragmentation after C 1s ionization, PEPIPICO
	IH&11	330	P	site-selective fragmentation after C 1s ionization, PEPIPICO
<b>C<sub>4</sub>H<sub>4</sub>FN<sub>3</sub>O</b>	FP&11	284-296	P	(5-methylcytosine), tautomerism in cytosines
<b>C<sub>4</sub>H<sub>4</sub>N<sub>2</sub>O<sub>2</sub></b>	FP&10	283-297	P,T	(cytosine), tautomerism
<b>C<sub>4</sub>H<sub>4</sub>O</b>	NIH86	275-325	E	(furan), absolute; compared to tetrahydro-furan, other heterocycles
	SMS91	280-320	E,P	comp of gas, monolayer on Ag(110); curve fits
	RH&02	285-292	P	partial electron yield; comp. to EELS (NIH86); Auger, XPS
<b>C<sub>4</sub>H<sub>4</sub>S</b>	H86b	275-325	E,R	(thiophene), comp. to thiolane, other heterocyclics
	HNS86	275-325	E,P	comp. to thiolane, solid, monolayer; MS-X $\alpha$ calc
	HT&90	275-325	E	absolute, 3-alkyl-thiophenes; no mod. of $\pi^*$ (cf. polymer cond.)
	HE91	(white)	P	(hv; $e_{Auger,ion}$ ) coinc.; mass spectra at C1s, S2p with Auger
	TG&18	284-291	P,T	TIY, DFT calc., compare C <sub>4</sub> H <sub>4</sub> S, C <sub>8</sub> H <sub>6</sub> S, C <sub>8</sub> H <sub>6</sub> S (S-hetero-rings)
<b>C<sub>4</sub>H<sub>4</sub>Se</b>	HTB89	275-325	E	(selenophene), comp to solid
<b>C<sub>4</sub>H<sub>5</sub>N</b>	HA&97	282-307	E,T	allyl-cyanide; relative; 0.25 eV fwhm; Z+1 calc'n; $\pi^*$ interactions; comp. of CH <sub>2</sub> =CHCN, C <sub>2</sub> H <sub>2</sub> (CN) <sub>2</sub> , CH <sub>2</sub> =CHCH <sub>2</sub> CN
<b>C<sub>4</sub>H<sub>5</sub>N</b>	PS&01	280-315	T	STEX, extensive series of C-N compounds
	NIH86	275-325	E	(pyrrole), absolute
	DH&98	280-330	E,T	relative, 0.2 eV fwhm, Z+1 HONDO, pyrrole vs. pyrazole
	PS&01	280-315	T	STEX, extensive series of C-N compounds
	SU&09	284-300	P,T	TEY, relative, compared to ISEELS (DH&98), liquid, DFT, 287.1 eV feature may be from gas phase dimer
<b>C<sub>4</sub>H<sub>5</sub>N</b>	PS&01	280-315	T	(1,3-pyrrole), STEX, extensive series of C-N compounds
<b>C<sub>4</sub>H<sub>5</sub>N</b>	PS&01	280-315	T	(2,4-pyrrole), STEX, extensive series of C-N compounds
<b>C<sub>4</sub>H<sub>5</sub>N<sub>3</sub>O</b>	FP&11	284-296	P	(5-fluorocytosine), tautomerism in cytosines
<b>C<sub>4</sub>H<sub>6</sub></b>	HB&84	280-325	E	(cis, trans-1,3-butadiene CH <sub>2</sub> CHCHCH <sub>2</sub> )
	SB85a	280-320	E	0.07eVFWHM, two $\pi^*$ levels observed
	L86	284-290	T	HAM/3 electron affinities, reassigned $\pi^*$ levels, comp. to HB&84
	MC&87	284-296	E	comp. to C <sub>4</sub> F <sub>6</sub> , reassigned 1s6 $\pi^*$ s
	RI&88	275-325	E	absolute, comp. to C <sub>4</sub> H <sub>6</sub> re perfluoro effect

(C <sub>4</sub> H <sub>6</sub> cont'd)	NS&92	280-330	P,T	ab initio, $\pi^*$ vib'n'l struct.; comp. to sol NEXAFS, re-assigns HB&84
	S92	280-320	E,R	comp. to polymer NEXAFS
	LA93	282-292	T	1-particle Green's function; comp. of C <sub>2</sub> H <sub>4</sub> , C <sub>4</sub> H <sub>6</sub> ,C <sub>6</sub> H <sub>8</sub> ; comp. to NS&92 (solid); claims relaxation shifts dominate; $\pi^*$ split small.
	MB&94b	280-320	P,T	<100 mV fwhm; ab initio; vibrn=l str.; comp. of C <sub>2</sub> H <sub>4</sub> , C <sub>3</sub> H <sub>3</sub> N,C <sub>4</sub> H <sub>6</sub> ,C <sub>4</sub> H <sub>8</sub>
	GA95	284-290	T	delocalization in polyenes; comp. of H-(CH=CH) <sub>n</sub> -H, n=1-5
	CA&95	280-320	T	polyenes, STEX, $\pi/\sigma$ convergence
	GYA96	285	T	X-ray emission as f(conjugation); $\pi$ -exciton effects; H(C <sub>2</sub> H <sub>2</sub> ) <sub>n</sub> H, n=1,10
	YA96	290-315	T	STEX; shake-up spectra related to NEXAFS; H(C <sub>2</sub> H <sub>2</sub> ) <sub>n</sub> H, n=1-5
	SO&96	284-286	P,T	decay of $\pi^*$ states; site selective; INDO calc.
	AJ&97a	283-292	P	relative; 0.6 eVsplit of $\pi^*(CH_2=, =CH-)$ ; vibrational resolved
	CPA01	280-320	T	STEX with screening; comp. to expt. (NS&92)
	BRB05	288-292	T	GOS; oscillations from Young-type interference
C <sub>4</sub> H <sub>6</sub>	RI&88	275-325	E	CH <sub>3</sub> C:::CCH <sub>3</sub> , 2-butyne, absolute, ref. per-F-2-butyne re per-F eff.
	S92	280-320	E,R	comp. to polymer NEXAFS
C <sub>4</sub> H <sub>6</sub> O <sub>3</sub>	LC&07	280-320	E,T	acetic anhydride; di-carbonyls; charge shifts for fingerprinting, GSCF3
C <sub>4</sub> H <sub>6</sub> O <sub>5</sub>	LCH03	280-320	E,T	MeO(CO)O(CO)OMe; di-carbonyls; charge shifts, GSCF3
	LC&07	280-320	E,T	MeO(CO)O(CO)OMe; di-carbonyls; charge shifts, GSCF3
C <sub>4</sub> H <sub>7</sub> N	PS&01	280-315	T	(2-pyrroline), STEX, extensive series of C-N compounds
C <sub>4</sub> H <sub>7</sub> N	PS&01	280-315	T	(3-pyrroline), STEX, extensive series of C-N compounds
C <sub>4</sub> H <sub>7</sub> NO <sub>2</sub>	LC&07	280-320	E,T	Me(CO)N(CO)Me; di-acetamide; di-carbonyls; charge shifts, GSCF3
C <sub>4</sub> H <sub>7</sub> NO <sub>4</sub>	UA&99	280-320	E	ethyl allophanate (NH <sub>2</sub> (CO)O(CO)OEt); absolute; polymer model
	UH&99	280-320	E,T	ethyl allophanate; absolute; GSCF3; comp. of urethane species
C <sub>4</sub> H <sub>8</sub>	HB&84	280-325	E	(1-butene CH <sub>2</sub> CHCH <sub>2</sub> CH <sub>3</sub> )
	MB&94b	280-320	P,T	<100 mV fwhm; ab initio; vib. structure; comp. of C <sub>2</sub> H <sub>4</sub> , C <sub>3</sub> H <sub>3</sub> N,C <sub>4</sub> H <sub>6</sub> ,C <sub>4</sub> H <sub>8</sub>
	FL96	282-294	T	absolute; $\Delta$ SCF-CI; comp. to XPS shake-up and expt. [S92]; n-C <sub>n</sub> H <sub>2n</sub> , n=3,4,5,6 compared
C <sub>4</sub> H <sub>8</sub>	HB&84	280-325	E	(cis-2-butene CH <sub>3</sub> CHCHCH <sub>3</sub> )
C <sub>4</sub> H <sub>8</sub>	HB&84	280-325	E	(trans-2-butene CH <sub>3</sub> CHCHCH <sub>3</sub> )
C <sub>4</sub> H <sub>8</sub>	HN&86	275-325	EPT	(cyclobutane), comp. to other cyclics, sol., calc., E( $\sigma^*$ ) $\alpha$ R
	H86	280-320	E,R	comp. to n-butane
	S92	280-320	E,R	comp. to polymer NEXAFS
C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> O <sub>3</sub>	GC&03	283-310	E,T	(glycyl-glycine),absolute, Gly, Gly-Gly; tri-gly(s); peptide bonds; GSCF3
	CG&04	282-304	E	comp. of Gly, Gly-gly, Gly <sub>3</sub> , gas-solid
	MG&16	284-310	P,T	comp Gly, Gly-gly
C <sub>4</sub> H <sub>8</sub> O	NIH86	275-325	E	(tetrahydrofuran)
	SY&89	280-320	P	comp to EELS, lower discrete/cont.;cont. flatter, O1s 2nd order
C <sub>4</sub> H <sub>8</sub> O	YA&96	280-320	T	iso-butanaldehyde; absolute; STEX; R <sub>2</sub> CO comparison
	YA&97	287	T	$\pi^*$ OS; test of initial and final state sum rules; comp to expt.
C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	SY&89	280-320	P	(p-dioxane), lower discrete/cont.; cont. flatter, O1s 2nd order
C <sub>4</sub> H <sub>8</sub> S	H86b	275-325	E,R	(thiolane), comp. to thiophene, other heterocyclics
	HNS86	275-325	E,P	$\sigma^*(C-S)$ , comp. to C <sub>4</sub> H <sub>4</sub> S
	HE91	(white)	P	(hv; $e_{Auger}$ ,ion) coinc.; mass spectra at C1s, S2p with Auger
C <sub>4</sub> H <sub>9</sub> N	NIH86	275-325	E	(pyrrolidine), absolute
	PS&01	280-315	T	STEX, extensive series of C-N compounds
C <sub>4</sub> H <sub>10</sub>	HI87	275-325	E	n-butane
	H86	280-320	E,R	comp. to cyclo-butane
	S92	280-320	E,T,R	MS-X $\alpha$ ; comp. of cyclic-C <sub>n</sub> alkanes
	WBW99	280-320	T	ab initio $\Delta$ SCF; comp to solid & clusters; conformational dep; Ryd persist in condensed phase
C <sub>4</sub> H <sub>10</sub>	HI87	275-325	E	iso-butane
	UG05	286-292	P,T	high-res, 40 meV; comparison of small alkanes; Ryd-val mix; GSCF3

<b>C<sub>4</sub>H<sub>10</sub>O</b>	IM&87	275-325	E	t-butanol, comp. to t-butyl-peroxide
<b>C<sub>4</sub>H<sub>10</sub>O</b>	SY&89	280-320	P	diethyl-ether, lower discrete/cont.; cont. flatter, O1s 2nd order
	UH&95b	280-320	E,T	absolute; EHMO; comp. to polyurethanes
	FB02	280-360	E	absolute; sum rule checked
<b>C<sub>4</sub>H<sub>12</sub>OSi</b>	UH94a	280-330	E	Me <sub>3</sub> Si(OMe);comp of Si-O-X species; inductive, resonance effects
	UT&97	283-303	P	absolute; Si-Si & Si-O-R
<b>C<sub>4</sub>H<sub>12</sub>Pb</b>	NK&89	50-600	P	Pb(CH <sub>3</sub> ) <sub>4</sub> ; total & partial ion d; no C1s signal (!); contaminated optics; core-site dependent fragmentation
<b>C<sub>4</sub>H<sub>12</sub>Si</b>	SD&84	280-380	E	(Me) <sub>4</sub> Si-TMS, methane-like spectrum
	SD&85	280-380	E	methane-like spectrum
	W92	280-320	E	absolute; comp. of Si(CH <sub>3</sub> ) <sub>4</sub> , Si <sub>2</sub> (CH <sub>3</sub> ) <sub>6</sub> and Si <sub>6</sub> (CH <sub>3</sub> ) <sub>6</sub> ; σ*(Si-Si)
	UX&94	280-330	E	absolute; comp. of edges of Si-Si compounds
<b>C<sub>4</sub>H<sub>12</sub>OSi</b>	UH94a	280-330	E	Me <sub>3</sub> Si(OMe);comp of Si-O-X species; inductive, resonance effects
<b>C<sub>4</sub>NiO<sub>4</sub></b>	CSB89	280-335	E	Ni(CO) <sub>4</sub> , high res., comp. to CO; vibrations resolved on π*
	H90a	280-325	E,R	absolute; comp. to TM-COs; relaxation and δ(R) for σ*(CO)
	HWR90a	280-325	E	absolute; comp. to TM-COs; f(π*) vs. extent of backbonding
	SLD95	287	T	absolute, DF-LCAO; OS for C1s, O1s → π*; orbital mapping
<b>C<sub>4</sub>N<sub>2</sub>O</b>	UH&95b	280-320	E,T	(NH <sub>2</sub> ) <sub>2</sub> C=O, urea; absolute; EHMO; comp. to polyurethanes
<b>C<sub>5</sub>Cl<sub>3</sub>H<sub>5</sub>Ti</b>	WH93	280-335	E	CpTiCl <sub>3</sub> , abs. comp. of Cp <sub>x</sub> TiCl <sub>4-x</sub> , x=0-2; diff '10Dq' at each edge
<b>C<sub>5</sub>F<sub>8</sub></b>	RI&88	280-330	E	perfluor-cyclopentene, absolute
<b>C<sub>5</sub>F<sub>10</sub></b>	IM&88	280-330	E	perfluoro-cyclopentane, comp. to per-F c-C <sub>2</sub> H <sub>2n+2</sub> ; strong σ*(C-F)
<b>C<sub>5</sub>F<sub>12</sub></b>	HFM87	280-320	E	comp. to other fluorocarbons; σ*(C-F) 'giant shape res.'
	IM&88	275-325	E	perfluoropentane, C <sub>x</sub> F <sub>2x+2</sub> series, σ*(C-F) dominated
<b>C<sub>5</sub>F<sub>12</sub></b>	IM&88	275-325	E	perfluoro-neo-pentane, σ*(C-F) dom.; comp. to C <sub>2</sub> F <sub>6</sub> , extra σ*(C-F)
<b>C<sub>5</sub>FeO<sub>5</sub></b>	EC&85	280-340	P	Fe(CO) <sub>5</sub> , ion & electron yield, comp. to free CO, CO/Cu, Cr(CO) <sub>6</sub>
	E87	280-340	P	ion yields, DES
	MSN89	270-520	P	total, partial ion yields; comp to CO, Fe <sub>2</sub> (CO) <sub>9</sub> ; EXAFS?
	H90a	280-325	E,R	absolute; comp. to TM-COs; relaxation and δ(R) for σ*(CO)
	HWR90a	280-325	E	absolute; comp. to TM-COs; f(π*) vs. extent of backbonding
	HW&90	280-530	E	EXEFS, comp. to simulation, C,O distances detected
	H92b	284-298	E,T	comp of <sup>3</sup> π- <sup>1</sup> π split. in CO and Fe(CO) <sub>5</sub> (1.30 eV); core hole relaxation investigated via EHMO calc
	WRH92	280-330	E	absolute, comp. to CxF(CO) <sub>3</sub> , COTFe(CO) <sub>3</sub> , Fe(Cp) <sub>2</sub> ; mix. lig. effect
	SLD95	287	T	absolute, DF-LCAO; OS for C1s, O1s → π*; orbital mapping
<b>C<sub>5</sub>H<sub>2</sub>N<sub>4</sub></b>	AGH93	280-320	E,P	dicyano-imidazole; absolute; gas-EELS; comp. to sol.-NEXAFS
	CPA01	395-428	T	STEX with screening; comp. to expt. (AGH93)
<b>C<sub>5</sub>H<sub>5</sub>N</b>	AV&85	285-305	P	(pyridine), absolute; comp. benzene, toluene & styrene; 1π* 0.5eV split
	HS&85	275-330	E,P	gas,solid monolayer comp., π* & σ* res. Identified
	HD&99	280-315	E,T	0.2 eV fwhm; Z+1 calc; comp to pyridazine; s-triazine
	CPA01	280-320	T	STEX with screening; comp. to expt. (HS&85)
	KP&01	280-310	P,T	relative; high res – 65 meV; DFT; vibrations resolved; π* intensities
	PS&01	280-315	T	STEX, extensive series of C-N compounds
	IH07	284-302	T	relative, Gaussian augmented plane wave (GAPW) - DFT; (-5 to +3 eV errors on 14 small molecules
	VG&08	284-330	P,T	relative, transmission, double ion cell, DEMON calc, comp of 5 aza-rings
	LG&09	283-287	P	relative, comparison of molecular and cluster π*, red-shift in cluster
<b>C<sub>5</sub>H<sub>5</sub>N<sub>5</sub>O</b>	PF&09	283-316	P,T	(guanine) Tautomerism, thermal gas, DFT calc; Boltzmann-weighted
<b>C<sub>5</sub>H<sub>6</sub></b>	H90a	272-320	E,R	cyclopentadiene, comp to Fe,Co,Ni metallocenes
	RWH91	280-320	E	absolute, comp. of CpH, di-CpH, C <sub>5</sub> H <sub>8</sub> re π* of Cp <sup>-</sup>
	PS&01	280-315	T	STEX, comp. to expt.; extensive series of C-N compounds
<b>C<sub>5</sub>H<sub>6</sub>S</b>	HT&90	280-330	E	3-Me-thiophene; absolute, comp. 3-alkylthiophenes; NEXAFS of poly.
<b>C<sub>5</sub>H<sub>6</sub>Se</b>	HTB89	275-325	E	(3-Me-selenophene), absolute, comp. to selenophene, solid

<b>C<sub>5</sub>H<sub>7</sub>N</b>	PS&01	280-315	T	(1,4-dihydropyridine), STEX, extensive series of C-N compounds
<b>C<sub>5</sub>H<sub>7</sub>N<sub>3</sub>O</b>	FP&11	284-296	P	(isocytosine), tautomerism in cytosines
<b>C<sub>5</sub>H<sub>8</sub></b>	H86b	280-320	E,R	comp. to solid, monolayer
	HN&86	275-325	E,P	(cyclopentene), $\sigma^*$ res./bond length, solid, monolayer comp.
	RWH91	280-320	E	absolute, comp. of CpH, di-CpH, C <sub>5</sub> H <sub>8</sub> re $\pi^*$ of Cp <sup>-</sup>
	PS&01	280-315	T	STEX, comp. to expt.; extensive series of C-N compounds
<b>C<sub>5</sub>H<sub>8</sub>O</b>	HI88a	275-325	E	(1,3-dihydropyran)
<b>C<sub>5</sub>H<sub>8</sub>O<sub>2</sub></b>	LC&07	280-320	E,T	Me(CO)Me(CO)Me; di-carbonyls; charge shifts, GSCF3
<b>C<sub>5</sub>H<sub>8</sub>O<sub>4</sub></b>	LC&07	280-320	E,T	MeO(CO)Me(CO)OMe; di-carbonyls; charge shifts, GSCF3
<b>C<sub>5</sub>H<sub>9</sub>N</b>	PS&01	280-315	T	(1,2,3,4-tetrahydropyridine), STEX, extensive series of C-N compounds
<b>C<sub>5</sub>H<sub>9</sub>N</b>	PS&01	280-315	T	(1,2,3,6-tetrahydropyridine), STEX, extensive series of C-N compounds
<b>C<sub>5</sub>H<sub>10</sub></b>	HN&86	275-325	E,P	(cyclopentane), $\sigma^*$ res./bond length, solid, monolayer comp.
	S92	280-320	E,T,R	MS-X $\alpha$ ; comp. of cyclic-C <sub>n</sub> alkanes
	PS&01	280-315	T	STEX, comp. to expt.; extensive series of C-N compounds
<b>C<sub>5</sub>H<sub>10</sub></b>	FL96	282-294	T	1-pentene; absolute; $\Delta$ SCF-Cl; comp. to XPS shake-up and expt. [S92]; n-C <sub>n</sub> H <sub>2n</sub> , n=3,4,5,6 compared
<b>C<sub>5</sub>H<sub>10</sub>O</b>	NIH86	275-325	E	(tetrahydropyran)
<b>C<sub>5</sub>H<sub>10</sub>O</b>	YA&96	280-320	T	diethylketone; absolute; STEX; R <sub>2</sub> CO comparison
	YA&97	287	T	$\pi^*$ OS; test of initial and final state sum rules; comp to expt.
<b>C<sub>5</sub>H<sub>10</sub>N<sub>2</sub></b>	HE&01	280-305	E	methyl-carbene; thermal decomposition of tetra-amino ethylene
<b>C<sub>5</sub>H<sub>11</sub>N</b>	NIH86	275-325	E	(piperidine), absolute, heterocycles
	PS&01	280-315	T	STEX, extensive series of C-N compounds
<b>C<sub>5</sub>H<sub>11</sub>NO<sub>2</sub></b>	PC&98	285-315	T	valine; (D,L-) STEX; comp. of NEXAFS, circ. Dichroism of amino acids
<b>C<sub>5</sub>H<sub>12</sub></b>	HI87	275-325	E	n-pentane
	LAL91	285-305	T	CNDO, systematic calc. of $\sigma^*$ energies; ISEELS, ETS for param. det.
	S92	280-320	E,T,R	MS-X $\alpha$ ; comp. of cyclic-C <sub>n</sub> alkanes
<b>C<sub>5</sub>H<sub>12</sub></b>	HI87	275-325	E	iso-pentane
<b>C<sub>5</sub>H<sub>12</sub></b>	HI87	275-325	E	neo-pentane
	UG05	286-292	P,T	high-res, 40 meV; comparison of small alkanes; Ryd-val mix; GSCF3
<b>C<sub>5</sub>H<sub>14</sub>O</b>	UHR95	280-320	E	sec-butyl ethyl ether; absolute
<b>C<sub>5</sub>H<sub>14</sub>OSi</b>	TC&02	280-320	E	Me <sub>3</sub> SiOEt; absolute; comp. to vinyl silanes
<b>C<sub>5</sub>H<sub>15</sub>NSi</b>	UH94b	280-330	E	Me <sub>3</sub> Si(NMe <sub>2</sub> ) <sub>2</sub> ; comp. of Si-N cmpds; models for SiN <sub>x</sub> O <sub>y</sub> films
<b>C<sub>5</sub>MnO<sub>5</sub>H</b>	HR89	280-320	E	Mn(CO) <sub>5</sub> H, absolute, $\pi^*$ intensity as measure of d $\pi$ -p $\pi$ backbonding
	RH89a	275-330	E	comp. to CO, Mn(CO) <sub>10</sub> & M(CO)s; E(ref); f( $\pi^*$ ) $\alpha$ backbond
	SLD95	287	T	absolute, DF-LCAO; OS for C1s, O1s $\rightarrow \pi^*$ ; orbital mapping
<b>C<sub>5</sub>H<sub>8</sub>MnO<sub>2</sub><sup>+</sup></b>	AG&23	528-540	P	Mn(acac); RASPT2 calc., compare m=1,2,3
<b>C<sub>6</sub>ClH<sub>5</sub></b>	HP&78	283-295	E	XPS-EELS chemical shifts comp.
	ES84	270-310	P	total, partial ion yield, site-selective frag., differs from (HP&78)
<b>C<sub>6</sub>CrO<sub>6</sub></b>	EC&84	287	P	Cr(CO) <sub>6</sub> , ion & electron yield, comp. to free CO, CO/Cu, Fe(CO) <sub>5</sub>
	CSB90	275-325	E	comp. of M(CO) <sub>6</sub> , M=Cr, Mo, W
	SLD95	287	T	absolute, DF-LCAO; OS for C1s, O1s $\rightarrow \pi^*$ ; orbital mapping
<b>C<sub>6</sub>D<sub>6</sub></b>	CS90	284-287	P	$\pi^*$ vib'nl isotope effect; symmetry breaking; localised core hole
	MS&89	284-287	P	30 meV fwhm; vib'nl isotope eff; symmetry breaking; local. hole
(C <sub>6</sub> D <sub>6</sub> cont'd)	MS&90	284-287	P	40 meV fwhm; $\pi^*$ vib'nl isotope eff; symmetry breaking; local hole
	MC&91	284-291	P	50 meV fwhm; $\pi^*$ & Ryd vibns; comp of C <sub>2</sub> H <sub>x</sub> &C <sub>2</sub> D <sub>x</sub> (isotope effect)
<b>C<sub>6</sub>FH<sub>5</sub></b>	HP&78	283-295	E	XPS-EELS chemical shifts comp.
	HFM87	280-320	E	comp. to other fluorocarbons; $\sigma^*(C-F)$ 'giant shape res.'
	HF&87	280-325	E	weak C-F $\sigma^*$ res.
	PY&97	280-310	T	STEX; C <sub>6</sub> H <sub>x</sub> F <sub>6-x</sub> isomers; comp to HF&87; test of building block; C-R shift; (C <sub>6</sub> H <sub>5</sub> X, X=F,NH <sub>2</sub> ,OH)
	SC&87	280-305	T	comp. of ab initio, EICVOM & g-Hartree, exp (HP&78); hole local.
	PP&00	285	T	MC-SCF Z+1 calc; vibrational structure, XPS better than NEXAFS

<b>C<sub>6</sub>F<sub>2</sub>H<sub>4</sub></b>	HFM87	280-320	E	comp. to other fluorocarbons; σ*(C-F) 'giant shape res.'
	HF&87	280-325	E	(1,4 = para-difluoro), weak C-F σ* res.
	PY&97	280-310	T	STEX; C <sub>6</sub> H <sub>x</sub> F <sub>6-x</sub> isomers; comp to HF&87; test of building block
<b>C<sub>6</sub>F<sub>3</sub>H<sub>3</sub></b>	HFM87	280-320	E	comp. to other fluorocarbons; σ*(C-F) 'giant shape res.'
	HF&87	280-325	E	(1,3,5-trifluoro), weak C-F σ* res.
	PY&97	280-310	T	STEX; C <sub>6</sub> H <sub>x</sub> F <sub>6-x</sub> isomers; comp to HF&87; test of building block
<b>C<sub>6</sub>F<sub>4</sub>H<sub>2</sub></b>	HFM87	280-320	E	comp. to other fluorocarbons; σ*(C-F) 'giant shape res.'
	HF&87	280-325	E	(1,2,4,5 = para-dihydro), weak C-F σ* res.
	PY&97	280-310	T	STEX; C <sub>6</sub> H <sub>x</sub> F <sub>6-x</sub> isomers; comp to HF&87; test of building block
<b>C<sub>6</sub>F<sub>5</sub>H</b>	HFM87	280-320	E	comp. to other fluorocarbons; σ*(C-F) 'giant shape res.'
	HF&87	280-325	E	weak C-F σ* res.
	PY&97	280-310	T	STEX; C <sub>6</sub> H <sub>x</sub> F <sub>6-x</sub> isomers; comp to HF&87; test of building block
	YP&97	280-310	T	comp. of phenol, aniline, fluorobenzene; substituent effects
<b>C<sub>6</sub>F<sub>6</sub></b>	HI86	290-700	E	extended fine structure
	HFM87	280-320	E	comp. to other fluorocarbons; σ*(C-F) 'giant shape res.'
	HF&87	280-325	E	weak C-F σ* res.
	H89	280-320	E,R	review of electron-beam core excitation spectroscopies (Aussois)
	H90a	290-320	E,R	absolute, pot. bar. effect on I{σ*(C-F)} through CF <sub>x</sub> series
	D92a	270-320	P,R	PEPICO, PEPIPICO; fragmentation mechanisms
	PY&97	280-310	T	STEX; C <sub>6</sub> H <sub>x</sub> F <sub>6-x</sub> isomers; comp to HF&87; test of building block
<b>C<sub>6</sub>F<sub>12</sub></b>	IM&88	275-325	E	(perfluoro-cyclohexane), σ*(C-F) dominated
	OS&90	280-320	P,T	PTFE(s), EY-NEXAFS, comp. to gas (IM&88); reassigned σ*s
<b>C<sub>6</sub>F<sub>14</sub></b>	HFM87	280-320	E	comp. to other fluorocarbons; σ*(C-F) 'giant shape res.'
	IM&88	275-325	E	(perfluoro-n-hexane), σ*(C-F) dominated
	AC&95	290-315	T	STEX ab initio; absolute; growth of poly-(CF <sub>2</sub> ) <sub>n</sub> by C <sub>2n</sub> F <sub>4n+2</sub> , n=1-5
<b>C<sub>6</sub>H<sub>4</sub>N<sub>2</sub>S</b>	HD&91	275-320	E	Bz(N-S) ring; comp. of S-N heterocycles, aromaticity
<b>C<sub>6</sub>H<sub>4</sub>N<sub>2</sub>S<sub>2</sub></b>	HD&91	275-320	E	Bz(N-S) ring; comp. of S-N heterocycles, aromaticity
<b>C<sub>6</sub>H<sub>4</sub>N<sub>2</sub>S<sub>3</sub></b>	HD&91	275-320	E	Bz(N-S) ring; comp. of S-N heterocycles, aromaticity
<b>C<sub>6</sub>H<sub>4</sub>O<sub>2</sub></b>	FH92	280-330	E,T	O=Bz=O; absolute; EHMO; comp. of BzOH, Bz(OH) <sub>2</sub> and quinone
<b>C<sub>6</sub>H<sub>5</sub>I</b>	HP&78	283-295	E	XPS-EELS chemical shifts comp.
<b>C<sub>6</sub>H<sub>5</sub>NO<sub>2</sub></b>	TUH96	280-320	E,T	absolute; EHMO; comp. to aniline, benzene and nitroanilines
<b>C<sub>6</sub>H<sub>6</sub></b>	HS90	280-345	E	CH <sub>3</sub> C/C-C/CCH <sub>3</sub> ; absolute; comp. to other X::X species; conj.
	S92	280-320	E,T,R	MS-Xα; comp to propyne, solid
<b>C<sub>6</sub>H<sub>6</sub></b>	EH&76	280-300	P	benzene, photoelectric yield
	HB77	280-340	E	cont. res.
	ES84	270-310	P	partial & total ion yields, e <sub>u</sub> π* res. anomalously weak
	SSH84a	295	T	σ*-res./bond length relationship
	AV&85	2-1000	P	absolute, discrete hv; 'MRV-Xα' calc.; σ* res. have diff. pol.
	GMT85	280-300	T	MSX-α; π levels only; assigns 289eV peak to π <sub>2</sub> (b <sub>2g</sub> ), comp. to ETS
	HS&85	275-330	E,P	gas, solid monolayer comp., π* & σ* res., MS X-α calc.
	DG&86	280-320	E	comp. to borazine, cyclohexane
	L86	284-290	T	HAM/3 electron affinities, reassigned π* levels, comp. to HB77
	HI86	290-700	E	extended fine structure
	HF&87	280-325	E	comp. to fluorobenzenes
	SC&87	280-305	T	comp. of ab initio, EICVOM & g-Hartree, exp (HP&78); core local.
	MF&88	280-320	P	ZEKE; XPS-sat & EELS/PA, higher Ryd., 2e & shake-up, PCI
	H89	280-320	E,R	review of electron-beam core excitation spectroscopies (Aussois)
	HR89	280-320	E	comp. of c-C <sub>6</sub> hydrocarbons; develop. of π* & σ* conjugation
	MS&89	284-287	P	30 meV fwhm, vib'ns; comp. to C <sub>2</sub> D <sub>4</sub> ; symmetry mod. by localised hole
	PF&89	280-360	P	partial X-sect. (main line, satellites), 293 eV peak is 2e-
	YS&89	280-320	P,T	yield NEXAFS of H-(C <sub>6</sub> H <sub>4</sub> ) <sub>n</sub> -H (N=1,3-6); comp. to benzene (HS&85),

				$\pi^*$ localisation, CNDO/S calc. (Z+1)
(C <sub>6</sub> H <sub>6</sub> .cont'd)	CS90	284-287	P	$\pi^*$ vib'nl isotope effect; symmetry breaking; localised core hole
	HW&90	300-700	E	EXELFS, comp. to NEXAFS of solid (77 K)
	MS&90	284-287	P	40 meV fwhm; $\pi^*$ vib'nl isotope eff.; symmetry breaking; local. hole
	BG&91	291	E	(e,e); comp. to calc.; suggests R-dependent interference in I(q)
	H91	280-320	E	comp. of c-C <sub>6</sub> HCs; development of $\pi^*$ & $\sigma^*$ conjugation
	LAL91	285-305	T	CNDO, systematic calc. of $\sigma^*$ energies; ISEELS, ETS for param. det.
	MC&91	284-291	P	50 meV fwhm; $\pi^*$ & Ryd vibns; comp of C <sub>2</sub> H <sub>x</sub> &C <sub>2</sub> D <sub>x</sub> (isotope effect)
	VNP91	280-320	P	comp. of BF <sub>3</sub> , BN(s) & borazine; edge resonances
	ME&92	282-292	P	comp. of gas (HB77) & sol.; H <sup>+</sup> yield; ultrafast C-H resonance decay
	HUR92	280-330	E,T	absolute, comp. of R-benzenes; EHMO; PET-polymer PEELS model
	RY&92	280-320	E	comp. of small mol. analogs with PET polymer
	S92	280-330	E,R	comp. of C <sub>2</sub> H <sub>x</sub> , x=2,4,6; $\sigma^*(C-C)$
	FE&94	284-286	E,T	<sup>3</sup> $\pi^*$ ; INDO calc; correl. of $\Delta(1,3)$ and $\pi^*$ osc. str.
	AVC95	280-314	T	absolute; $\Delta$ SCF with Stieltjes continuum; comp. of benzene, naphthalene, anthracene, tetracene and pyrene; comp. to expt. reinterpret HS&85
	SG&95b	284-310	P,T	resonant X-ray emission (RIXS); unbroken symmetry; states assigned
	HC96	285	T	DFT calc.; <sup>3</sup> $\pi^{-1}\pi$ split = 0.41 eV
	TUH96	280-320	E,T	absolute, EHMO, comp. to aniline, nitrobenzene and nitroanilines
	PY&97	280-310	T	STEX; C <sub>6</sub> H <sub>x</sub> F <sub>6-x</sub> isomers; comp to HF&87
	UT&97	282-303	P	absolute; reference for Ph <sub>3</sub> Si-X, Me <sub>3</sub> Si-X
	OM&98	280-310	T	GSCF3; DOUS modified by core hole effect; compared to condensed ring systems: chrysene, perylene, coronene
	KK&99	290-360	P	absolute; main line partial cross-sections; disputes shape res. existence
	DF&00	280-320	E,T	relative, Z+1 ab initio; C <sub>2v</sub> sym. Ass.; Ryd-val mix; 289 peak = 2e-
	RK&00a	282-800	P	absolute; high-res (50 meV), partial X-sect; $\beta$ ; EXAFS; resonant Auger; no SR; explains 298 continuum peak
	PS&01	280-315	T	STEX, comp. to expt.; extensive series of C-N compounds
	FG&03b	284-286	P	partial ion yield; molecule, di-cluster compared, 90 meV shift
	GT&03a	280-320	E	absolute; comp. to X-ray Raman spectra
	CG&04	282-304	E	comp. of alanine, benzene, phenylalanine - additivity
	PK&04	284-291	P,T	high res. (60 meV), TIY, TD-DFT
	KP&06	283-293	P, T	relative, hi-res; comp. of C <sub>6</sub> -ring molecules; DFT-TS accurate to 0.2 eV
	GW09	288-296	T	DFT, comp of C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub> , C <sub>6</sub> H <sub>6</sub> , C <sub>8</sub> H <sub>10</sub> O <sub>2</sub> , C <sub>8</sub> H <sub>11</sub> N, C <sub>9</sub> H <sub>11</sub> NO <sub>2</sub>
	CS&20	620-670	P,T	XFEL, K <sup>-2</sup> V (double core excitation)
C <sub>6</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub>	TUH96	280-320	E,T	(1,2)-nitroaniline; absolute, EHMO, comp. to aniline, nitrobenzene
	H00	282-298	E,T,R	isomer effects on spectra; EHMO calculations
C <sub>6</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub>	TUH96	280-320	E,T	(1,3)-nitroaniline; absolute, EHMO, comp. to aniline, nitrobenzene
	H00	282-298	E,T,R	isomer effects on spectra; EHMO calculations
C <sub>6</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub>	TUH96	280-320	E,T	(1,4)-nitroaniline; absolute, EHMO, comp. to aniline, nitrobenzene
	H00	282-298	E,T,R	isomer effects on spectra; EHMO calculations
C <sub>6</sub> H <sub>6</sub> O	FH92	280-330	E,T	phenol; absolute; EHMO; comp. of BzOH, Bz(OH) <sub>2</sub> and quinone
	PY&97	280-310	T	STEX; C-R shift; (C <sub>6</sub> H <sub>5</sub> X, X=F,NH <sub>2</sub> ,OH)
	YP&97	280-310	T	comp. of phenol, aniline, fluorobenzene; substituent effects
	PP&00	285	T	MC-SCF Z+1 calc; vibrational structure, XPS better than NEXAFS
	LL&14a	284-298	P	TIY, PIY
C <sub>6</sub> H <sub>6</sub> O <sub>2</sub>	FH92	280-330	E,T	HO-Bz-OH; EHMO; comp. of BzOH, Bz(OH) <sub>2</sub> and quinone
C <sub>6</sub> H <sub>7</sub> N	HUR93	280-330	E	aniline, comp. to dimethylaniline
	LA&95	284-296	P,T	RIXS; comp. to benzene; interference between (C-H, C-R) $\pi^*$ states
	LAG96	284-294	T	absorption; RIXS; polarisation anisotropy
	TUH96	280-320	E,T	absolute, EHMO, comp. to nitrobenzene and nitroanilines
	NG&97	284-294	P,R	resonant X-ray emission (RIXS); comp. to benzene

C <sub>6</sub> H <sub>7</sub> N cont'd)	PY&97	280-310	T	STEX; C-R shift; (C <sub>6</sub> H <sub>5</sub> X, X=F,NH <sub>2</sub> ,OH) comp. of phenol, aniline, fluorobenzene; substituent effects
	YP&97	280-310	T	MC-SCF Z+1 calc; vibrational structure, XPS better than NEXAFS
	PP&00	285	T	STEX with screening; comp. to expt. (HUR93)
	CPA01	280-320	T	(1,3-cyclohexadiene), comp. of c-C <sub>6</sub> HCs; $\pi^*$ & $\sigma^*$ conjugation
<b>C<sub>6</sub>H<sub>8</sub></b>	HR89	280-320	E	comp. of c-C <sub>6</sub> HCs; development of $\pi^*$ & $\sigma^*$ conjugation
	H91	275-335	E	relative, hi-res; comp. of C <sub>6</sub> -ring molecules; DFT-TS accurate to 0.2 eV
	KP&06	283-293	P, T	polyenes, STEX, $\pi/\sigma$ convergence
	CA&95	280-320	T	STEX, comp. to expt.; extensive series of C-N compounds
	PS&01	280-315	T	(1,4-cyclohexadiene), comp. of c-C <sub>6</sub> HCs; $\pi^*$ & $\sigma^*$ conjugation
<b>C<sub>6</sub>H<sub>8</sub></b>	HR89	280-320	E	comp. of c-C <sub>6</sub> HCs; development of $\pi^*$ & $\sigma^*$ conjugation
	H91	275-335	E	STEX, comp. to expt.; extensive series of C-N compounds
	PS&01	280-315	T	relative, hi-res; comp. of C <sub>6</sub> -ring molecules; DFT-TS accurate to 0.2 eV
<b>C<sub>6</sub>H<sub>8</sub></b>	KP&06	283-293	P, T	1,3,5-hexatriene; solid NEXAFS; vibn'l struct., ab initio
C <sub>6</sub> H <sub>8</sub>	NS&92	280-330	P,T	1-particle Green's function; comp. of C <sub>2</sub> H <sub>4</sub> , C <sub>4</sub> H <sub>6</sub> ,C <sub>6</sub> H <sub>8</sub> ; comp. to NS&92 (solid); claims relaxation shifts dominate; $\pi^*$ split small.
	LA93	282-292	T	delocalization in polyenes; comp. of H-(CH=CH) <sub>n</sub> -H, n=1-5
	GA95	284-290	T	X-ray emission as f(conjugation); $\pi$ -exciton effects; H(C <sub>2</sub> H <sub>2</sub> ) <sub>n</sub> H, n=1,10
	GYA96	285	T	STEX; shake-up spectra related to NEXAFS; H(C <sub>2</sub> H <sub>2</sub> ) <sub>n</sub> H, n=1-5
<b>C<sub>6</sub>H<sub>8</sub>O</b>	UHR99	280-320	E	2-cyclohexene-1-one; absolute; conjugation test
<b>C<sub>6</sub>H<sub>8</sub>O<sub>2</sub></b>	FH94	280-330	E,T	1,2-chclohexanedione, absolute; eff. of cong.; enol-form
<b>C<sub>6</sub>H<sub>8</sub>O<sub>2</sub></b>	FH94	280-330	E,T	1,3-chclohexanedione, absolute; eff. of cong.; keto-form
<b>C<sub>6</sub>H<sub>8</sub>O<sub>2</sub></b>	FH94	280-330	E,T	1,4-chclohexanedione, absolute; eff. of cong.; keto-form
C <sub>6</sub> H <sub>9</sub> N <sub>3</sub> O <sub>3</sub>	UA&99	280-340	E	trimethyl-isocyanurate; absolute; polymer model
C <sub>6</sub> H <sub>9</sub> S	HT&90	275-325	E	3-Ethyl-thiophene; absolute, no mod. of $\pi^*$ (cf. polymer cond.)
<b>C<sub>6</sub>H<sub>10</sub></b>	HN&86	275-325	E,P	(cyclohexene), res./bond length
	HR89	280-320	E	comp. of c-C <sub>6</sub> hydrocarbons; development of $\pi^*$ & $\sigma^*$ conjugation
	H91	275-335	E	absolute, comp. of c-C <sub>6</sub> hydrocarbons; $\pi^*$ & $\sigma^*$ conjugation
	PS&01	280-315	T	STEX, comp. to expt.; extensive series of C-N compounds
	KP&06	283-293	P, T	relative, hi-res; comp. of C <sub>6</sub> -ring molecules; DFT-TS accurate to 0.2 eV
<b>C<sub>6</sub>H<sub>10</sub></b>	EL&98	280-320	E	dimethylcyclobutene; absolute; comp with tetramethylcyclobutene
<b>C<sub>6</sub>H<sub>10</sub>O</b>	FH94	280-330	E,T	(cyclohexanone); absolute; comp. to o,m,p-cyclohexanedione
<b>C<sub>6</sub>H<sub>10</sub>O</b>	UHR99	280-320	E	4-hexene-3-one; absolute; conjugation test
C <sub>6</sub> H <sub>12</sub>	DG&86	280-330	E	(cyclohexane), comp. to borazine, benzene, claims giant resonance
	HN&86	275-325	E,P	$\delta$ -R; solid, monolayer comp., MS-X $\alpha$ calc.
	HI86	290-700	E	extended fine structure
	H89	280-320	E,R	review of electron-beam core excitation spectroscopies (Aussois)
	HR89	280-320	E	comp. of c-C <sub>6</sub> hydrocarbons; development of $\pi^*$ & $\sigma^*$ conjugation
	H91	275-335	E	absolute, comp. of cyclic-hexa-hydrocarbons; $\pi^*$ & $\sigma^*$ conjugation
	LAL91	285-305	T	CNDO, systematic calc. of $\sigma^*$ energies; ISEELS, ETS for param. det.
	S92	280-320	E,T,R	MS-X $\alpha$ ; comp. of cyclic-C <sub>n</sub> alkanes
	PS&01	280-315	T	STEX, comp. to expt.; extensive series of C-N compounds
	KP&06	283-293	P, T	relative, hi-res; comp. of C <sub>6</sub> -ring molecules; DFT-TS accurate to 0.2 eV
C <sub>6</sub> H <sub>12</sub>	FL96	282-294	T	1-hexene; absolute; $\Delta$ SCF-Cl; comp. to XPS shake-up and expt. [S92]; n-C <sub>n</sub> H <sub>2n</sub> , n=3,4,5,6 compared
<b>C<sub>6</sub>H<sub>12</sub>N<sub>2</sub></b>	RUH95	280-320	E	DABCO; absolute
<b>C<sub>6</sub>H<sub>14</sub></b>	HI87	275-325	E	n-hexane, C <sub>x</sub> H <sub>2x+2</sub> series
	HI88b	275-335	E	absolute, comp. to c-C <sub>6</sub> H <sub>x</sub> , evolution of conjugation
C <sub>6</sub> H <sub>14</sub> N <sub>4</sub> O <sub>2</sub>	LH&12	287-293	T	(arginine), gas-solid comparison
<b>C<sub>6</sub>H<sub>14</sub>O</b>	UHR92	280-330	E	i-Pr-ether, absolute; modelling of PEELS of polyurethane
	UH&95a	280-330	E	absolute; modelling of PEELS of polyurethane
	UH&95b	280-330	E	absolute; polyurethane models

<b>C<sub>6</sub>H<sub>16</sub>N<sub>2</sub>Si</b>	UH&94b	390-420	E	bis(dimethylamino)dimethylsilane; explore Si-N bond
<b>C<sub>6</sub>H<sub>16</sub>OSi</b>	UH94a	280-330	E	Et <sub>3</sub> SiOH; comp of Si-O-X species; inductive, resonance effects
<b>C<sub>6</sub>H<sub>18</sub>OSi<sub>2</sub></b>	UH94a	280-330	E	Me <sub>3</sub> SiOSiMe <sub>3</sub> ; comp of Si-O-X species; inductive, resonance effects
	UT&97	282-303	P	absolute; Ph <sub>3</sub> Si-X, Me <sub>3</sub> Si-X
<b>C<sub>6</sub>H<sub>18</sub>O<sub>3</sub>Si<sub>3</sub></b>	UH94a	280-330	E	c-(SiMe <sub>2</sub> O) <sub>3</sub> ; comp of Si-O-X species; inductive, resonance effects
<b>C<sub>6</sub>H<sub>18</sub>Si<sub>2</sub></b>	W92	280-320	E	absolute; comp. of Si(CH <sub>3</sub> ) <sub>4</sub> , Si <sub>2</sub> (CH <sub>3</sub> ) <sub>6</sub> and Si <sub>6</sub> (CH <sub>3</sub> ) <sub>6</sub> ; σ*(Si-Si)
	UX&94	280-330	E	absolute; comp. of edges of Si-Si compounds
	UT&97	282-303	P	absolute; reference for Ph <sub>3</sub> Si-X, Me <sub>3</sub> Si-X
<b>C<sub>6</sub>MoO<sub>6</sub></b>	CSB90	275-325	E	comp. of M(CO) <sub>6</sub> , M=Cr, Mo, W
	SLD95	287	T	absolute, DF-LCAO; OS for C1s, O1s → π*; orbital mapping
<b>C<sub>6</sub>O<sub>6</sub>V</b>	TD&92a	280-330	P,E	V(CO) <sub>6</sub> , absolute
<b>C<sub>6</sub>O<sub>6</sub>W</b>	CSB90	275-325	E	W(CO) <sub>6</sub> , comp. of M(CO) <sub>6</sub> , M=Cr, Mo, W
<b>C<sub>7</sub>CoH<sub>5</sub>O<sub>2</sub></b>	HW&90	300-530	E	CoCp(CO); EXELFS; C-C detected; strong C-Co backscatter
	RWH91	270-350	E	absolute; comp. to other mixed-Cp, CO species
	H92b	281-307	E,R	absolute, comp. of CpCo(CO) <sub>2</sub> , Co <sub>2</sub> (CO) <sub>8</sub> and Co(Cp) <sub>2</sub>
<b>C<sub>7</sub>F<sub>5</sub>N</b>	IO&99	278-292	P	C <sub>6</sub> F <sub>5</sub> CN; TIY; mass spec at π* <sub>ring</sub>
<b>C<sub>7</sub>FeH<sub>6</sub>O<sub>3</sub></b>	RH92	280-330	E	C <sub>4</sub> H <sub>6</sub> -Fe(CO) <sub>3</sub> ; comp. of Fe(CO) <sub>5</sub> , RFe(CO) <sub>3</sub> , Fe(Cp) <sub>2</sub> ; mix. lig. effect
<b>C<sub>7</sub>H<sub>5</sub>N</b>	H92a	275-340	E,T	(benzonitrile), absolute; EHMO
	PS&01	280-315	T	STEX, extensive series of C-N compounds
<b>C<sub>7</sub>H<sub>6</sub>O</b>	HUR92	280-330	E,T	benzaldehydye; absolute, comp. of R-Bz; EHMO; poly-PET PEELS
	RY&92	280-320	E	comp. of small mol. analogs with PET polymer
<b>C<sub>7</sub>H<sub>7</sub>NO<sub>2</sub></b>	UH&95b	280-330	E	NH <sub>2</sub> -CO <sub>2</sub> Ph, absolute; modelling of polyurethane PEELS
<b>C<sub>7</sub>H<sub>8</sub></b>	AV&85	285-305	P	toluene; absolute, comp. of benzene, polystyrene & toluene
	CH07	275-340	E	absolute
<b>C<sub>7</sub>H<sub>8</sub></b>	HS90	275-340	E	1,6-heptadiyne; absolute; conjugation as f(chain length)
<b>C<sub>7</sub>H<sub>8</sub>O</b>	UHR97	280-320	E	anisole (Ph-OMe); absolute
<b>C<sub>7</sub>H<sub>8</sub>N<sub>2</sub>O</b>	UH&95a	280-320	E	phenylurea; absolute; modelling of polyurethane PEELS
	UH&95b	280-320	E	phenylurea; absolute; distinguishing urea/urethane
<b>C<sub>7</sub>H<sub>9</sub>N</b>	UH96	280-320	E	N-methyl aniline; absolute
<b>C<sub>7</sub>H<sub>10</sub></b>	WH&90	280-320	E	norbornene; absolute; comp. of NB, 2-CH <sub>3</sub> -NB & 2-CF <sub>3</sub> -NB
	H92b	280-320	E,R	comp. of NB, 2-Me-NB, 2-CF <sub>3</sub> -NB; core vs. valence
<b>C<sub>7</sub>H<sub>12</sub>O<sub>2</sub></b>	LUH97	280-320	E	butyl acrylate; absolute; polymer model
<b>C<sub>7</sub>H<sub>12</sub>O<sub>4</sub></b>	LC&07	280-320	E, T	(dimethyl malonate), comp of di-carbonyls, GSCF3
<b>C<sub>7</sub>H<sub>14</sub>O</b>	YA&96	280-320	T	dipropylketone; absolute; STEX; R <sub>2</sub> CO comparison
	YA&97	287	T	π* OS; test of initial and final state sum rules; comp to expt.
<b>C<sub>7</sub>H<sub>18</sub>N<sub>3</sub>Si</b>	UH&94b	280-320	E	tris(dimethylamino)methylsilane; exploring Si-N bond
<b>C<sub>8</sub>Cl<sub>2</sub>H<sub>6</sub>O<sub>2</sub></b>	HUR92	275-340	E	ClCO-Bz-ClCO (terphthalic Cl); absolute; comp. to polymer EELS
	RY&92	280-320	E	comp. of small mol. analogs with PET polymer
<b>C<sub>8</sub>ClH<sub>18</sub>P</b>	HH&98	284-304	E	(tBu) <sub>2</sub> PCl; absolute; comp. to PMe <sub>3</sub>
<b>C<sub>8</sub>Co<sub>2</sub>O<sub>8</sub></b>	H90a	280-325	E,R	absolute; comp. to TM-COs; relaxation and δ(R) for σ*(CO)
	HWR90a	280-325	E	absolute; comp. to TM-COs; f(π*) vs. extent of backbonding
	RWH91	270-350	E	Co <sub>2</sub> (CO) <sub>8</sub> ; absolute; comp. to mixed-Cp, CO species
	H92b	281-307	E,R	absolute, comp. of CpCo(CO) <sub>2</sub> , Co <sub>2</sub> (CO) <sub>8</sub> and Co(Cp) <sub>2</sub>
<b>C<sub>8</sub>F<sub>3</sub>H<sub>9</sub></b>	WH&90	280-320	E	CF <sub>3</sub> -norbornene; absolute; comp. of NB, 2-CH <sub>3</sub> -NB & 2-CF <sub>3</sub> -NB
	H92b	280-320	E,R	comp. of NB, 2-Me-NB, 2-CF <sub>3</sub> -NB; core vs. valence
<b>C<sub>8</sub>F<sub>18</sub></b>	AC&95	290-315	T	STEX ab initio; absolute; growth of poly-(CF <sub>2</sub> ) <sub>n</sub> by C <sub>2n</sub> F <sub>4n+2</sub> , n=1-5
<b>C<sub>8</sub>H<sub>6</sub></b>	LUH99	280-320	E,T	phenylacetylene; absolute; GSCF3, low-lying π*
	CP&98	280-320	P,T	relative, TIY, STEX, good agreement of 1s → π* expt, theory
<b>C<sub>8</sub>H<sub>6</sub>S</b>	TG&18	284-291	P,T	benzo(b)thiophene, TIY, DFT calc., compare C <sub>4</sub> H <sub>4</sub> S, C <sub>8</sub> H <sub>6</sub> S, C <sub>8</sub> H <sub>6</sub> S (S-hetero-rings)

<b>C<sub>8</sub>H<sub>6</sub>O<sub>2</sub></b>	HUR92 RY&92 YP&97	275-340 280-320 280-320	E E T	CHO-Bz-CHO (Terphthaldehyde); absolute; comp. to polymer EELS comp. of small mol. analogs with PET polymer ortho, para terphthaldehyde; substituent effects; comp. to HUR92
<b>C<sub>8</sub>H<sub>8</sub></b>	HN&86	275-325	E,P	(cyclo-octatetraene), σ*-E,R; solid, monolayer comp.
C <sub>8</sub> H <sub>8</sub>	AV&85 KP&06	285-305 283-293	P P, T	(C <sub>6</sub> H <sub>5</sub> CH-CH <sub>2</sub> -), polystyrene, comp. to benzene, pyridine & toluene relative, hi-res; comp. of C <sub>6</sub> -ring molecules; DFT-TS accurate to 0.2 eV
<b>C<sub>8</sub>H<sub>8</sub>O</b>	HH13	275-345	E	(phenyl-methyl-ketone), absolute
<b>C<sub>8</sub>H<sub>9</sub>NO</b>	UH&95b	275-330	E	benzyl carbamate; absolute; modelling polyurethanes
C <sub>8</sub> H <sub>9</sub> NO	TC&16	283-295	P,T	acetanilide; TIY; TD-LB94/6-31+G(d,p); comp to cis-Nbenzylacetamide
<b>C<sub>8</sub>H<sub>9</sub>NO<sub>2</sub></b>	GH01 GC&04	280-320 280-320	E E	phenylalanine, comp. of amino acids additivity test: phenylalanine ~ benzene + alanine
<b>C<sub>8</sub>H<sub>10</sub></b>	CA&95 GA95 GYA96 YA96	280-320 284-290 285 290-315	T T T T	polyenes, STEX, π/σ convergence delocalization in polyenes; comp. of H-(CH=CH) <sub>n</sub> -H, n=1-5 X-ray emission as f(conjugation); π-exciton effects; H(C <sub>2</sub> H <sub>2</sub> ) <sub>n</sub> H, n=1,10 STEX; shake-up spectra related to NEXAFS; H(C <sub>2</sub> H <sub>2</sub> ) <sub>n</sub> H, n=1-5
<b>C<sub>8</sub>H<sub>10</sub></b>	EH&98	275-325	E	o-xylene (Me-C <sub>6</sub> H <sub>4</sub> -Me); absolute; weak ring substitution effects
<b>C<sub>8</sub>H<sub>10</sub></b>	HE&98	284-388	E,T	m-xylene; absolute; subst. isomer effects on π* shape
<b>C<sub>8</sub>H<sub>10</sub></b>	EH&98	275-325	E	m-xylene (Me-C <sub>6</sub> H <sub>4</sub> -Me); absolute; weak ring substitution effects
<b>C<sub>8</sub>H<sub>10</sub></b>	HE&98	284-388	E,T	m-xylene; absolute; subst. isomer effects on π* shape
<b>C<sub>8</sub>H<sub>10</sub></b>	EH&98	275-325	E	p-xylene (Me-C <sub>6</sub> H <sub>4</sub> -Me); absolute; weak ring substitution effects
<b>C<sub>8</sub>H<sub>10</sub></b>	HE&98	284-388	E,T	m-xylene; absolute; subst. isomer effects on π* shape
<b>C<sub>8</sub>H<sub>10</sub></b>	KP&06	283-293	P, T	(ethylbenzene- C <sub>6</sub> H <sub>5</sub> -CH <sub>2</sub> CH <sub>3</sub> ); relative, hi-res; comp. of C <sub>6</sub> -ring molecules; DFT-TS accurate to 0.2 eV
C <sub>8</sub> H <sub>10</sub> O <sub>2</sub>	GW09	288-296	T	1-phenyl, ethanoic acid, DFT, comp of C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub> , C <sub>6</sub> H <sub>6</sub> , C <sub>8</sub> H <sub>10</sub> O <sub>2</sub> , C <sub>8</sub> H <sub>11</sub> N, C <sub>9</sub> H <sub>11</sub> NO <sub>2</sub>
<b>C<sub>8</sub>H<sub>11</sub>N</b>	HUR93	275-330	E	N,N-dimethylaniline, absolute
C <sub>8</sub> H <sub>11</sub> N	GW09	288-296	T	phenylethylamine, DFT, comp of C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub> , C <sub>6</sub> H <sub>6</sub> , C <sub>8</sub> H <sub>10</sub> O <sub>2</sub> , C <sub>8</sub> H <sub>11</sub> N, C <sub>9</sub> H <sub>11</sub> NO <sub>2</sub>
<b>C<sub>8</sub>H<sub>12</sub></b>	WH&90 H92b	280-320 280-320	E E,R	CH <sub>3</sub> -norbornene; absolute; comp. of NB, 2-CH <sub>3</sub> -NB & 2-CF <sub>3</sub> -NB comp. of NB, 2-Me-NB, 2-CF <sub>3</sub> -NB; core vs. valence
C <sub>8</sub> H <sub>12</sub> O <sub>3</sub> Si	TC&02	280-320	E	(CH <sub>2</sub> =CH)Si(OAc) <sub>3</sub> ; absolute; vinyl silanes
<b>C<sub>8</sub>H<sub>12</sub>S</b>	HT&90	275-325	E	3-butyl thiophene; absolute; no mod. of π* (cf. polymer cond.)
<b>C<sub>8</sub>H<sub>12</sub>Si</b>	HS90	280-345	E	HC/C-CH <sub>2</sub> -C/CSi(CH <sub>3</sub> ) <sub>3</sub> ; absolute; comp. of X:::X species
<b>C<sub>8</sub>H<sub>14</sub></b>	EL&98	280-320	E	cis-tetramethylcyclobutene; comp of cis, trans, dimethylcyclobutene
<b>C<sub>8</sub>H<sub>14</sub></b>	EL&98	280-320	E	trans-tetramethylcyclobutene; comp of cis, trans, dimethylcyclobutene
C <sub>8</sub> H <sub>16</sub> O	UHR92	280-330	E	di(sec-butyl)ether; absolute; modelling of polyurethane PEELS
C <sub>8</sub> H <sub>18</sub>	SK&22c	290-315	T	octane (1 of 22,155 molecules calculated); CASTEP, HF
<b>C<sub>8</sub>H<sub>18</sub>O<sub>2</sub></b>	IM&87	275-325	E	(bis-(t-Bu)peroxide) low-lying σ*(O-O)
C <sub>8</sub> H <sub>18</sub> O <sub>3</sub> Si	TC&02	280-320	E	(CH <sub>2</sub> =CH)Si(OEt) <sub>3</sub> ; absolute
C <sub>8</sub> H <sub>24</sub> N <sub>4</sub> Si	UH94b	280-330	E	Si(NMe <sub>2</sub> ) <sub>4</sub> ; comp. of Si-N cmpds; models for SiN <sub>x</sub> O <sub>y</sub> films
<b>C<sub>8</sub>H<sub>24</sub>O<sub>4</sub>Si<sub>4</sub></b>	UH94a	280-330	E	c-(SiMe <sub>2</sub> O) <sub>4</sub> ; comp of Si-O-X species; inductive, resonance effects
C <sub>9</sub> CrH <sub>6</sub> O <sub>3</sub>	W92	280-330	E	BzCr(CO) <sub>3</sub> , absolute; comp to CrBz <sub>2</sub>
	WHR92	280-330	E	BzCr(CO) <sub>3</sub> , absolute; comp to CrBz <sub>2</sub>
<b>C<sub>9</sub>FeH<sub>8</sub>O<sub>3</sub></b>	WRH92	280-330	E	CxFe(CO) <sub>3</sub> ; comp. of Fe(CO) <sub>5</sub> , RFe(CO) <sub>3</sub> , Fe(Cp) <sub>2</sub> ; mix. lig. effect
C <sub>9</sub> Fe <sub>2</sub> O <sub>9</sub>	MSN89	270-520	P	total, partial ion yields; comp to Fe(CO) <sub>5</sub> ; EXAFS?
	WRH92	280-330	E	absolute, comp. with Fe(CO) <sub>5</sub> , RFe(CO) <sub>3</sub> , Fe(Cp) <sub>2</sub> ; mix. lig. effect
<b>C<sub>9</sub>H<sub>5</sub>O<sub>4</sub>V</b>	WHR92	280-320	E	cyclopentadienyl vanadium tetracarbonyl
<b>C<sub>9</sub>H<sub>6</sub>N<sub>2</sub>O<sub>2</sub></b>	UHR99	280-320	E,T	2,4-TDI, absolute; isomeric effect
<b>C<sub>9</sub>H<sub>6</sub>N<sub>2</sub>O<sub>2</sub></b>	UHR99	280-320	E,T	2,6-TDI, absolute; isomeric effect
<b>C<sub>9</sub>H<sub>7</sub>MnO<sub>3</sub></b>	W92	280-330	E	Me-CpMn(CO) <sub>3</sub> , absolute
<b>C<sub>9</sub>H<sub>8</sub>O<sub>2</sub></b>	LUH97	280-320	E	vinyl benzoate; absolute; model for PET X-ray damage
C <sub>9</sub> H <sub>9</sub> N	ZC&09	283-305	P	(3-methyl indone); tautomers, comp aromatic amino acids

<b>C<sub>9</sub>H<sub>10</sub>O<sub>2</sub></b>	HUR92	275-340	E	Ethylbenzoate; absolute; comp. to PET polymer EELS; EHMO
	RY&92	280-320	E	comp. of small mol. analogs with PET polymer
	H00	282-294	E,T,R	delocalization effects on spectra; GSCF3 calculations
C <sub>9</sub> H <sub>11</sub> NO	TC&16	283-295	P,T	cis-N-benzylacetamide ; TIY; TD-LB94/6-31+G(d,p); comp to acetanilide
C <sub>9</sub> H <sub>11</sub> NO <sub>5</sub> P	LC&25	294-291	P,T	protonated phosphotyrosine, NEXAMS, TIY, PIY; conformer calc
C <sub>9</sub> H <sub>12</sub> NO	LKC16	285-290	P, T	TEMPO, relative, ΔDFT-GGA, complex spectra
<b>C<sub>9</sub>H<sub>11</sub>NO<sub>2</sub></b>	CG&04	282-304	E	(phenylalanine), comp. of alanine, benzene, phenylalanine – additivity
	GW09	288-296	T	DFT, comp of C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub> , C <sub>6</sub> H <sub>6</sub> , C <sub>8</sub> H <sub>10</sub> O <sub>2</sub> , C <sub>8</sub> H <sub>11</sub> N, C <sub>9</sub> H <sub>11</sub> NO <sub>2</sub>
	ZC&09	283-305	P	tautomers, comp aromatic amino acids
<b>C<sub>9</sub>H<sub>11</sub>NO<sub>2</sub></b>	UH&95b	280-330	E	Ph-NH-CO <sub>2</sub> Et, absolute; modelling of polyurethane PEELS
C <sub>9</sub> H <sub>11</sub> NO <sub>3</sub>	ZC&09	283-305	P	(tyrosine) tautomers, comp aromatic amino acids
C <sub>9</sub> H <sub>27</sub> NSi <sub>3</sub>	UH94b	280-330	E	N(SiMe <sub>3</sub> ) <sub>3</sub> ; comp. of Si-N cmpds; models for SiN <sub>x</sub> O <sub>y</sub> films
C <sub>10</sub> ClCo <sub>3</sub> O <sub>9</sub>	HM&93	280-330	E,P,T	Cl-C-[Co(CO) <sub>3</sub> ] <sub>3</sub> , abs.; gas(E,P-ions), sol(P); PIPICO, TOF-MS
C <sub>10</sub> Cl <sub>2</sub> H <sub>10</sub> Ti	WH93	280-335	E	Cp <sub>2</sub> TiCl <sub>2</sub> , abs. comp. of Cp <sub>x</sub> TiCl <sub>4-x</sub> , x=0-2; diff '10Dq' at each edge
C <sub>10</sub> Cl <sub>2</sub> H <sub>10</sub> V	WRH89	274-340	E	Cp <sub>2</sub> TiCl <sub>2</sub> , absolute
C <sub>10</sub> CoH <sub>10</sub>	HR89	280-320	E	cobaltocene, absolute, strong C1s6e <sub>1g</sub> (M3d)
	RH89b	275-325	E	comp. of Fe, Co, Ni metallocenes
	H92b	281-307	E,R	absolute, comp. of CpCo(CO) <sub>2</sub> , Co <sub>2</sub> (CO) <sub>8</sub> and Co(Cp) <sub>2</sub>
C <sub>10</sub> CrH <sub>8</sub> O <sub>3</sub>	WRH89	280-330	E	toluene-Cr(CO) <sub>3</sub> , comp. to Bz <sub>2</sub> Cr
C <sub>10</sub> CrH <sub>10</sub>	HWR89	275-325	E	chromocene, comp. of V, Cr, Mn
C <sub>10</sub> F <sub>4</sub> H <sub>8</sub>	UH96	280-320	E	dimethyl-tetrafluoro-benzocyclobutane; model for dielectric polymer
C <sub>10</sub> F <sub>16</sub>	HI88a	275-335	E	per-fluoro-adamantine, strong σ*(C-F)
C <sub>10</sub> F <sub>8</sub>	RI&88	275-325	E	per-fluoro-naphthalene, low-lying σ*(C-F), perfluoro-effect
	LAL91	280-300	T	CNDO, pred. of π* and σ* energies
C <sub>10</sub> F <sub>22</sub>	AC&95	290-315	T	STEX ab initio; absolute; growth of poly-(CF <sub>2</sub> ) <sub>n</sub> by C <sub>2n</sub> F <sub>4n+2</sub> , n=1-5
<b>C<sub>10</sub>FeH<sub>10</sub></b>	HR89	280-320	E	ferrocene, absolute, strong C1s6e <sub>1g</sub> (M3d)
	RH89b	275-325	E	comp. of Fe, Co, Ni
	H90a	275-322	E,R	absolute, comp. of Fe,Co,Ni metallocenes versus Cp-H
	RH&93b	282-312	P	absolute, comp of TEY, TIY, PIPICO yields; TOF-MS
	WRH92	280-330	E	absolute, comp. of organo-iron complexes, ligand interaction effects
C <sub>10</sub> GeH <sub>20</sub> N <sub>2</sub>	LU&99	282-309	E,T	c-Ge(RNCH=CHNR), R=tBu, comp. cyclic diamino C:, Si:, Ge: ; GSCF3
C <sub>10</sub> GeH <sub>22</sub> N <sub>2</sub>	LU&99	282-309	E,T	c-Ge(RNCH <sub>2</sub> CH <sub>2</sub> NR), R=tBu, comp. cyclic diamino C:, Si:, Ge: ; GSCF3
C <sub>10</sub> GeH <sub>22</sub> N <sub>2</sub>	LU&99	282-309	E,T	c-H <sub>2</sub> Ge(RNCH=CHNR), R=tBu, comp. cyclic diamino C: Si: Ge: ; GSCF3
C <sub>10</sub> GeH <sub>24</sub> N <sub>2</sub>	LU&99	282-309	E,T	c-H <sub>2</sub> Ge(RNCH <sub>2</sub> CH <sub>2</sub> NR), R=tBu, comp. cyclic diamino C: Si: Ge: GSCF3
<b>C<sub>10</sub>H<sub>8</sub></b>	RI&88	275-325	E,T	naphthalene, five π* res., HAM/3 calc., comp. to per-F-nap.
	HT&89	275-325	E,T	comp. to azulene; comp to polymer
	AVC95	280-314	T	absolute; ΔSCF with Steltjes cont.; comp. of aromatics; comp. to RI&88
	SB&02	278-320	E	variable angle; dipole forbidden transition identified
	GT&03a	280-320	E, T	absolute; GSCF3; comp. to X-ray Raman spectra
	FM&04	280-320	P,T	50 meV, v <sub>C-C</sub> vibrational progressions in π*; comp. to hi-res XPS
	MG&04	284-298	P, T	high res. 50 meV; vibrations, chem.. shifts, comp. to PES
<b>C<sub>10</sub>H<sub>8</sub></b>	HT&89	275-325	E,T	azulene, comp. to naphthalene; comp to polymer
	LAL91	285-305	T	CNDO, systematic calc. of σ* energies; ISEELS, ETS for param. det.
<b>C<sub>10</sub>H<sub>10</sub>Mg</b>	WRH89	274-340	E	Cp <sub>2</sub> Mn, absolute
<b>C<sub>10</sub>H<sub>10</sub>Mn</b>	HWR89	275-325	E	manganocene, comp. of V, Cr, Mn
	H90a	275-322	E,R	absolute, comp. of Fe,Co,Ni metallocenes versus Cp-H
	S92	280-320	E,R	comp. to free CO and CO/Mo; σ*(CO) shift
<b>C<sub>10</sub>H<sub>10</sub>Ni</b>	HR89	280-320	E	absolute, strong C1s6e <sub>1g</sub> (M3d)
	RH89b	275-325	E	nickelocene, comp. of Fe, Co, Ni
	H90a	275-322	E,R	absolute, comp. of Fe,Co,Ni metallocenes versus Cp-H
	RH&93b	282-312	P	absolute, comp of TEY, TIY, PIPICO yields; TOF-MS

<b>C<sub>10</sub>H<sub>10</sub>O<sub>4</sub></b>	UH&96	280-296	E,T	p-dimethylphthalate (MeO <sub>2</sub> C-C <sub>6</sub> H <sub>4</sub> -CO <sub>2</sub> Me); ab initio; isomer effects in o-, m-, p-phthalates; comp. to polymer
	RH&97	275-325	E,P,T	absolute; comp. to solid; NEXAFS, PEELS, STXM of PET; radiation damage quantified
	UH&97	280-310	E,T	absolute; ab initio; comp. to oligimer NEXAFS
	HE&98	284-288	E,T	GSCF3; comp. to polymer
	H00	282-294	E,T,R	delocalization effects on spectra; GSCF3 calculations
<b>C<sub>10</sub>H<sub>10</sub>O<sub>4</sub></b>	UH&96	280-296	E,T	o-dimethylphthalate (MeO <sub>2</sub> C-C <sub>6</sub> H <sub>4</sub> -CO <sub>2</sub> Me); ab initio; isomer effects in o-, m-, p-phthalates; comp. to polymer
	UH&97	280-310	E,T	absolute; ab initio; comp. to oligimer NEXAFS
<b>C<sub>10</sub>H<sub>10</sub>O<sub>4</sub></b>	UH&96	280-296	E,T	m-dimethylphthalate (MeO <sub>2</sub> C-C <sub>6</sub> H <sub>4</sub> -CO <sub>2</sub> Me); ab initio; isomer effects in o-, m-, p-phthalates; comp. to polymer
	UH&97	280-310	E,T	absolute; ab initio; comp. to oligimer NEXAFS
<b>C<sub>10</sub>H<sub>10</sub>V</b>	HWR89	275-325	E	vanadocene, comp. of V, Cr, Mn
<b>C<sub>10</sub>H<sub>11</sub>N<sub>2</sub>O<sub>2</sub></b>	LKC16	285-290	P, T	nit8, TEMPO, relative, ΔDFT-GGA, complex spectra
<b>C<sub>10</sub>H<sub>12</sub></b>	CA&95	280-320	T	polyenes, STEX, $\pi/\sigma$ convergence
	GA95	284-290	T	delocalization in polyenes; comp. of H-(CH=CH) <sub>n</sub> -H, n=1-5
	GYA96	285	T	X-ray emission as f(conjugation); $\pi$ -exciton effects; H(C <sub>2</sub> H <sub>2</sub> ) <sub>n</sub> H, n=1,10
	YA96	290-315	T	STEX; shake-up spectra related to NEXAFS; H(C <sub>2</sub> H <sub>2</sub> ) <sub>n</sub> H, n=1-5
<b>C<sub>10</sub>H<sub>12</sub></b>	RWH91	280-320	E	(CpH) <sub>2</sub> (Diels-alder dimer); comp. of CpH, di-CpH, C <sub>5</sub> H <sub>8</sub> ; Cp <sup>-</sup> ( $\pi^*$ )
<b>C<sub>10</sub>H<sub>12</sub>N</b>	UH98	280-320	E	1234-tetrahydro-1-naphthyl-amine, absolute
<b>C<sub>10</sub>H<sub>13</sub>O</b>	OJ&16	283-290	P,T	S+-carvone, TIY, optical fluorescence, TDDFT, chiral signal not seen
<b>C<sub>10</sub>H<sub>13</sub>NO<sub>2</sub></b>	UH&95b	280-330	E	Ph-N(CH <sub>3</sub> ) <sub>2</sub> -CO <sub>2</sub> Et, absolute; modelling of polyurethane PEELS
<b>C<sub>10</sub>H<sub>13</sub>N<sub>2</sub>O<sub>2</sub></b>	LKC16	285-290	P, T	nit9, TEMPO, relative, ΔDFT-GGA, complex spectra
<b>C<sub>10</sub>H<sub>14</sub>O</b>	OJ&16	283-290	P,T	R(+)-limonene, TIY, optical fluorescence, TDDFT, chiral signal not seen
<b>C<sub>10</sub>H<sub>16</sub></b>	HI88a	275-325	E	adamantane, (tri-cyclo 3,3,1 <sup>3,7</sup> )-decane
<b>C<sub>10</sub>H<sub>16</sub>MnO<sub>4</sub><sup>+</sup></b>	AG&23	275-325	P	Mn(acac) <sub>2</sub> ; RASPT2 calc., compare m =1,2,3
<b>C<sub>10</sub>H<sub>16</sub>O</b>	OJ&16	283-290	P,T	(-) -fenchone, TIY, optical fluorescence, TDDFT, chiral signal not seen
<b>C<sub>10</sub>H<sub>17</sub></b>	OJ&16	283-290	P,T	(-) -a-pinene, TIY, optical fluorescence, TDDFT, chiral signal not seen
<b>C<sub>10</sub>H<sub>17</sub>S</b>	HT&90	275-325	E	3-hexyl-thiophene; absolute; no mod. of $\pi^*$ (cf. polymer cond.)
<b>C<sub>10</sub>H<sub>19</sub>O<sub>4</sub></b>	LC&07	280-320	E,T	'BuO(CO)NH(CO)O'Bu; di-carbonyls; charge shifts, GSCF3
<b>C<sub>10</sub>H<sub>20</sub>N<sub>2</sub></b>	LU&99	282-309	E	tBu-NC=CN-tBu; absolute; model for ring of cyclic diamino C:,Si:,Ge:
	HE&01	280-305	E	reference for thermal decomposition of tetra-amino ethylene
<b>C<sub>10</sub>H<sub>20</sub>N<sub>2</sub>Si</b>	UH&98	283-302	E,T	c-Si(RNCH=CHNR), R=tBu, silylene; absolute; delocal. in Si-N-C=C
	LU&99	280-305	E,T	absolute; comparison of cyclic diamino C:, Si:, Ge: ; GSCF3 ab initio
<b>C<sub>10</sub>H<sub>22</sub>N<sub>2</sub></b>	LU&99	280-305	E	tBu-NCH <sub>2</sub> CH <sub>2</sub> N-tBu; absolute; ligand rel. to cyclic diamino C:,Si:,Ge.
<b>C<sub>10</sub>H<sub>22</sub>N<sub>4</sub></b>	HE&01	280-305	E	tetra-amino ethylene; used for thermal decomposition to form carbene
<b>C<sub>10</sub>H<sub>22</sub>N<sub>2</sub>Si</b>	UH&98	283-302	E,T	c-Si(RNCH <sub>2</sub> CH <sub>2</sub> NR), R=tBu, unsat. silylene; absolute;
	LU&99	280-305	E,T	absolute; comparison of cyclic diamino C:, Si:, Ge: ; GSCF3 ab initio
<b>C<sub>10</sub>H<sub>22</sub>N<sub>2</sub>Si</b>	UH&98	283-302	E,T	c-H <sub>2</sub> Si(RNCH=CHNR), R=tBu, silylene; absolute; no delocal.
	LU&99	280-305	E,T	absolute; comparison of cyclic diamino C:, Si:, Ge: ; GSCF3 ab initio
<b>C<sub>10</sub>H<sub>24</sub>N<sub>2</sub>Si</b>	UH&98	283-302	E,T	c-H <sub>2</sub> Si(RNCH <sub>2</sub> CH <sub>2</sub> NR), R=tBu, unsat. silylene; absolute;
	LU&99	280-305	E,T	absolute; comparison of cyclic diamino C:, Si:, Ge: ; GSCF3 ab initio
<b>C<sub>10</sub>H<sub>22</sub>O</b>	HI88a	275-325	E	decyl alcohol
<b>C<sub>10</sub>Mn<sub>2</sub>O<sub>10</sub></b>	HR89	280-320	E	absolute, $\pi^*$ intensity as measure of d $\pi$ -p $\pi$ backbonding
	RH89a	275-330	E	Mn <sub>2</sub> (CO) <sub>10</sub> , comp. CO, other M(CO)s; E(ref); f( $\pi^*$ ) $\alpha$ backbond
<b>C<sub>11</sub>Co<sub>3</sub>H<sub>3</sub>O<sub>10</sub></b>	HM&93	280-330	E,P	CH <sub>3</sub> O-C-[Co(CO) <sub>3</sub> ] <sub>3</sub> ; abs.; comp. of gas (E), sol (P-TEY)
<b>C<sub>11</sub>FeH<sub>8</sub>O<sub>3</sub></b>	WRH92	280-330	E	COT-Fe(CO) <sub>3</sub> ; comp. of Fe(CO) <sub>5</sub> , RFe(CO) <sub>3</sub> , Fe(Cp) <sub>2</sub> ; mix. lig. effect
<b>C<sub>11</sub>H<sub>12</sub>N<sub>2</sub>O<sub>2</sub></b>	ZC&09	283-305	P	(tryptophan) tautomers, comp aromatic amino acids
<b>C<sub>11</sub>H<sub>14</sub>N<sub>2</sub>O<sub>4</sub></b>	UHR99	280-320	E	TDI-bis-methyl urethane; absolute
<b>C<sub>11</sub>H<sub>20</sub>N<sub>2</sub></b>	LU&99	282-309	E,T	c-C:(RNCH=CHNR), R=tBu, carbene; absolute;
<b>C<sub>11</sub>H<sub>22</sub>N<sub>2</sub></b>	LU&99	282-309	E,T	c-C:(RNCH <sub>2</sub> CH <sub>2</sub> NR), R=tBu, absolute;

C <sub>11</sub> H <sub>24</sub> N <sub>2</sub>	LU&99	282-309	E,T	c-H <sub>2</sub> C:(RNCH <sub>2</sub> CH <sub>2</sub> NR), R=tBu, hydrogenated carbene (ref.)
C <sub>12</sub> CrH <sub>12</sub>	W92	280-330	E	CrBz <sub>2</sub> ; absolute; comp to BzCr(CO) <sub>3</sub>
	WRH92	275-330	E	CrBz <sub>2</sub> ; comp. to benzene
C <sub>12</sub> FeH <sub>12</sub>	WRH92	280-330	E	CH <sub>2</sub> =CH-CpFeCp; comp. of organo-irons; ligand interaction effects
C <sub>12</sub> Fe <sub>3</sub> O <sub>12</sub>	EC&84	280-340	P	Fe <sub>3</sub> (CO) <sub>12</sub> , ion & electron yield, comp. to free CO, CO/Cu, Cr(CO) <sub>6</sub>
C <sub>12</sub> F <sub>10</sub>	WC&05	284-308	E,T	biphenyl, absolute, GSCF <sub>3</sub> , ring-ring-interactions (comp to o,o-dibromo)
C <sub>12</sub> H <sub>8</sub> S	TG&18	284-291	P,T	dibenzothiophene, TIY; DFT calc, compare C <sub>4</sub> H <sub>4</sub> S, C <sub>8</sub> H <sub>6</sub> S, C <sub>8</sub> H <sub>6</sub> S (Srings)
C <sub>12</sub> H <sub>10</sub>	WC&05	284-308	E,T	biphenyl, absolute, GSCF <sub>3</sub> , ring-ring-interactions (comp to o,o-dibromo), compared to hexa-phenylbenzene (s)
	FM&04	280-320	P,T	50 meV, v <sub>C-C</sub> vibrational progressions in π*; comp. to hi-res XPS; no dihedral modes (weakening ring-ring delocalization does not excite torsion) dibenzothiophene (DBT); OLED, XPS
C <sub>12</sub> H <sub>18</sub> PO	GZ&20	284-292	P,T	(BzO) <sub>2</sub> CO (phenyl carbonate); absolute; comp. to polymer EELS
C <sub>12</sub> H <sub>10</sub> O <sub>3</sub>	HUR92	275-340	E	X-ray emission as f(conjugation); π-exciton effects; H(C <sub>2</sub> H <sub>2</sub> ) <sub>n</sub> H, n=1,10
C <sub>12</sub> H <sub>14</sub>	GYA96	285	T	Cπ*ReN <sub>2</sub> O <sub>2</sub> , abs.; mixed ligand; chem. shift of N <sub>a</sub> -N <sub>b</sub>
C <sub>12</sub> H <sub>15</sub> N <sub>2</sub> O <sub>2</sub> Re	HS92	280-330	E	diphenylether, TIY, TD-DFT (Q-CHEM 4.1)
C <sub>12</sub> H <sub>18</sub> O	LL&14b	284-299	P,T	3-octyl-thiophene; absolute, no mod. of π* (cf. polymer cond.)
C <sub>12</sub> H <sub>21</sub> S	HT&90	275-325	E	absolute; comp. of Si(CH <sub>3</sub> ) <sub>4</sub> , Si <sub>2</sub> (CH <sub>3</sub> ) <sub>6</sub> and Si <sub>6</sub> (CH <sub>3</sub> ) <sub>12</sub> ; σ*(Si-Si)
C <sub>12</sub> H <sub>36</sub> Si <sub>5</sub>	W92	280-320	E	absolute; comp. of edges of Si-Si compounds
	UX&94	280-330	E	c-(SiMe <sub>2</sub> ) <sub>6</sub> ; comp. of edges of Si-Si compounds
C <sub>12</sub> H <sub>36</sub> Si <sub>6</sub>	UX&94	280-330	E	relative, electron yield, multiple π* res.; relaxation
C <sub>12</sub> O <sub>12</sub> Ru <sub>3</sub>	SF&90	275-325	P	(C <sub>6</sub> H <sub>5</sub> O) <sub>2</sub> C=O; absolute; comp. to methyl carbonate
C <sub>13</sub> H <sub>10</sub> O <sub>3</sub>	HW&91	280-340	E	(diphenoxymethanone), comp of di-carbonyls, GSCF <sub>3</sub>
C <sub>13</sub> H <sub>10</sub> O <sub>3</sub>	LC&07	280-320	E, T	(Ph-NH) <sub>2</sub> C=O, absolute; modelling of polyurethane PEELS
C <sub>13</sub> H <sub>12</sub> N <sub>2</sub> O	UH&95b	280-330	E	Ph-CH <sub>2</sub> -Ph; absolute; modelling of polyurethane PEELS
C <sub>13</sub> H <sub>12</sub>	UH&93	280-330	E	Cπ*Mn(CO) <sub>3</sub> ; absolute
C <sub>13</sub> H <sub>15</sub> MnO <sub>3</sub>	WRH89	275-325	E	Bu-cpFeCp; organo-iron complexes, ligand interaction effects
C <sub>14</sub> FeH <sub>18</sub>	WRH92	280-330	E	anthracene; absolute; ΔSCF with Stieljes cont.; comp. of aromatics
C <sub>14</sub> H <sub>10</sub>	AVC95	280-314	T	absolute; GSCF <sub>3</sub> ; comp. to X-ray Raman spectra
	GT&03a	280-320	E, T	phenanthrene; absolute; GSCF <sub>3</sub> ; comp. to X-ray Raman spectra
C <sub>14</sub> H <sub>10</sub>	GT&03a	280-320	E, T	vibrational-resolved NEXAFS
C <sub>14</sub> H <sub>12</sub>	FB&03	283-291	P,T	cis-stilbene, relative, TIY, StoBe DFT, 7 1s→1π* transitions, 2 peak, compared to cis-stilbene on Si(100)
C <sub>14</sub> H <sub>12</sub>	PS&17	283-289	P,T	trans-stilbene, relative, TIY, StoBe DFT, 7 1s→1π* transitions, 1 peak compared to cis-stilbene on Si(100)
C <sub>14</sub> H <sub>10</sub> O <sub>3</sub>	LUH97	280-320	E	benzoic anhydride; absolute; polymer model
C <sub>14</sub> H <sub>25</sub> S	HT&90	275-325	E	3-decyl-thiophene, absolute, comp. of 3-alkyl-thiophenes; no change of π* (polymer cond.)
C <sub>15</sub> H <sub>24</sub> O	LUH97	280-320	E	butylated hydroxy toluene; absolute; polymer model
C <sub>15</sub> H <sub>24</sub> MnO <sub>6</sub> <sup>+</sup>	AG&23	528-540	P	Mn(acac) <sub>3</sub> ; RASPT2 calc., compare m=1,2,3
C <sub>16</sub> H <sub>10</sub>	AVC95	280-314	T	tetracene; absolute; ΔSCF with Stieljes cont.; comp. of aromatics
C <sub>16</sub> H <sub>18</sub>	GYA96	285	T	X-ray emission as f(conjugation); π-exciton effects; H(C <sub>2</sub> H <sub>2</sub> ) <sub>n</sub> H, n=1,10
C <sub>16</sub> H <sub>19</sub> N <sub>4</sub> O <sub>2</sub>	XX04	280-320	E	toluene ethyl urea, absolute
C <sub>18</sub> H <sub>12</sub>	AVC95	280-314	T	pyrene; absolute; ΔSCF with Stieljes cont.; comp. of aromatics
	GT&03a	280-320	E	absolute; comp. to X-ray Raman spectra
C <sub>18</sub> H <sub>12</sub>	GT&03a	280-320	E, T	triphenylene. absolute; GSCF <sub>3</sub> ; comp. to X-ray Raman spectra
C <sub>18</sub> H <sub>12</sub>	GT&03a	280-320	E, T	1,2-benzanthracene. absolute; GSCF <sub>3</sub> ; comp. to X-ray Raman spectra
C <sub>18</sub> H <sub>12</sub>	OM&96	280-294	P,T	chrysene; GSCF <sub>3</sub> calc. of DOUS and excitation; comp. to solid, pol. dep. (π* most intense at normal incidence); large core-hole effect
	OM&98	280-310	T	GSCF <sub>3</sub> ; DOUS mod. by core hole; comp. of chrysene, perylene, coronene
C <sub>18</sub> H <sub>14</sub> O <sub>2</sub>	LL&14B	284-301	P,T	1,3-diphenoxylbenzene, TIY, TD-DFT (Q-CHEM-4.1)
C <sub>18</sub> H <sub>15</sub> PO	GZ&20	284-295	P,T	triphenylphosphine (TP); OLED, XPS

<b>C<sub>18</sub>H<sub>16</sub>OSi</b>	UT&97	280-320	E	triphenylsilanol; absolute; Si-Si, Si-O-R systems
C <sub>19</sub> H <sub>22</sub> O <sub>3</sub>	AP&20	287-295	P	avobenzone, PEPICO, fragmentation, PES-derived
C <sub>20</sub> H <sub>12</sub>	OM&96	280-294	P,T	perylene; GSCF3 calc. of DOUS and excitation; comp. to solid, pol. dep. ( $\pi^*$ most intense at normal incidence); large core-hole effect
	OM&98	280-310	T	GSCF3; DOUS modified by core hole effect; compared to condensed ring systems: chrysene, perylene, coronene
C <sub>20</sub> H <sub>22</sub>	GA95	284-290	T	delocalization in polyenes; comp. to H-(CH=CH) <sub>n</sub> -H, n=1-5
	GYA96	285	T	X-ray emission as f(conjugation); $\pi$ -exciton effects; H(C <sub>2</sub> H <sub>2</sub> ) <sub>n</sub> H, n=1,10
<b>C<sub>21</sub>H<sub>15</sub>N<sub>3</sub>O<sub>3</sub></b>	UHR92	275-325	E	(Bz-O) <sub>3</sub> C <sub>3</sub> N <sub>3</sub> (tri-phenoxy-triazine); polyurethane modelling
	UA&99	280-320	E	tritylilisocyanurate; absolute, polymer model
C <sub>24</sub> H <sub>12</sub>	OM&96	280-294	P,T	coronene; GSCF3 calc. of DOUS and excitation; comp. to solid, pol. dep. ( $\pi^*$ most intense at normal incidence); large core-hole effect
	OM&98	280-310	T	GSCF3; DOUS mod. by core hole; comp.of chrysene, perylene, coronene
	FB&03	283-291	P,T	vibrational-resolved NEXAFS
	RB&14	283-305	P,T	TIY, PIY, NEXAMS
	RB&15	283-305	P,T	TIY, PIY, NEXAMS, H-loss dominates over H <sub>2</sub> -loss at high T-int
<b>C<sub>24</sub>H<sub>21</sub>N<sub>3</sub>O<sub>3</sub></b>	UA&99	280-320	E	tritylilisocyanurate; absolute, polymer model
C <sub>26</sub> H <sub>36</sub> N <sub>3</sub> O <sub>7</sub>	GR&12	282-290	P	leucine enkephaline ([YGGFL+H] <sup>+</sup> , 5-AA peptide, NEXAMS
C <sub>27</sub> H <sub>35</sub> N <sub>5</sub> O <sub>7</sub> S	DS&21	284-296	P,T	[LeuEnk+H], ENK-Tyr-Gly-Gly-Phe); NEXAFS mass spec; DFT/ROCIS
C <sub>27</sub> H <sub>35</sub> N <sub>5</sub> O <sub>7</sub> S	ES&16	284-296	P,T	[LeuEnk+H], compared to 7 other proteins; NEXAMS, size effect
C <sub>28</sub> H <sub>37</sub> N <sub>5</sub> O	DS&21	284-296	P,T	MetEnk+H], ENK = Tyr-Gly-Gly-Phe); NEXAFS mass spec; DFT/ROCIS
<b>C<sub>29</sub>H<sub>20</sub>O</b>	LUH99	280-320	E,T	tetraphenyl-cyclopentadienone; low-lying $\pi^*$
<b>C<sub>30</sub>H<sub>30</sub>Si<sub>2</sub></b>	UT&97	282-303	P	Ph <sub>3</sub> Si-SiPh <sub>3</sub> ; absolute; reference for Ph <sub>3</sub> Si-X, Me <sub>3</sub> Si-X
C <sub>32</sub> H <sub>16</sub> N <sub>8</sub>	RSH93	280-316	E	phythalocyanine; compared to solid
C <sub>32</sub> H <sub>16</sub> N <sub>8</sub> Fe	RSH93	280-316	E	Fe-phythalocyanine; compared to solid
C <sub>32</sub> H <sub>16</sub> N <sub>8</sub> Ni	RSH93	50-450	E	Ni-phythalocyanine; compared to solid
C <sub>32</sub> H <sub>16</sub> N <sub>8</sub> Zn	RSH93	280-316	E	Zn-phythalocyanine; compared to solid
C <sub>32</sub> H <sub>28</sub> P <sub>2</sub> O <sub>2</sub>	GZ&20	284-292	P,T	2,8-bis- (diphenylphosphoryl)-dibenzo[b,d]thiophene (PPT); OLED, XPS
C <sub>42</sub> H <sub>52</sub> FeN <sub>8</sub> O <sub>6</sub> S <sub>2</sub>	MC12	283-305	P	cytochrome c (12 kDa), NEXAMS
	MG&16	280-302	P	NEXAMS
C <sub>131</sub> H <sub>229</sub> N <sub>39</sub> O <sub>31</sub> <sup>+</sup>	EB&18	283-305	P	Melittin protein, NEXAMS, PIY
	BE&18	280-300	P	Melittin protein, NEXAMS, PIY
C <sub>60</sub>	KB&93a	280-296	P	gas, solid essentially identical; intramolecular e- correl.; XPS, Auger
	KB&93b	280-296	P	gas comp. to EELS of solid; plasmon at 6 eV higher in gas
	JT94a	284-290	T	relative, $\pi^*$ transitions; minimal many-electron effects
	AN&95	280-313	P	TOF mass spec; partial ion yields; (C <sub>2</sub> ) <sub>n</sub> losses dominate
	LP&95	290-320	P	partial PI X-sect (main, sat.); $\beta$ s; $\beta < 2$ at 300 eV interpreted as SR
	BS96	290-320	P,R	absolute; cross-sections, $\beta$ 's compared to solid
	B97	270-320	P	total and partial ion yields; lumiescence; plasmasa resonance sought
	KN&97a	280-296	P	pulse, PEPICO TOF; discrete, cont. frag; plasmon res. ~20 eV > IP; PCI
C <sub>400</sub> N <sub>110</sub> O <sub>150</sub> S <sub>3</sub>	MN&15	282-302	P	ubiquitin protein (formula is approx); electrospray MS, and partial ion yield

#### Cesium 4d (85eV)

CsBr	WS76	70-180	P	photographic, gas-solid comp.
	KR&02a	76-86	P	partial electron yield from 2D (e-hv) maps, relative, gas jet
CsCl	RS74	78-92	P	photographic, gas-solid comp.
	RS76	70-180	P	photographic, gas-solid comp.
CsF	WS76	70-180	P	photographic, gas-solid comp.
CsI	R74	160-175	P	photographic

Chlorine 2p, 2s (205, 278 eV)

BCl <sub>3</sub>	FB70	190-210	P	pressure dependence
	II&80	190-280	P	absolute
	UC&94b	190-208	P	absolute, resonance Auger; spectator only; localised decay
BrCClH <sub>2</sub>	SR&94	195-225	P	TIY; PEPICO; PEPI3CO; selective fragment.; Br(CH <sub>2</sub> ) <sub>n</sub> Cl, n=1-3
	NM96	220	P,R	mass spectra; comp. of Br 3d/Cl2p for Br(CH <sub>2</sub> ) <sub>n</sub> Cl n=1-3
	MS&98a	219	P	Auger-ion coincidence; strong site selectivity from site specific Auger
	MS&98b	220	P	ES-AEPICO, PE, site-selective fragmentation & kinetics
BrC <sub>2</sub> ClH <sub>4</sub>	SR&94	195-225	P	TIY; PEPICO; PEPI3CO; selective fragment.; Br(CH <sub>2</sub> ) <sub>n</sub> Cl, n=1-3
	NM96	220	P,R	mass spectra; comp. of Br 3d/Cl2p for Br(CH <sub>2</sub> ) <sub>n</sub> Cl n=1-3
BrC <sub>3</sub> ClH <sub>6</sub>	SR&94	195-225	P	TIY; PEPICO; PEPI3CO; selective fragment.; Br(CH <sub>2</sub> ) <sub>n</sub> Cl, n=1-3
	NM96	220	P,R	mass spectra; comp. of Br 3d/Cl2p for Br(CH <sub>2</sub> ) <sub>n</sub> Cl n=1-3
CClF <sub>2</sub> H	CD78	120-270	P	absolute
CClF <sub>3</sub>	CD78	120-270	P	absolute
	ZIB92	190-290	E	absolute, high res. (70 meV), pot. bar., comp. of CCl <sub>x</sub> F <sub>4-x</sub> , x=1-4
	YL94	195-240	E	absolute GOS; comp. of CF <sub>4-n</sub> Cl <sub>n</sub> (n=0-4); σ*(C-Cl) GOS changes
	SS&95	190-280	P	PIPICO; start = selective ion gate; PIPICO yields; comp of Cl2p, C1s, F1s edges; only selective at Cl 2p edge
CClH <sub>3</sub>	SSB99	200-220	P	TIY, PIY; comp of CF <sub>x</sub> Cl <sub>4-x</sub> x=1-3; site selective fragmentation
	HB78a	190-290	E	revised assignment of Cl 1s spectrum of HG76
	HB78b	190-290	E	extended fine structure (EXAFS)
	CG&88	160-240	P	DES, resonant Auger, βs, spectator dominates
	TSH94	196-210	P	PEPICO, TEY, KERDs; ultrafast decay; supports scheme 2 of H78a
	CP&07	190-2800	P	relative; TIY, PIY +ve, -ve; state-selective frag.
CCl <sub>2</sub> F <sub>2</sub>	CD78	120-270	P	absolute
	S82b	200-208	P	laser plasma source, comp. to Cl-atom calc.s
	ZIB92	190-290	E	absolute, high res. (70 meV), pot. bar., comp. of CCl <sub>x</sub> F <sub>4-x</sub> , x=1-4
	BSS93b	50-1500	P	partial ion yields at coarse resolution
	SBS94a	185-285	P	partial ion yields; site-selective frag. at C 1s, Cl 2p, F 1s
	SSB94	185-285	P	partial ion-pair yields; site-selective frag.
	YL94	195-240	E	absolute GOS; comp. of CF <sub>4-n</sub> Cl <sub>n</sub> (n=0-4); σ*(C-Cl) GOS changes
	SSB99	200-220	P	TIY, PIY; comp of CF <sub>x</sub> Cl <sub>4-x</sub> x=1-3; site selective fragmentation
	H19	680-730	E	Freon152, absolute
CCl <sub>2</sub> F <sub>2</sub> H	CD78	120-270	P	absolute
CCl <sub>2</sub> F <sub>3</sub> P	HBC96	190-240	P	TIY, PIY, PEPICO; comp. of PCl <sub>3</sub> , PF <sub>3</sub> , CF <sub>3</sub> PCl <sub>2</sub>
	NJ&98	180-240	P,T	absolute; GSCF3 calc.; LS-state; comp of PX <sub>3</sub> , YPF <sub>3</sub> . X=Cl,F, Y=O,S)
CCl <sub>2</sub> H <sub>2</sub>	HB78b	190-290	E	extended fine structure (EXAFS)
	CG&88	160-240	P	DES, resonant Auger, βs, spectator dominates
CCl <sub>2</sub> O	HUR92	180-290	E	absolute, comp. to terphthaloylchloride; EHMO
CCl <sub>3</sub> F	CD78	120-270	P	absolute
	ZIB92	190-290	E	absolute, high res. (70 meV), pot. bar., comp. of CCl <sub>x</sub> F <sub>4-x</sub> , x=1-4
	YL94	195-240	E	absolute GOS; comp. of CF <sub>4-n</sub> Cl <sub>n</sub> (n=0-4); σ*(C-Cl) GOS changes
	SS97	198-225	P	PIPICO branching ratios; partial X-sect.; site-specific fragmentation
	SS98b	180-240	P	PIY, comp of C 1s, F1s, Cl 2p
	SSB99	200-220	P	TIY, PIY; comp of CF <sub>x</sub> Cl <sub>4-x</sub> x=1-3; site selective fragmentation
CCl <sub>3</sub> H	HB78b	190-290	E	extended fine structure (EXAFS)
	W80	220-290	E	extended fine structure (EXAFS)
	CG&88	160-240	P	DES, resonant Auger, βs, spectator dominates
CCl <sub>4</sub>	P34	180-300	P	photographic; <b>FIRST MOLECULAR CORE EXCITATION</b>

(CCl <sub>4</sub> .cont'd)	N71a	190-205	P	10eV below IP
	CD78	120-270	P	absolute
	HB78b	150-400	E	pot. bar. effects, extended fine structure (EXAFS)
	CKS80	178-207	P	photographic, laser bombardment X-ray light source
	W80	220-290	E	extended fine structure (EXAFS)
	S82b	200-208	P	laser plasma source, comp. to Cl-atom calc.s
	CG&88	160-240	P	DES, resonant Auger, $\beta$ s, spectator dominates
	ZIB92	190-290	E	absolute, high res. (70 meV), pot. bar., comp. of CCl <sub>x</sub> F <sub>4-x</sub> , x=1-4
	BC&94	0-400	E	absolute; comp. to atomic (25% too high); (e,e') = absorption; (e,e+ion)=PIMS; dipole breakdown scheme
	YL94	195-240	E	absolute GOS; comp. of CF <sub>4-n</sub> Cl <sub>n</sub> (n=0-4); $\sigma^*(C-Cl)$ GOS changes
	H98	6-250	P	absolute; OOS extrapolation to test TKR; Rydberg assignments
	FM&01	220	P	Auger-ion coincidence
	IP&12	197-210	P	TIY, Auger (220), and resonant Auger (198)
C <sub>2</sub> ClF <sub>5</sub>	CD78	120-270	P	absolute
C <sub>2</sub> ClH <sub>3</sub>	SBK88	190-260	E	v vinyl chloride, comp. other vinyl halides, strong cont. res. $\sigma^*(C=C)$ ?
C <sub>2</sub> ClH <sub>5</sub>	FL02	190-220	E	absolute, GOS profiles compared of C 1s, Cl 2p & valence
<b>C<sub>2</sub>ClF<sub>3</sub></b>	H14	180-280	E	trifluoro-chloroethylene, absolute
C <sub>2</sub> Cl <sub>2</sub> F <sub>4</sub>	CD78	120-270	P	absolute
C <sub>2</sub> Cl <sub>2</sub> H <sub>4</sub>	H92	120-270	P	dichloroethane; comp. to NEXAFS
C <sub>2</sub> Cl <sub>2</sub> H <sub>6</sub> Si	CL&05	190-230	P	SiMe <sub>2</sub> Cl <sub>2</sub> , luminescence yield, Si*, Si <sup>+</sup> , CH*, H*, excited diatomic
C <sub>2</sub> Cl <sub>3</sub> H	WH90	160-280	E	Cl <sub>2</sub> C=CClH
C <sub>2</sub> Cl <sub>3</sub> N	IO&99	190-280	P	absolute; selected E mass spec; no site-specific fragmentation
<b>C<sub>5</sub>Cl<sub>3</sub>H<sub>5</sub>Ti</b>	W92	196-250	E	CpTiCl <sub>3</sub> , absolute
	WH93	196-250	E	abs. comp. of Cp <sub>x</sub> TiCl <sub>4-x</sub> , x=0-2; diff '10Dq' at each edge
C <sub>6</sub> H <sub>5</sub> Cl	HP&78	195-215	E	comp. with carbon 1s near-edge features
C <sub>8</sub> Cl <sub>2</sub> H <sub>4</sub> O	HUR92	180-290	E	para-Bz(COCl) <sub>2</sub> ; absolute, comp. to phosgene
<b>C<sub>8</sub>ClH<sub>18</sub>P</b>	HH&98	130-220	E	(t-Bu) <sub>2</sub> PCl; comp. to PCl <sub>3</sub>
<b>C<sub>10</sub>ClCo<sub>3</sub>O<sub>9</sub></b>	HM&93	180-280	E	Cl-C-[Co(CO) <sub>3</sub> ] <sub>3</sub> , abs.; gas(E,P-ions), sol(P); PIPICO, TOF-MS
<b>C<sub>10</sub>Cl<sub>2</sub>H<sub>10</sub>Ti</b>	WH93	196-250	E	Cp <sub>2</sub> TiCl <sub>2</sub> , abs.; comp. of Cp <sub>x</sub> TiCl <sub>4-x</sub> , x=0-2; diff '10Dq' at each edge
CID	KA&96a	201,203	P	ultrafast decay, comp. of resonant Auger, PES; D-isotope enhances molecular features (slower dissoc.)
	KA&96d	202-207	P	res. Auger; TIY; high res. (45 mV); comp. to HCl; mol. field splitting; $\Gamma(4s)=95(10)$ meV
	FB&02	190, 200.6	P	resonant PES; spin-orbit selectivity in 2p <sup>-1</sup> $\sigma^*$ state; in Auger the valence, core holes are aligned
ClF	MM12	68-72	P,R	ultra-fast decay (HBr-Br3d; DCl, HCl-Cl2p; H <sub>2</sub> S - S2p, O <sub>2</sub> -O1s)
	FSD99	200-300	T	absolute; ab initio Cl; DFT for cont.; comp of ClF, ClF <sub>3</sub> ; F-cage effects
ClF <sub>3</sub>	BS87	190-230	E	high res.
	SB89	190-230	E	high res., partial bar. Effects
	FSD99	200-300	T	absolute; ab initio Cl; DFT for cont.; comp of ClF, ClF <sub>3</sub> ; F-cage effects
ClH	HB72	200-210	P	photoelectric yield, absolute, Rydberg analysis IP (207.1, 208.7)
	S74	196-210	T	Z+1 analogy
	R75	200-210	T	alternate assignment of HB72
	S75a,b	200-210	T	Z+1 analogy calc., alternate assignment of HB72
	S76a	200-210	T	Z+1 analogy, EICVOM
	GKM77b	198-215	P	comp. to Cl <sub>2</sub> spectrum
	NI&81	198-280	P	absolute, Rydberg analysis IP (207.3, 208.9)
	SYD82	190-225	T	ab initio, absolute, comp. to expt (HB72)
	DBH83	198-214	E	0.11eV FWHM
	KM83	190-220	T	Green's function theory - general formulation for near-edge & EXAFS
	SC&84	198-209	E	75meV FWHM, Rydberg IP [3/2=207.40(3), 1/2=209.03(3)]

(HCl cont'd)	AA&90b	200-202	P,T	DES at $\sigma^*$ ; ultra-fast decay and normal compete
	YPD91	200-230	T	SCF-Cl; vib'n'l effects; comp. to expt. (SC&84)
	AA&92a	198-214	P,T	PIPICO; partial & total ion yields; $\sigma^*$ , Ryd. differ; HCl <sup>2+</sup> pot. curves
	AA&92c	200-203	P	resonant AI; comp. of HCl, Cl <sub>2</sub> , H <sub>2</sub> S
	KA&93	198-214	P	0.2 eV fwhm; resonant AI of Rydbergs; molecular NOT ultrafast
	BM95	199,200	P	resonant Auger; ang. dist.; ultrafast atomic decay 6 large alignment
	LB&95	195-250	T	MS-X $\alpha$ ; comp. of XH <sub>n</sub> (X=Si,P,S,Cl)
	KA&96a	201,203	P	ultrafast decay, comp. of resonant Auger, PES
	KA&96b	201,203	P	resonant Auger-Raman narrowing is selective; in 4s $\sigma$ not $\sigma^*$ ; reflects relative widths of Franck-Condon to dissoci. states
	KA&96d	202-207	P	resonant Auger; TIY; high res. (45 mV); comp. to HCl; mol. field splitting; 95(10) meV 4s natural linewidth
	BS&97	199-202	P	resonant X-ray scattering; ultra-fast decay; Auger as f(detune from $\sigma^*$ )
	SA97	201,204	P	Auger resonant Raman; line narrowing at 4s $\sigma$ but not at $\sigma^*$
	FS&98	200-210	T	DFT, CI; discrete states
	KK&98	196-200	P	angle resolved PI; asymmetric; ultrafast decay
	KW&98	198-212	P	angle-resolved 2d map of Auger; resonant AI, etc; $\beta$ s
	MK&98a	203-205	P	resonant Auger; ang. distr; intermediate states identified
	FKA99	203-206	T	absolute; relativistic; core-level only; S-O coupling
	GTM99	204	T	wave packet description of ultrafast decay; detune effects; general theory
	FB&00	200-202	P	resonant Auger; ultrafast; atomic-molecular interference; detuning
	FB&02	190, 200.6	P	resonant PES; spin-orbit selectivity in 2p <sup>-1</sup> $\sigma^*$ state; in Auger the valence, core holes are aligned
	SS&05	202-211	P	neutral, luminescence and ion yield; metastable H at IPs
	LP&12	196	P	ultra-fast decay, Auger, AI and atomic decay lines, 12 meV.
Cl <sub>2</sub>	MM12	68-72	P,R	ultra-fast decay (HBr-Br3d; DCI, HCl-Cl2p; H <sub>2</sub> S - S2p, O <sub>2</sub> -O1s)
	G77	196-214	P	Rydberg analysis IP (208.0, 209.6)
	GKM77b	196-214	P	Rydberg analysis IP (208.0, 209.6)
	KMN80b	196-215	T	ab initio calc., comp. to experiment (GKM77)
	SKR80	197-210	E	Z+1 analogy, <70meV FWHM, Ryd. analysis IP (207.80, 209.42)
	NI&81	198-280	P	absolute, Rydberg analysis IP (208.3, 209.8)
	AA&92c	198-202	P	resonant AI; comp. of HCl, Cl <sub>2</sub> , H <sub>2</sub> S
	LB&95	195-250	T	MS-X $\alpha$ ; comp. to XH <sub>n</sub> (X=Si,P,S,Cl)
	SG&02	195-215	P	TIY, angle resolved, exchange & S-O splittings,
Cl <sub>2</sub> Fe	CK&83	200-240	T	absolute, energy dependent Dirac calc, spin-dependence
Cl <sub>3</sub> OP	TKM82	198-215	T	X- $\alpha$ (MSM calc.), comp. to expt (K77)
	YM&84	198-215	P	comp. of fluorescence, PES & calc to TKM82
	SB85d	195-295	E	d-cont. res.
	NJ&98	180-240	P,T	absolute; GSCF3 calc.; LS-state; comp of PX <sub>3</sub> , YPF <sub>3</sub> . X=Cl,F, Y=O,S)
ClO <sub>2</sub>	FPR06	200-260	P	PIY, TIY; ionization yield; PEPICO, PIPICO
Cl <sub>3</sub> P	MK80	198-216	P	comp. to P 2p spectrum
	TKM81	198-216	P	comp to P2p
	SB85c	190-290	E	0.18eV FWHM, in PX <sub>3</sub> series
	II&87	130-270	P	absolute, high res. (0.03-0.07 eV), comp. to SB85c
	HBC96	190-240	P	TIY, PIY, PEPICO; comp. of PCl <sub>3</sub> , PF <sub>3</sub> , CF <sub>3</sub> PCl <sub>2</sub>
	AB97	0-350	E	absolute; total and partial ion yield; (e,e+ion); dipole breakdown
	OC&97b	5-200	E,R	absolute, VTKR sum rule; derived molecular properties
	HH&98	130-220	E	absolute; comp. to (t-Bu) <sub>2</sub> PCl
Cl <sub>3</sub> PS	TKM82	198-215	T	X- $\alpha$ (MSM calc.), comp. to expt (K77)
	NJ&98	180-240	P,T	absolute; GSCF3 calc.; LS-state; comp of PX <sub>3</sub> , YPF <sub>3</sub> . X=Cl,F, Y=O,S)
Cl <sub>4</sub> Ge	GD&96	100-300	E	non-statistical 3/2:1/2 intensities; comp. to Cl 1s, Ce2p/3p of GeCl <sub>4</sub>
Cl <sub>4</sub> Na <sub>4</sub>	YS&02	190-230	T	relative; MS-X $\alpha$ plus DFT; geometry dependence

(ClNa) <sub>n</sub>	MC&99 NR&99	190-235 190-235	P P,T	relative, PIY, comp. to thin film, solid TEY relative, PIY, comp. to thin film, solid TEY; MS cluster calc
<b>Cl<sub>4</sub>Si</b>	BT&87	200-225	P,T	0.4 eV FWHM res., not analysed
	AS&88	200-225	P	DES, spectator decay dominates
	CG&88	200-225	P,T	DES, βs, spectator dominates
	TL&89	190-240	T	absolute, X-α calc; cont. & discrete; Rydbergs
	W92	190-240	E	comp of SiCl <sub>4</sub> and Si <sub>2</sub> Cl <sub>6</sub>
	Cl <sub>4</sub> Ti	196-250	E	TiCl <sub>4</sub> , absolute, comp. to CpTiCl <sub>3</sub>
Cl <sub>6</sub> Si <sub>2</sub>	WH93	196-250	E,T	absolute; comp. of Cp <sub>x</sub> TiCl <sub>4-x</sub> , x=0-2; diff '10Dq' at each edge
	W92	190-240	E	comp of SiCl <sub>4</sub> and Si <sub>2</sub> Cl <sub>6</sub>
<u>Chlorine 1s (2830 eV)</u>				
AsCl <sub>3</sub>	GDT97	2.81-2.85	P,T	relative; TIY, MS-Xα; pot. barr.; AsCl <sub>3</sub> , PCl <sub>3</sub> , GeCl <sub>4</sub> , SnCl <sub>4</sub> comp.; σ*(X-Cl) bond length correlation
CCl <sub>3</sub> H <sub>3</sub>	SBB68	2.81-2.85	P	gas-solid comp.
	BS&69	2.81-2.85	P	assignment of SBB68
	N71	2.82-2.83	P	10eV below IP
	HG76	2.81-2.84	P	absolute
	PB&85	2.81-2.85	P	comp. to fluorescence, weak shake-up features identified
	D86b	2.81-2.85	P	abs., emission comp. [PB&85]; state-selected fluorescence
	LC&88a	2.81-2.85	P,T	relative, polarised fluorescence with tuned excitation, MO calc
	LC&88b	2.81-2.85	P	relative, polar. fluorescence, MO symmetries, sat.-free Fl spectrum
	L89	2.80-2.84	P	abs., emission comp.; state-selected fluorescence; polarisation
	LC&91	2.81-2.84	P	relative; abs. vs. fluorescence; polarised at σ*(C-Cl)
	PF&94	2.80-2.93	P	thresh. PES; comp. of CH <sub>x</sub> Cl <sub>4-x</sub> , x=0-3; CF <sub>x</sub> Cl <sub>4-x</sub> , x=1-3; I(IP) α #-Cl
CCl <sub>2</sub> H <sub>2</sub>	HC&99	2.82-2.84	P	relative; TIY, PIY; branching ratios; PEPICO; KERD; mechanisms
	PF&94	2.80-2.93	P	thresh. PES; comp. of CH <sub>x</sub> Cl <sub>4-x</sub> , x=0-3; CF <sub>x</sub> Cl <sub>4-x</sub> , x=1-3; I(IP) α #-Cl
	LD&06	2.81-2.86	P	relative, TIY, PIY, +ve and -ve ions, strong PCI type effect
CCl <sub>2</sub> F <sub>2</sub>	ZK&15	2.82-2.83	P	nexafs & RIXS, core hole clock; compare 11 Cl compounds
	HG76	2.81-2.84	P	absolute
	LC&91	2.81-2.84	P	relative; abs. vs. fluorescence; polarised at σ*(C-Cl)
	PC&91	2.81-2.84	P	relative; abs. vs. fluorescence; σ*(C-Cl)
	PF&94	2.80-2.93	P	thresh. PES; comp. of CH <sub>x</sub> Cl <sub>4-x</sub> , x=0-3; CF <sub>x</sub> Cl <sub>4-x</sub> , x=1-3; I(IP) α #-Cl
	LAG96	2.81-2.85	T	resonant & non-resonant X-ray emission; polarization anisotropy in 1-step (RIXS) and generalised 2-step models
CCl <sub>3</sub> F	LC&91	2.81-2.84	P	relative; abs. vs. fluorescence; polarised at σ*(C-Cl)
	PC&91	2.81-2.84	P	relative; abs. vs. fluorescence; σ*(C-Cl)
	PF&94	2.80-2.93	P	thresh. PES; comp. of CH <sub>x</sub> Cl <sub>4-x</sub> , x=0-3; CF <sub>x</sub> Cl <sub>4-x</sub> , x=1-3; I(IP) α #-Cl
CCl <sub>3</sub> H	SBB68	2.81-2.85	P	(chloroform) gas-solid comp.
	BS&69	2.81-2.85	P	assignment of SBB68
	PF&94	2.80-2.93	P	thresh. PES; comp. of CH <sub>x</sub> Cl <sub>4-x</sub> , x=0-3; CF <sub>x</sub> Cl <sub>4-x</sub> , x=1-3; I(IP) α #-Cl
	LS&05	2.81-2.85	P	TIY, PIY, more fragmentation in continuum, state selective frag.
	ZK&15	2.82-2.83	P	nexafs & RIXS, core hole clock; compare 11 Cl compounds
CCl <sub>3</sub> H <sub>3</sub> Si	FBN90	2.81-2.89	P	MeCl <sub>3</sub> Si, discrete & cont. shape res.; strong double excitation
	SBB68	2.81-2.85	P	gas-solid comp.
	BS&69	2.81-2.85	P	assignment of SBB68
	N71	2.83	P	10eV below IP
	LG&86	2.8-3.0	P	XANES, EXAFS, ionization yield
	PF&94	2.80-2.93	P	thresh. PES; comp. of CH <sub>x</sub> Cl <sub>4-x</sub> , x=0-3; CF <sub>x</sub> Cl <sub>4-x</sub> , x=1-3; I(IP) α #-Cl
CCl <sub>4</sub>	ZK&15	2.82-2.83	P	nexafs & RIXS, core hole clock; compare 11 Cl compounds

C <sub>2</sub> ClH <sub>5</sub>	ZK&15	2.82-2.83	P	Chloroethane, nexafs & RIXS, core hole clock; compare 11 Cl compounds
C <sub>2</sub> Cl <sub>2</sub> H <sub>6</sub> Si	FBN90	2.81-2.89	P	Me <sub>2</sub> Cl <sub>2</sub> Si, discrete & cont. shape res.; strong double excitation
C <sub>2</sub> Cl <sub>2</sub> H <sub>2</sub>	ZK&15	2.82-2.83	P	chloro-ethene, nexafs & RIXS, core hole clock; compare 11 Cl compounds
C <sub>2</sub> Cl <sub>2</sub> H <sub>4</sub>	LG&86	2.8-3.0	P	1,2, dichloroethane, XANES, EXAFS, ionization yield
	ZK&15	2.82-2.83	P	nexafs & RIXS, core hole clock; compare 11 Cl compounds
C <sub>2</sub> Cl <sub>3</sub> H	HG76	2.81-2.84	P	absolute
C <sub>2</sub> Cl <sub>3</sub> H <sub>3</sub>	ZK&15	2.82-2.83	P	nexafs & RIXS, core hole clock; compare 11 Cl compounds
C <sub>2</sub> Cl <sub>5</sub> H	HG76	2.81-2.84	P	absolute
C <sub>3</sub> ClH <sub>5</sub> O	LDN07	2.81-2.85	P	epichlorohyrin – CH <sub>3</sub> (CH-O-CH <sub>2</sub> ); TIY, PEPICO, possible alignment
C <sub>3</sub> ClH <sub>9</sub> Si	FBN90	2.81-2.89	P	Me <sub>3</sub> ClSi; discrete & cont. shape res.; strong double excitation
C <sub>6</sub> H <sub>5</sub> Cl	ZK&15	2.82-2.83	P	nexafs & RIXS, core hole clock; compare 11 Cl compounds
CID	DA&98c	2.82-2.84	P	TIY, PIY, neutral D observed; $\beta$ for fragmentation
ClF	FSD99	2.81-2.85	T	absolute; ab initio CI, DFT continuum; comp of ClF, ClF <sub>3</sub> ; F-cage
ClF <sub>3</sub>	LC&87	2.82-2.86	P	comp. of abs. & fl.; res. effects; strong polarisation
	PC&87	2.81-2.84	P	abs., emission comp.; state-selected fluorescence
	SL&91a	2.81	P	anisotropy of fluorescence at $\sigma^*(C-Cl)$ ; matches classical oscillator pred. (2-step model)
	LC&91	2.81-2.84	P	relative; abs. vs. fluorescence; polarised at $\sigma^*(C-Cl)$
	PC&91	2.81-2.84	P	relative; abs. vs. fluorescence; $\sigma^*(C-Cl)$
	LM&94	2.824	P	ion yields at $\sigma^*(C-Cl)$ ; Auger-ion coincidence
	PF&94	2.80-2.93	P	thresh. PES; comp. of CH <sub>x</sub> Cl <sub>4-x</sub> , x=0-3; CF <sub>x</sub> Cl <sub>4-x</sub> , x=1-3; I(IP) $\alpha$ #-Cl
	LAG96	2.81-2.85	T	resonant & non-resonant X-ray emission; polarization anisotropy in 1-step (RIXS) and generalised 2-step models
ClH	LN43	2.8-3.2	P	comp. to Cl <sub>2</sub>
	SKN51	2.81-2.83	P	20eV around edge, comp. to Cl <sub>2</sub>
	BN66	2.81-2.85	P	relative, see SYD82
	SBB68	2.81-2.85	P	gas-solid comp.
	BS&69	2.81-2.85	P	assignment of SBB68
	G70	2.81-2.84	P	relative absorption
	SM&70	2.81-2.85	P	comp. to Cl 1s emission
	MN&75	2.81-2.85	T	one-centre SCF-MO calc., geometry optimized
	SYD82	2.81-2.85	T	ab initio, absolute, comp. to expt (BN66)
	D86b	2.81-2.84	P	abs., emission comp. [G70]; multi-vacancy effects
	BM&90	2.81-2.86	P	absolute; HCl, Cl <sub>2</sub> comp; KV 2e-; sym.-broken states in 2e delocal?
	LM&94	2.824	P	ion yields at $\sigma^*(H-Cl)$ ; Auger-ion coincidence
	FPS95b	2.82-2.83	T	MS-X $\alpha$ ; non-MT and SCF required to model expt.
	DA&98c	2.82-2.84	P	TIY, PIY, neutral H observed; $\beta$ for fragmentation
	FS&98	2.81-1.85	T	DFT, CI; discrete states; comp to BM&90; absolute 1s ioniz. X-sect
	HA&98a	2.82-2.85	P	TIY, PIY, neutral H-decay at 6 $\sigma^*$ ; ultrafast decay
	HA&98b	2.82-2.84	P	Cl <sup>n+</sup> n=1-5 yields, PCI
ClF <sub>5</sub> S	RB&92	2.8-3.1	P,T	relative; comp. to SF <sub>6</sub> ; EXAFS
Cl <sub>2</sub>	LN43	2.81-3.20	P	comp. with early EXAFS theory
	SKN51	2.81-2.84	P	30eV around edge, comp. with early EXAFS theory
	SBB68	2.81-2.85	P	gas-solid comp.
	BS&69	2.81-2.85	P	assignment of SBB68
	SM&70	2.81-2.85	P	comp. to Cl 1s emission
	MS&73	2.81-2.85	T	semiempirical calc.
	B80	2.81-3.20	P,R	review, (SKN51 data)
	LG&86	2.8 -3.0	P	XANES, EXAFS, ionization yield
	BM&90	2.81-2.86	P	absolute; HCl, Cl <sub>2</sub> comp; KV 2e-; sym.-broken states in 2e delocal?
	FPS95a	2.82-2.83	T	MS-X $\alpha$ ; non-MT and SCF required to model expt.
	NM96	2.81-2.86	P,R	absolute; XAFS (BM&90 data)

Cl <sub>2</sub> (cont'd)	MS&97b	2.81-2.86	P,T	RIXS; pol. dep.; non-dipole features associated with phase variation over molecular size; complicates use of RIXS for state symmetry determination
Cl <sub>2</sub> OS	HBT87	2.81-2.86	P	comp. to other S,Cl,O cmpds, $\sigma^*(Cl-S)$ dominates
Cl <sub>2</sub> OS <sub>2</sub>	HBT87	2.81-2.86	P	comp. to other S,Cl,O cmpds, $\sigma^*(Cl-S)$ dominates
Cl <sub>2</sub> S	HBT87	2.81-2.86	P	comp. to other S,Cl,O cmpds, $\sigma^*(Cl-S)$ dominates
Cl <sub>2</sub> S <sub>2</sub>	HBT87	2.81-2.86	P	comp. to other S,Cl,O cmpds, $\sigma^*(Cl-S)$ dominates
Cl <sub>3</sub> P	GDT97	2.81-2.85	P,T	relative; TIY, MS-X $\alpha$ ; pot. barr.; AsCl <sub>3</sub> , PCl <sub>3</sub> , GeCl <sub>4</sub> , SnCl <sub>4</sub> comp.; $\sigma^*(X-Cl)$ bond length correlation
Cl <sub>4</sub> Ge	GD&96	2.81-2.85	P,T	ab initio calc; comp. to all other edges
	GDT97	2.81-2.85	P,T	relative; TIY, MS-X $\alpha$ ; pot. barr.; AsCl <sub>3</sub> , PCl <sub>3</sub> , GeCl <sub>4</sub> , SnCl <sub>4</sub> comp.; $\sigma^*(X-Cl)$ bond length correlation
Cl <sub>4</sub> Si	BF&87	2.81-2.88	P	split first res., comp. to Si 1s
	TL&89	2.81-2.88	T	absolute, X- $\alpha$ calc; cont. & discrete; Rydbergs
	FBN90	2.81-2.89	P	discrete & cont. shape res.; strong double excitation
	GDT97	2.81-2.85	P,T	relative; TIY, MS-X $\alpha$ ; pot. barr.; AsCl <sub>3</sub> , PCl <sub>3</sub> , GeCl <sub>4</sub> , SnCl <sub>4</sub> comp.; $\sigma^*(X-Cl)$ bond length correlation
Cl <sub>4</sub> Sn	GDT97	2.81-2.85	P,T	relative; TIY, MS-X $\alpha$ ; pot. barr.; AsCl <sub>3</sub> , PCl <sub>3</sub> , GeCl <sub>4</sub> , SnCl <sub>4</sub> comp.; $\sigma^*(X-Cl)$ bond length correlation

### Chromium 2p (574, 584 eV)

CrCl <sub>2</sub> O <sub>2</sub>	DF&94	570-575	T	ab initio CI; relaxed orb.; MO <sub>x</sub> X <sub>y</sub> (Ti,V,Cr,Mn); covalency incr. as Cl 6 F
CrF <sub>2</sub> O <sub>2</sub>	DF&94	570-575	T	Cr(NO) <sub>4</sub> ; absolute; ab initio-SCF-CI; comp. of 3d spectra of 5 TM
CrN <sub>4</sub> O <sub>4</sub>	DFL92	570-575	T	compounds; supports MO-model for edge structure
	FD&93	570-575	T	LCAO-SCF-CI; comp. of L-edges of organometallics

### Chromium 1s (5.99 keV)

Cr(CO) <sub>6</sub>	JP58	5.98-6.02	P	40eV about edge, gas-solid comp.
	N70	5.98-6.02	T	pot. bar. effects, MO interpretation
	FDL93	5.98-6.04	T	absolute; LCAO-SCF-CI; comp. to Cr 2p results; Ni, Fe, Cr cmpds
	DF&94	5.98-6.00	T	ab initio CI; relaxed orb.; MO <sub>x</sub> X <sub>y</sub> (Ti,V,Cr,Mn); covalency incr. as Cl 6 F
CrCl <sub>2</sub> O <sub>2</sub>	FDL93	5.98-6.04	T	absolute; LCAO-SCF-CI; comp. to Cr 2p results; Ni, Fe, Cr cmpds
	DF&94	5.98-6.00	T	ab initio CI; relaxed orb.; MO <sub>x</sub> X <sub>y</sub> (Ti,V,Cr,Mn); covalency incr. as Cl 6 F
CrF <sub>2</sub> O <sub>2</sub>	DF&94	5.98-6.00	T	ab initio CI; relaxed orb.; MO <sub>x</sub> X <sub>y</sub> (Ti,V,Cr,Mn); covalency incr. as Cl 6 F
Cr(NO) <sub>4</sub>	FDL93	5.98-6.04	T	absolute; LCAO-SCF-CI; comp. to Cr 2p results; Ni, Fe, Cr cmpds

### Cobalt 3p (55 eV)

C <sub>7</sub> CoH <sub>5</sub> O <sub>2</sub>	HWR90b	30-280	E	CoCp(CO) <sub>2</sub> ; absolute; comp. to other mixed-Cp, CO species
C <sub>8</sub> CoO <sub>8</sub>	HWR90b	30-280	E	Co <sub>2</sub> (CO) <sub>8</sub> ; absolute; comp. to mixed-Cp, CO species
C <sub>10</sub> ClCoO <sub>9</sub>	HM&93	30-280	E,P,T	Cl-C-[Co(CO) <sub>3</sub> ] <sub>3</sub> , abs.; gas(E,P-ions), sol(P); PIPICO, TOF-MS
C <sub>10</sub> CoH <sub>10</sub>	HWR90b	30-280	E	CoCp <sub>2</sub> ; absolute; comp. to mixed-Cp, CO species
C <sub>11</sub> Co <sub>3</sub> H <sub>3</sub> O <sub>10</sub>	HM&93	30-280	E,P	CH <sub>3</sub> O-C-[Co(CO) <sub>3</sub> ] <sub>3</sub> ; abs.; comp. of gas (E), sol (P-TEY)

### Cobalt 2p (775, 790 eV)

C <sub>7</sub> CoH <sub>5</sub> O <sub>2</sub>	WRH89	750-820	E	CoCp(CO) <sub>2</sub> ; absolute; comp. to other mixed-Cp, CO species
C <sub>8</sub> Co <sub>2</sub> O <sub>8</sub>	WRH89	750-820	E	Co <sub>2</sub> (CO) <sub>8</sub> ; absolute; comp. to mixed-Cp, CO species
C <sub>10</sub> ClCo <sub>3</sub> O <sub>9</sub>	HM&93	750-820	E,P,T	Cl-C-[Co(CO) <sub>3</sub> ] <sub>3</sub> , abs.; gas(E,P-ions), sol(P); PIPICO, TOF-MS
C <sub>10</sub> CoH <sub>10</sub>	HWR90b	750-820	E	CoCp <sub>2</sub> ; absolute; comp. to mixed-Cp, CO species

<b>C<sub>11</sub>Co<sub>3</sub>H<sub>3</sub>O<sub>10</sub></b>	HM&93 C <sub>32</sub> H <sub>28</sub> Co <sup>+</sup>	750-820 770-810	E,P P	CH <sub>3</sub> O-C-[Co(CO) <sub>3</sub> ] <sub>3</sub> ; abs.; comp. of gas (E), sol (P-TEY) Co-porphyrin ION; NEXAMS (PIY), TIY
--	--	--------------------	----------	--

### Cobalt 1s (7709 keV)

Co <sub>2</sub>	WRE89a	7.70-7.74	T	DVM-X $\alpha$ ; XANES; comp. of Co <sub>2</sub> , Mn <sub>2</sub> , Ni <sub>2</sub>
-----------------	--------	-----------	---	--

### Fluorine 1s (690 eV)

<b>BF<sub>3</sub></b>	ZV72 SDD81 SSH84a VA&85 NAV88a NAV88b PV&90 SU&97	680-710 680-715 690 680-720 688-708 688-708 680-700 680-710	P,R T T P,R P P P P	pot. bar. effects MSM X- $\alpha$ calc., shape res., comp. to experiment(ZV72) $\sigma^*$ -res./bond length relationship comp. of BF <sub>3</sub> , N <sub>2</sub> , NO <sub>3</sub> <sup>-</sup> ; shape resonances comp. to KNO <sub>3</sub> , NaNO <sub>3</sub> (O1s - sol); $\delta(\pi-\sigma)$ versus R comp. to KNO <sub>3</sub> , NaNO <sub>3</sub> (O1s - sol); $\delta(\pi-\sigma)$ versus R comp. to NO <sub>2</sub> <sup>-</sup> , NO <sub>3</sub> <sup>-</sup> ; $\delta(\pi-\sigma)$ versus R PEPICO - E-resolved; partial X-sect.; ang. dist.; dynamics of 2a <sub>2</sub> state
BeF <sub>2</sub>	CC84	686	T	delta SCF, F1s->5 $\sigma^*$ at 685.3 (T=6.27eV), excited & ion state diss.
CCl <sub>3</sub>	ZIB92 SS&95	680-740 290-325	E P	absolute, high res. (70 meV), pot. bar., comp. of CCl <sub>x</sub> F <sub>4-x</sub> , x=1-4 PIPICO; start = selective ion gate; PIPICO yields; comp of Cl2p, C1s, F1s edges; only selective at Cl 2p edge
CCl <sub>2</sub> F <sub>2</sub>	SS97a SSB99 ZIB92 BSS93b SBS94a SSB94 SS97 SSB99	680-750 680-710 680-740 50-1500 670-730 670-730 680-750 680-710	P P E P P P P P	PIPICO, BR and X-sect.; site-specific fragmentation TIY, PIY; comp of CF <sub>x</sub> Cl <sub>4-x</sub> x=1-3; site selective fragmentation absolute, high res. (70 meV), pot. bar., comp. of CCl <sub>x</sub> F <sub>4-x</sub> , x=1-4 partial ion yields at coarse resolution partial ion yields; site-selective frag. at C 1s, Cl 2p, F 1s partial ion-pair yields; site-selective frag. PIPICO, BR and X-sect.; site-specific fragmentation TIY, PIY; comp of CF <sub>x</sub> Cl <sub>4-x</sub> x=1-3; site selective fragmentation
CCl <sub>2</sub> F <sub>3</sub>	HBC96	670-740	P	TIY, PIY, PEPICO; comp. of PCl <sub>3</sub> , PF <sub>3</sub> , CF <sub>3</sub> PCl <sub>2</sub>
CCl <sub>3</sub> F	ZIB92 SS97 SS98b SSB99	680-740 680-750 680-730 680-710	E P P P	absolute, high res. (70 meV), pot. bar., comp. of CCl <sub>x</sub> F <sub>4-x</sub> , x=1-4 PIPICO, BR and X-sect.; site-specific fragmentation PIY, comp of C 1s, F1s, Cl 2p TIY, PIY; comp of CF <sub>x</sub> Cl <sub>4-x</sub> x=1-3; site selective fragmentation
<b>CFHO</b>	IH87 RI&88	670-730 670-730	E E	HCOF - formyl fluoride absolute
<b>CFH<sub>3</sub></b>	HC96 L73 HB78a SSH84a	688 670-780 680-700 690	T P E T	DFT, $\Delta^3\pi^{-1}\pi = 0.10$ eV res. at thr. res. at thr. $\sigma^*$ -res./bond length relationship
CF <sub>2</sub> H <sub>2</sub>	US&96 L73 SSH84a	682-696 670-780 690	P,T P T	TEY; Auger, AI; ultrafast decay proposed; SCF calc. res. at thr. $\sigma^*$ -res./bond length relationship
<b>CF<sub>2</sub>O</b>	US&96 RI&88 HC96	682-696 680-730 688	P,T E T	TEY; Auger, AI; ultrafast decay proposed; SCF calc. C-F $\sigma^*$ res., absolute, perfluoro effect DFT, $\Delta^3\pi^{-1}\pi = 0.010$ eV
<b>CF<sub>3</sub>H</b>	L73 SSH84a HN86 US&96	670-780 690 680-720 682-696	P T E P,T	res. at thr., extended fine structure (EXAFS) $\sigma^*$ -res./bond length relationship absolute TEY; Auger, AI; ultrafast decay proposed; SCF calc.
<b>CF<sub>3</sub>NO</b>	HIR89	680-730	E	absolute, $\sigma^*(C-F)$ dominates

<b>CF<sub>4</sub></b>	L73	670-780	P	absolute, res. at thr., extended fine structure (EXAFS)
	WB74d	685-725	E	strong t <sub>2</sub> res.
	BH81	680-740	E,R	wide range
	HS&81	685-705	T	X- $\alpha$ calc, comp. to WB74d
	SSH84a	690	T	$\sigma^*$ -res./bond length relationship
	SA&86b	690-780	P	absolute, t <sub>2</sub> res., comp. to C 1s
	SDD86	690-720	T	MS-X $\alpha$ calc, $\beta$ , partial X-sections, comp. to WB74d
	HI88b	600-1200	E	exelfs, q-dependence
	LM&89	625-825	P	total ion yield, TOF mass spec at 693, 742 eV
	ZC&89	670-740	E	absolute, check on conv. to absolute, comp. to PA (SA&86b, L73)
	HM94	670-750	E,R	absolute; improved method for X-section detection; this bibliography!!
	SBS94b	44-1500	P	partial & total ion yields; site-selective fragmentation; PEPICO; (F <sup>+</sup> , CF <sub>2</sub> <sup>+</sup> ), (F <sup>+</sup> , CF <sup>+</sup> ) only produced at F 1s edge
	SBS95	684-718	P	PEPICO and KERD's; (C,F) site differences probed
	US&96	682-696	P,T	TEY; Auger, AI; ultrafast decay proposed; SCF calc.
	MU&99	686-700	P,T	TIY; ang. dep. by fast ion collection; F1s $\rightarrow\sigma^*$ CF anisotropic; 42% core-hole localization; symmetry breaking
	TF&99	688-703	P	relative; TIY, threshold EY, TPEPICO; kinematics; branching ratios
	PUT04	686-701	P	TIY, Auger, and AEICO with F <sup>+</sup> , ultrafast fragmentation
<b>CF<sub>4</sub>O</b>	IM&87	670-730	E	CF <sub>3</sub> OF, low-lying $\sigma^*$ (O-F)
CF <sub>8</sub> S	IS&05	680-730	P	PEPICO, PIPICO, site-selective fragmentation
<b>C<sub>2</sub>FH<sub>3</sub></b>	MC&87	680-730	E	$\sigma^*$ (C-F)
<b>C<sub>2</sub>F<sub>2</sub>Cl<sub>2</sub></b>	H19	680-730	E	Freon152, absolute
<b>C<sub>2</sub>F<sub>2</sub>H<sub>2</sub></b>	MC&87	680-730	E	(CH <sub>2</sub> =CF <sub>2</sub> ), $\sigma^*$ (C-F)
<b>C<sub>2</sub>F<sub>2</sub>H<sub>2</sub></b>	MC&87	680-730	E	(CHF=CFH), $\sigma^*$ (C-F)
<b>C<sub>2</sub>F<sub>2</sub>H<sub>4</sub></b>	H19	680-730	E	1,2di-fluoro-ethne, absolute, compare to
<b>C<sub>2</sub>F<sub>3</sub>H</b>	MC&87	680-730	E	$\sigma^*$ (C-F)
<b>C<sub>2</sub>F<sub>3</sub>HO<sub>2</sub></b>	RI&88	630-730	E	CF <sub>3</sub> COOH, perfluoro effect
<b>C<sub>2</sub>F<sub>3</sub>H<sub>3</sub></b>	MS&84	606-777	P	ZEKE, mass spectrum at $\sigma^*$ (C-F), site-selective fragmentation
<b>C<sub>2</sub>F<sub>3</sub>H<sub>3</sub>O<sub>3</sub>S</b>	HH14	640-720	E	(Methyl trifluoromethanesulfonate), absolute, comp to Nafion
<b>C<sub>2</sub>F<sub>3</sub>N</b>	HS90	680-728	E	CF <sub>3</sub> CN, absolute, comp. to CF <sub>3</sub> C:::CH
<b>C<sub>2</sub>F<sub>4</sub></b>	MC&87	680-730	E	$\sigma^*$ (C-F)
<b>C<sub>2</sub>F<sub>6</sub></b>	HFM87	680-730	E	comp. of perfluoro-n-alkanes. $\sigma^*$ (C-F)
	IM&88	680-730	E	$\sigma^*$ (C-F), $\sigma^*$ (C-F) dominated
	AC&95	685-710	T	STEX ab initio; absolute; growth of poly-(CF <sub>2</sub> ) <sub>n</sub> by C <sub>2n</sub> F <sub>4n+2</sub> , n=1-5
<b>C<sub>2</sub>F<sub>6</sub>O<sub>2</sub></b>	H86b	680-730	E	bis(trifluoromethyl)peroxide, orbital mapping
	IM&87	680-730	E	low-lying $\sigma^*$ (O-O)
	HM&89	680-730	P	absolute; total, partial ion yields; PIPICO, diss. IY; sel. frag.
<b>C<sub>3</sub>F<sub>3</sub>H</b>	HS90	680-728	E	CF <sub>3</sub> CCH, absolute, comp. to CF <sub>3</sub> CN
<b>C<sub>3</sub>F<sub>6</sub></b>	IM&88	680-730	E	perfluorocyclopropane, comp. to C <sub>4</sub> F <sub>8</sub> , C <sub>6</sub> F <sub>12</sub> , $\sigma^*$ (C-F) dominated
<b>C<sub>3</sub>F<sub>6</sub>O</b>	RI&88	680-730	E	(perfluoroacetone), intense $\sigma^*$ (C-F) res., perfluoro effect
<b>C<sub>3</sub>F<sub>8</sub></b>	HFM87	680-730	E	comp. of perfluoro-n-alkanes. $\sigma^*$ (C-F)
	IM&88	680-730	E	C <sub>x</sub> F <sub>2x+2</sub> series, $\sigma^*$ (C-F) dominated
<b>C<sub>4</sub>F<sub>6</sub></b>	MC&87	680-730	E	perfluorobutadiene
<b>C<sub>4</sub>F<sub>6</sub></b>	RI&88	680-730	E	CF <sub>3</sub> C:::CCF <sub>3</sub>
<b>C<sub>4</sub>F<sub>8</sub></b>	RI&88	680-730	E	CF <sub>3</sub> C=FCFCF <sub>3</sub>
<b>C<sub>4</sub>F<sub>8</sub></b>	IM&88	680-730	E	perfluorocyclobutane, comp. to C <sub>3</sub> F <sub>6</sub> & C <sub>6</sub> F <sub>12</sub> , $\sigma^*$ (C-F) dominated
<b>C<sub>4</sub>F<sub>10</sub></b>	HFM87	680-730	E	comp. of perfluoro-n-alkanes. $\sigma^*$ (C-F)
	IM&88	680-730	E	C <sub>x</sub> F <sub>2x+2</sub> series, $\sigma^*$ (C-F) dominated
	AC&95	685-710	T	STEX ab initio; absolute; growth of poly-(CF <sub>2</sub> ) <sub>n</sub> by C <sub>2n</sub> F <sub>4n+2</sub> , n=1-5
<b>C<sub>5</sub>F<sub>10</sub></b>	RI&88	680-730	E	perfluorocyclopentene
<b>C<sub>5</sub>F<sub>12</sub></b>	RI&88	680-730	E	perfluorocyclopentane

<b>C<sub>5</sub>F<sub>12</sub></b>	HFM87	680-730	E	comp. of perfluoro-n-alkanes. $\sigma^*(C-F)$
	IM&88	680-730	E	per-F-n-pentane, C <sub>x</sub> F <sub>2x+2</sub> series, $\sigma^*(C-F)$ dominated
<b>C<sub>5</sub>F<sub>12</sub></b>	IM&88	680-730	E	perfluoro-neo-pentane, comp. to C <sub>2</sub> F <sub>6</sub> , additional low-lying $\sigma^*(C-F)$
<b>C<sub>6</sub>FH<sub>5</sub></b>	HF&87	680-730	E	weak $\sigma^*(C-F)$
	PY&97	684-700	T	STEX, comp to HF&87
<b>C<sub>6</sub>F<sub>2</sub>H<sub>4</sub></b>	HF&87	680-730	E	(1,4 = para-difluoro), weak $\sigma^*(C-F)$
<b>C<sub>6</sub>F<sub>3</sub>H<sub>3</sub></b>	HF&87	680-730	E	(1,3,5-trifluoro), weak $\sigma^*(C-F)$
<b>C<sub>6</sub>F<sub>4</sub>H<sub>2</sub></b>	HF&87	680-730	E	(1,2,4,5 = para-dihydro), weak $\sigma^*(C-F)$
<b>C<sub>6</sub>F<sub>5</sub>H</b>	HF&87	680-730	E	weak $\sigma^*(C-F)$
<b>C<sub>6</sub>F<sub>6</sub></b>	HF&87	680-730	E	weak $\sigma^*(C-F)$
	D92a	689	P	PEPICO, PEPIPICO at $\pi^*$ res.; comp. to C 1s
<b>C<sub>6</sub>F<sub>12</sub></b>	IM&88	680-730	E	perfluoro-cyclohexane, comp. to C <sub>3</sub> F <sub>6</sub> , C <sub>4</sub> F <sub>8</sub> , $\sigma^*(C-F)$ dominated
<b>C<sub>6</sub>F<sub>14</sub></b>	HFM87	680-730	E	comp. of perfluoro-n-alkanes. $\sigma^*(C-F)$
	IM&88	680-730	E	perfluoro-n-hexane, $\sigma^*(C-F)$ dominated
	AC&95	685-710	T	STEX ab initio; absolute; growth of poly-(CF <sub>2</sub> ) <sub>n</sub> by C <sub>2n</sub> F <sub>4n+2</sub> , n=1-5
<b>C<sub>8</sub>F<sub>18</sub></b>	AC&95	685-710	T	STEX ab initio; absolute; growth of poly-(CF <sub>2</sub> ) <sub>n</sub> by C <sub>2n</sub> F <sub>4n+2</sub> , n=1-5
<b>C<sub>10</sub>F<sub>8</sub></b>	RI&88	680-730	E	perfluoronaphthalene, F1s--> $\pi^*$
<b>C<sub>10</sub>F<sub>16</sub></b>	HI88a	680-730	E	perfluoroadamantine; absolute
<b>C<sub>10</sub>F<sub>22</sub></b>	AC&95	685-710	T	STEX ab initio; absolute; growth of poly-(CF <sub>2</sub> ) <sub>n</sub> by C <sub>2n</sub> F <sub>4n+2</sub> , n=1-5
<b>C<sub>12</sub>F<sub>10</sub></b>	WC&05	686-708	E,T	biphenyl, absolute, GSCF <sub>3</sub> , ring-ring-interactions (comp to o,o-dibromo)
ClF <sub>3</sub>	BS87	680-730	E	high res.
	SB89	680-730	E	high res., partial bar. effects
<b>FH</b>	DC76	690-700	T	ab initio calc.
	MK&76	690-700	T	ab initio calc., oscillator strengths
	HB81b	680-720	E	comp. to F <sub>2</sub> spectrum
	B82a	680-720	E,R	comp. to F <sub>2</sub> spectrum, review (HB81b data)
	BD&82	680-720	E,R	review (HB81b data)
	SYD82	685-700	T	ab initio, absolute
	CC85	694	T	vibrational linewidths of discrete peak ( $\sigma^*(HF)$ ), dissociative state
	CH&85	685-695	T	ab initio, CI, reassigns HB81b spectrum
	S92	680-720	E,R	comp. of HX (X=CH <sub>3</sub> , NH <sub>2</sub> , OH, F)
	PB&99	684-694	T	variable resonant Auger if narrow band excite; time domain; excitation-decay interference
	PCT99	684-694	P	resonant Auger; dipole excitation computed; comp. to HB81; time domain; wave-packet dynamics; $^3\Sigma$ excited on low-E side of 687 band
<b>FH<sup>+</sup></b>	C05	690	T	DFT, small molecule BE and excitation energies
	MR&21	670-740	P,T	PIY, PEPIPICO, KER, compared to HO
<b>F<sub>2</sub></b>	HB81b	670-720	E	discrete $\sigma^*$ shape res.
	B82a	670-720	E,R	discrete $\sigma^*$ shape res., review (HB81b data)
	BD&82	680-720	E,R	review (HB81b data)
	SSH84b	690	T	prediction of $\sigma^*$ energy from E(Z,R)
	SG&89	680-700	T	$\sigma^*$ shape res.; pos. & shape as f(R); approx. cyl. well & ab initio
	S92	694	E,R	$\sigma^*$ position
<b>F<sub>2</sub>O</b>	IM&87	675-715	E	low-lying $\sigma^*(C-F)$
F <sub>3</sub> N	VZ&74	675-725	P	pot. bar. effects, cont. res.
	BD&82	670-770	E,R	cont. shape res., pot. bar. effects
	SBC84	680-770	E	discrete $\sigma^*$ res., shake-up cont. comp. to XPS satellite
	SSH84a	690	T	$\sigma^*$ -res./bond length relationship
<b>F<sub>4</sub>N<sub>2</sub></b>	HIR89	680-740	E	perfluoro-hydrazine, comp. to N <sub>2</sub> H <sub>4</sub>

<b>F<sub>3</sub>P</b>	SB85c	685-760	E	comp. to PX <sub>3</sub> series
	HBC96	670-740	P	TIY, PIY, PEPIPICO; comp. of PCl <sub>3</sub> , PF <sub>3</sub> , CF <sub>3</sub> PCl <sub>2</sub>
	NJ&98	670-720	P,T	absolute; GSCF3 calc.; LS-state; comp of PX <sub>3</sub> , YPF <sub>3</sub> . X=Cl,F, Y=O,S)
<b>F<sub>3</sub>OP</b>	SB85c	675-775	E	pot. bar. effects
<b>F<sub>5</sub>P</b>	SB85c	675-775	E	pot. bar. effects
<b>F<sub>2</sub>OS</b>	BHK92	680-700	T	ΔSCF, comp of all edges
<b>F<sub>4</sub>S</b>	BH87	680-750	E	comp. to S2p, S2s, S1s
	KBH90	680-700	T	ab initio, comp. to BH87; revised σ*(S-F) assignments
	BHK92	680-700	E,T	ΔSCF, comp of all edges
<b>F<sub>4</sub>Si</b>	VZ71a	680-745	P	cont. res., pot. bar. effects
	ZV71	680-750	P,R	pot. bar. effects
	ZV72	680-750	P,R	pot. bar. effects
	R75	680-700	T	alternate assignment of ZV72
	PV&82	680-720	P,T	relative, pot. bar. effects, comp. to theory
	LM&89	660-800	P	total ion yield, TOF MS; F <sup>2+</sup> yield up x2 in cont.; sel. frag.
<b>F<sub>5</sub>I</b>	CZB95	670-760	E	centrifugal pot. barrier; I 4f cont. res.; comp. to TeF <sub>6</sub> , XeF <sub>4</sub>
<b>F<sub>6</sub>S</b>	VZF71	680-760	P	absolute, pot. bar. effects, extended fine structure (EXAFS)
	D72	680-760	P,R	pot. bar. effects
	GGL72	680-770	T	ab initio calc., pot. bar. effects
	L72	680-780	P	relative, pot. bar. effects
	VZ72	.01-1.5	P	absolute, characteristic line measurements
	ZV72	675-760	P,R	pot. bar. effects
	B76b	680-1.03	E	cont. shape res., extended fine structure (EXAFS)
	H77b	680-720	T	HF improved VO; comp. to expt.
	HB78c	680-780	E	pot. bar. effects, extended fine structure (EXAFS)
	BD&82	680-690	E	calibration (a <sub>1g</sub> =688.3eV)
	GN&83	680-750	P,T	comp. of core & valence cont. shapes
	SB84	688.27(s)	E	calibration standard (a <sub>1g</sub> )
	VA&85	680-730	P,R	comp. to BF <sub>3</sub> , N <sub>2</sub> , NO <sub>3</sub> <sup>-</sup> ; KPF <sub>6</sub> (s); shape resonances
	KBH90	680-700	T	ab initio, comp. to SF <sub>4</sub> (BH87)
	NMA90	680-750	T	MS-Xα calc.; order of res. identified; comp. to expt. (ZV71)
	SB90	680-780	E	comp of TeF <sub>6</sub> , SeF <sub>6</sub> , SF <sub>6</sub> ; Z-dependence of pot. bar.s
	NMA91	680-740	T	absolute; DV-Xα; comp. to expt. (ZV71)
	BHK92	680-700	E,T	ΔSCF, comp. to expt (all edges)
	HS&93	680-735	P	relative; 0.3 eV fwhm; no vib. str; comp to (GGL72;H77;NMA90,91)
	SA93	650-750	P	XPS shakeup comp to ISEELS (HB78c); shape res. in shake spectra
	FT&95	680-720	E,T	dipole and non-dipole spectra same; 5 dipole allowed states; ΔSCF calc
	US&97	680-730	P,T	relative; TIY; polarized for energetic ions - changes observed !; βs; comp. to localized core hole calc; vibronically induced core hole localization
	FM&98	680-900	E	4 keV impact; Auger, no bound SF <sub>6</sub> <sup>++</sup> states
	U98	680-730	P,R,T	total ion yields; symmetry breaking
	EF&00	675-715	E	GOS; fifth state identified
	PS&05	680-740	P	relative, TIY, PIY, all +ves and S <sup>-</sup> , F <sup>-</sup> ; anion signals specific to shape resonances
	PU&05	687-689	P	3D ion momentum AEPIPICO, detuning energy creates fragmentation
<b>F<sub>6</sub>Se</b>	SB90	680-780	E	comp of TeF <sub>6</sub> , SeF <sub>6</sub> , SF <sub>6</sub> ; Z-dependence of potential barrriers
<b>F<sub>6</sub>Te</b>	SB90	680-780	E	comp of TeF <sub>6</sub> , SeF <sub>6</sub> , SF <sub>6</sub> ; Z-dependence of potential barrriers

#### Gadolinium 4d (145 eV)

GdF<sub>3</sub>      CP84      120-190      P      4d->f cont. res., comp. to lineshape of C84, no F-influence

Gallium 3d (19 eV)

C <sub>3</sub> H <sub>9</sub> Ga	NS&89	14-31	P	Ga(CH <sub>3</sub> ) <sub>3</sub> ; threshold e-; PI efficiency; orbital rationale of fragmentation
	NS&90	14-31	P	ZEKE, PI yield, BR, comp. of methyl-metal frag. (Bi,Ga,Zn,Ge,Sn,Pb)

Gallium 3p, 3s (102, 160 eV)

C <sub>3</sub> H <sub>9</sub> Ga	US&90c	90-260	P	Ga(CH <sub>3</sub> ) <sub>3</sub> , total & partial IYs; PIPICO; H <sup>+</sup> enhanced by sec. proc.
----------------------------------	--------	--------	---	--

Gallium 1s (10.37 keV)

AsGa	BF&93	10.3-11.1	P	GaAs; EXAFS; in situ monitor of CVD; fluorescence detection
------	-------	-----------	---	---

Germanium 3d (30 eV)

C <sub>4</sub> GeH <sub>12</sub>	NSK88	28-41	P	Ge(Me) <sub>4</sub> , thresh. e-; ionic frag.; comp. of M(Me) <sub>4</sub> M=Ge,Sn,Pb
	NS&90	28-41	P	ZEKE, PI yield, BR, comp. of M(Me) <sub>x</sub> frag. (Bi, Ga, Zn, Ge, Sn, Pb)
	BS&02B	50-450	P, T	GeMe <sub>4</sub> ; PEPPIPICO, PIPICO, partial ion yields; EICVOM calc
Cl <sub>4</sub> Ge	SN&86	21-42	P	threshold e-; review of apparatus

Germanium 3p, 3s (125,180 eV)

C <sub>4</sub> GeH <sub>12</sub>	BS&02B	50-450	P, T	GeMe <sub>4</sub> ; PEPPIPICO, PIPICO, partial ion yields; EICVOM calc
C <sub>4</sub> GeH <sub>12</sub>	KN&13	125-135	P,T	enhanced resolution,2d PES to defeat super-Coster-Kornig broaden
C <sub>10</sub> GeH <sub>20</sub> N <sub>2</sub>	LU&99	110-140	E	unsaturated germylene; broad
C <sub>10</sub> GeH <sub>22</sub> N <sub>2</sub>	LU&99	110-140	E	saturated germylene; broad
Cl <sub>4</sub> Ge	GD&96	100-300	E,T	comp. to Cl 2p, Ge2p/3p of GeCl <sub>4</sub> ; comp. to ETS
GeH <sub>4</sub>	HBK71	120-130	P	two lines at 124.7 & 129.7 eV

Germanium 2p, 2s (1210, 1420 eV)

C <sub>3</sub> ClGeH <sub>9</sub>	GD&96	1.21-1.27	P,T	ab initio SCF; comp. of GeCl <sub>4</sub> , GeH <sub>4</sub> , GeMe <sub>3</sub> Cl
Cl <sub>4</sub> Ge	M66	1.20-1.50	P	extended fine structure (EXAFS)
	PV&79	1.20-1.25	T	X- $\alpha$ (MSM) calc. of cont. shape, comp. to experiment (M66)
	GD&96	1.21-1.27	P,T	ab initio SCF; comp. of GeCl <sub>4</sub> , GeH <sub>4</sub> , GeMe <sub>3</sub> Cl
	GDT97	1.21-1.27	P,T	relative; TIY, MS-X $\alpha$ ; pot. barr.; AsCl <sub>3</sub> , PCl <sub>3</sub> , GeCl <sub>4</sub> , SnCl <sub>4</sub> comp.;
F <sub>4</sub> Ge	PV&79	1.20-1.25	T	X- $\alpha$ (MSM) calc. of cont. shape
GeH <sub>4</sub>	GD&96	1.21-1.27	P,T	ab initio SCF; comp. of GeCl <sub>4</sub> , GeH <sub>4</sub> , GeMe <sub>3</sub> Cl

Germanium 1s (11.17 keV)

GeH <sub>4</sub>	G51	11.1-12.0	P	comp. to GeCl <sub>4</sub> , absence of EXAFS
	NM&81	11.1-11.2	T	X- $\alpha$ (MSM) calc., comp. to experiment (G51)
	BB&88	11.0-11.3	P	EXAFS, expt test of multiple scat. (v.v. weak); $\sigma^*$ (Ge-Cl)
	GD&96	11.1-11.2	T	ab initio SCF; comp. to 2p, 2s calc; 2p experimental
ClGeH <sub>3</sub>	BB&88	11.0-11.3	P	EXAFS, expt test of multiple scat. (v.v. weak); $\sigma^*$ (Ge-Cl)
Cl <sub>4</sub> Ge	G51	11.1-12.0	P	(EXAFS)
	KE75	11.1-12.0	P	(EXAFS), comp. to theory
	NM&81	11.1-12.0	P	MSX- $\alpha$ ; comp. to experiment (G51, KE75)
	BB&88	11.0-11.3	P	EXAFS, experimental test of mult. scattering (v.v. weak); $\sigma^*$ (Ge-Cl)
	BM&89b	11.0-11.3	P	EXAFS, experimental test of multiple scattering (v.v. weak)

Cl <sub>4</sub> Ge (cont'd)	K92	11.0-11.3	R	survey of numerical XANES
	TH&92a	11.0-12.0	P,T	MS calc. of XFS amplitude red. factor; comp. of Br <sub>2</sub> , GeCl <sub>4</sub> , SF <sub>6</sub>
	GD&96	11.1-11.2	T	ab initio, comp. to Cl 2p, Ge2p/3p of GeCl <sub>4</sub>
	FA98	11.0-11.2	P	EXAFS; MSX $\alpha$ ; high precision – 0.1 pm accuracy; comp to ED

#### Iodine 4d (55 eV)

BrC <sub>2</sub> H <sub>4</sub> I	TH&92	50-61	P	CH <sub>2</sub> Br-CH <sub>2</sub> I; TEY; TOF-MS & PIPICO; sel. frag.; pref. Br <sup>+</sup> , I <sup>+</sup> -loss
CH <sub>3</sub> I	HB78a	45-300	E	cont. res.
	CKS80	40-120	P	photographic, laser bombardment X-ray light source
	S82	45-150	P	photographic, laser-plasma source, cont. res.; 1.72(5) eV s-o split
	LK&84	50-250	P	absolute, photoemission (TOF), d-->ef res.
	BD&85	30-60	P	ion yields, PIPICO, selective fragmentation
	DH&86	40-60	P	ion yields, PIPICO, selective fragmentation
	MN87	43-58	P	TPES, DES at σ*(C-I) res., no dissociation prior to AI
	OCB98	5-480	E	absolute; (e,2e); (e,e+ion); ion yields, dipole induced breakdown
CIN	ML&94a	40-70	P	ICN; fluor.-photoion coinc (260-600 nm); excited parent & fragment ions
	ML&95	45,95	P	fluorescence-ion coinc.; complements PEPICO and (Auger, ion)
	SL&96	95	P,R	PE3PICO; atomic fragmentation; non-Coulombic mech.; impulsive model
C <sub>2</sub> H <sub>3</sub> I	SBK88	45-100	E	high res., comp. to other vinyl halides
C <sub>6</sub> H <sub>5</sub> I	HP&78	46-62	E	cont. res.
F <sub>5</sub> I	CZB95	40-100	E	centrifugal pot. barrier; I 4f cont. res.; comp. to TeF <sub>6</sub> , XeF <sub>4</sub>
HI	KL86	50-100	T	atomic type d-->f res.; distinguished from molecular shape res.
	MN87	43-58	P	TPES, DES at σ*(C-I) res., no dissociation prior to AI
I <sub>2</sub>	CNS73	45-160	P,T	absolute, gas-solid comp., Rydberg analysis IP (57.25, 58.95)
	MB87	25-130	E	thr. electron impact; I <sup>+</sup> -yield follows 4d structure

#### Iodine 3d (650 eV)

CHI <sup>+</sup>	SG&19	610-670	P,T	I <sup>+</sup> , PIY, DFT calc; compare CH <sub>x</sub> I <sup>+</sup> (x = 0–3)
CH <sub>2</sub> I <sup>+</sup>	SG&19	610-670	P,T	I <sup>+</sup> , PIY, DFT calc; compare CH <sub>x</sub> I <sup>+</sup> (x = 0–3)
CH <sub>3</sub> I	HB78a	615-705	E	cont. res.
CH <sub>3</sub> I <sup>+</sup>	SG&19	610-670	P,T	I <sup>+</sup> , PIY, DFT calc; compare CH <sub>x</sub> I <sup>+</sup> (x = 0–3)
HI <sup>+</sup>	KG&18	610-680	P,T	PIY, compare PIY for I <sup>+</sup> and HI <sup>+</sup>
F <sub>5</sub> I	CZB95	610-720	E	centrifugal pot. barrier; I 4f cont. res.; comp. to TeF <sub>6</sub> , XeF <sub>4</sub>

#### Iodine 1s (33.2 keV)

IBr	C37	33.2	P	50 eV about edge, gas-solid comp., edge shape
I <sub>2</sub>	C37	33.2	P	50 eV about edge, gas-solid comp., edge shape

#### Iron 3p (60 eV)

B <sub>5</sub> C <sub>19</sub> FeH <sub>17</sub> O <sub>2</sub> P	HLD91	40-180	E	Cp(CO) <sub>2</sub> FeB <sub>5</sub> H <sub>2</sub> P(Ph) <sub>2</sub>
C <sub>5</sub> FeO <sub>5</sub>	MSN89	40-180	P	total, partial IYs; comp to Fe, Fe <sub>2</sub> (CO) <sub>9</sub> ; mol. giant res.
	HWR90b	50-90	E	comp. to other Fe-org, Fe2p; ligand effect on metal np
	WRH92	50-90	E	absolute, comp. of organo-iron complexes, ligand interaction effects
C <sub>7</sub> FeH <sub>6</sub> O <sub>3</sub>	WRH92	50-90	E	RFe(CO) <sub>3</sub> , R=butadiene; absolute, organo-irons; ligand interactions
C <sub>9</sub> FeH <sub>8</sub> O <sub>3</sub>	HWR90b	50-90	E	CxFe(CO) <sub>3</sub> ; comp. to other Fe-org, Fe2p; ligand effect on metal np
	WRH92	50-90	E	absolute, organo-irons; ligand interactions
C <sub>9</sub> Fe <sub>2</sub> O <sub>9</sub>	MSN89	40-180	P	total, partial IYs; comp to Fe, Fe(CO) <sub>5</sub> ; mol. giant res.
	WRH92	50-90	E	absolute, organo-irons; ligand interactions

$C_{10}FeH_{10}$	HWR90b	50-90	E	comp. to other Fe-org, Fe2p; ligand effect on metal np
	WRH92	50-90	E	absolute, organo-irons; ligand interactions
$C_{11}FeH_6O_3$	WRH92	50-90	E	RFe(CO) <sub>3</sub> , R=COT; absolute, organo-irons; ligand interactions
$C_{12}FeH_{12}$	WRH92	50-90	E	RCpFeCp R=ethylene; absolute, organo-irons; ligand interactions
$C_{14}FeH_{18}$	WRH92	50-90	E	RCpFeCp R=butane; absolute, organo-irons; ligand interactions
<b>Iron 2p, 2s (707,720, 845 eV)</b>				
$B_5C_{19}FeH_{17}O_2P$	HLD91	650-760	E	Cp(CO) <sub>2</sub> FeB <sub>5</sub> H <sub>2</sub> P(Ph) <sub>2</sub>
$C_2FeN_2O_4$	DFL92	660-670	T	Fe(CO) <sub>2</sub> (NO) <sub>2</sub> ; absolute; ab initio-SCF-CI; comp. of 3d spectra of 5 TM compounds; supports MO-model for edge resonances
$C_5FeO_5$	MSN89	650-760	P	total, partial ion yields; comp to Fe, Fe <sub>2</sub> (CO) <sub>9</sub>
	HWR90b	650-760	E	comp. to other Fe-org, Fe2p; ligand effect on metal np
( $C_5FeO_5$ cont'd)	WRH92	650-760	E	absolute, comp. of organo-iron complexes, ligand interaction effects
	FD&93	704-714	T	LCAO-SCF-CI; comp. of L-edges of organometallics
$C_7FeH_6O_3$	WRH92	650-760	E	RFe(CO) <sub>3</sub> , R=butadiene; absolute, organo-irons; ligand interactions
$C_9FeH_8O_3$	HWR90b	650-760	E	CxFe(CO) <sub>3</sub> ; comp. to other Fe-org, Fe2p; ligand effect on metal np
	WRH92	650-760	E	absolute, organo-irons; ligand interactions
$C_9Fe_2O_9$	MSN89	650-760	P	total, partial ion yields; comp to Fe, Fe(CO) <sub>5</sub>
	WRH92	650-760	E	absolute, organo-irons; ligand interactions
$C_{10}FeH_{10}$	HWR90b	650-760	E	comp. to other Fe-org, Fe2p; ligand effect on metal np
	WRH92	650-760	E	absolute, organo-irons; ligand interactions
	FD&93	704-714	T	LCAO-SCF-CI; comp. of L-edges of organometallics
	HR&93b	704-734	P	total ion yield; absolute; comp. of NiCP <sub>2</sub> , FeCp <sub>2</sub>
	G94	700-740	R	atomic multiplet calc.; review of 2p spectra of all TM cmpds
	KYN09	704-726	P, T	Fe(Cp*) <sub>2</sub> , double excitations; comp of FeCp <sub>2</sub> * <sup>+</sup> , FeCp <sub>2</sub> , FeCp <sub>2</sub> (PF <sub>6</sub> )
$C_{11}FeH_8O_3$	WRH92	650-760	E	RFe(CO) <sub>3</sub> , R=COT; absolute, organo-irons; ligand interactions
$C_{12}FeH_{12}$	WRH92	650-760	E	RCpFeCp R=ethylene; absolute, organo-irons; ligand interactions
$C_{14}FeH_{18}$	WRH92	650-760	E	RCpFeCp R=butane; absolute, organo-irons; ligand interactions
$C_{20}FeH_{30}$	KYN09	704-726	P, T	Fe(Cp*) <sub>2</sub> , double excitations; comp of FeCp <sub>2</sub> * <sup>+</sup> , FeCp <sub>2</sub> , FeCp <sub>2</sub> (PF <sub>6</sub> )

### Iron 1s (7.11 keV)

Fe(CO) <sub>5</sub>	JP58	7.10-7.15	P	gas-solid comp.
	K87	7.10-7.14	P	gas-liquid comp., identification of Rydbergs
	FDL93	7.10-7.14	T	absolute; LCAO-SCF-CI; comp. to Cr 2p results; Ni, Fe, Cr cmpds
Fe(Cp) <sub>2</sub>	JP58	7.10-7.15	P	gas-solid comp.
	FDL93	7.10-7.14	T	absolute; LCAO-SCF-CI; comp. to Cr 2p results; Ni, Fe, Cr cmpds
FeCl <sub>2</sub>	CK&83	7.10-7.13	T	absolute, energy dependent Dirac calc, spin-dependence
Fe <sub>2</sub>	WRE89b	7.10-7.15	T	DV-X $\alpha$ ; XANES; discrete res.; comp. to Ni <sub>2</sub> , Ni <sub>3</sub>

### Krypton 3d (92 eV)

ArKr	UF&08	262	P,T	PEPIPICO, interatomic coulomb decay (ICD); spin conserved processes faster than spin-flip processes; dipole forbidden processes observed
Kr <sub>2</sub>	UF&08	262	P,T	PEPIPICO, interatomic coulomb decay (ICD); spin conserved processes faster than spin-flip processes; dipole forbidden processes observed
Kr <sub>n</sub>	KWR98	89-96	P	TEY; Kr <sub>2</sub> <sup>+</sup> yield as f(<size>); site specific spectral features (surf, bulk)
Kr <sub>n</sub>	TL&02	90-93	P	surface & bulk PES peaks; do not resolve in Xe 4d – puzzle
	NHK08	90-95	P	<n>=15, exchange interaction, ion yield, Rydberg shifts
	NH&11	90-95	P	clusters, exchange interaction, ion yield, Rydberg shifts
	PT&03	90-95	P	atom vs. <N>=1000, 4000

### Krypton 2p (1680 eV)

Kr<sub>n</sub> SG&95a 1660-1760 P gas,cluster comparison, 3d exciton in cluster is 0.5 eV above gas

### Krypton 1s (14.11 keV)

(ArKr) <sub>n</sub>	NM&08	14.3-14.4	P	<n>=100; ionic fragmentation; singly charged atomic ions dominate
Kr <sub>n</sub>	SG&95a	14.3-14.4	P	gas,cluster comparison, 3d exciton in cluster is 0.5 eV above gas
	FPH97	14.2-14.9	P,T	clusters trapped in Be, Si; Feff; no EXAFS detected; shift in second XANES peak 6 NN contraction; T-dep. used to estimate DW factor
KrF <sub>2</sub>	KE&83	14.3-14.4	P	gas-solid comp., near-edge res.
	CK&85	14.3-14.4	T	absolute, shape res. at edge

### Lanthanum 4d (100 eV)

LaF<sub>3</sub> CP&80 95-145 P comp. to gas (R79) & metal La, no fluorine effect

### Lead 5d (20 eV)

C <sub>4</sub> H <sub>12</sub> Pb	NSK87	14-30	P	Pb(CH <sub>3</sub> ) <sub>4</sub> ; thresh. e-; TEPICO, ionic frag.
	NSK88	28-41	P	thresh. e-, ionic frag. yields, comp. of M(Me) <sub>4</sub> M=Ge,Sn,Pb
	NK&89	28-41	P	ZEKE, PI yield, BR, comp. of M(Me) <sub>x</sub> frag. (Bi, Ga, Zn, Ge, Sn, Pb)
	NS&90	28-41	P	ZEKE, PI yield, BR, comp. of M(Me) <sub>x</sub> frag. (Bi, Ga, Zn, Ge, Sn, Pb)

### Lead 5p,5s,4f (90,120,170 eV)

C<sub>4</sub>H<sub>12</sub>Pb NS&90 50-200 P total & partial ion yields, site/core-hole selective frag.

### Lithium 1s (55 eV)

LiCl	RS74	55-70	P	comp. to theory
LiCl	RS&76	55-70	P	photographic, gas-solid comp., Z+1 analogy
LiF	RS&76	55-70	P	photographic, gas-solid comp., Z+1 analogy
	SC76	55-65	T	multi-configuration calc. of core-excited states
LiH	SWD75	55-70	T	ab initio
	KW81	55-70	T	ab initio calc. of pot. curves (LiH, LiH <sup>+</sup> )
	DYM86	55-70	T	valence bond, ab initio, comp. to Li
Li <sub>2</sub>	SC76	55-65	T	multi-configuration calc. of core-excited states
	SB&78	56-63	P	photographic, vibnl structure, ab initio theory, pressure dependence
	DCZ83	50-110	T	one-electron, cont. X-sect.; 2 near-edge at. peaks, no shape res.
Li <sub>2</sub> Cl <sub>2</sub>	RS&76	55-70	P	comp. to N <sub>2</sub> , Li & N, no Cooper minimum
				photographic, gas-solid comp., Z+1 analogy

### Manganese 3p (60 eV)

C <sub>5</sub> MnO <sub>5</sub> Br	HSW89	40-90	E	Mn(CO) <sub>5</sub> Br, comp. to Mn(CO) <sub>10</sub>
C <sub>9</sub> H <sub>7</sub> MnO <sub>3</sub>	W92	40-90	E	Me-CpMn(CO) <sub>3</sub> , absolute
C <sub>10</sub> Mn <sub>2</sub> O <sub>10</sub>	HSW89	40-90	E	Mn <sub>2</sub> (CO) <sub>10</sub> , absolute, comp to CO, Mn(CO) <sub>5</sub> Br
C <sub>13</sub> H <sub>15</sub> MnO <sub>3</sub>	WRH89	40-90	E	Cπ*Mn(CO) <sub>3</sub> ; absolute

### Manganese 2p (645, 665 eV)

<b>C<sub>5</sub>MnO<sub>5</sub>Br</b>	RH89	620-665	E	Mn(CO) <sub>5</sub> Br, comp. to Mn(CO) <sub>10</sub>
	HWR90b	620-665	E	comp. to metal 2p; ligand effect on metal np
<b>C<sub>9</sub>H<sub>7</sub>MnO<sub>3</sub></b>	W92	620-665	E	Me-CpMn(CO) <sub>3</sub> , absolute
<b>C<sub>10</sub>Mn<sub>2</sub>O<sub>10</sub></b>	RH89	620-665	E	Mn <sub>2</sub> (CO) <sub>10</sub> , absolute, comp to CO, Mn(CO) <sub>5</sub> Br
	HWR90b	630-670	E	comp. to metal 2p; ligand effect on metal np
<b>C<sub>13</sub>H<sub>15</sub>MnO<sub>3</sub></b>	WRH89	630-670	E	C $\pi^*$ Mn(CO) <sub>3</sub> ; absolute
ClMnO <sub>3</sub>	DF&94	640-660	T	ab initio CI; relaxed orb.; trends in MO <sub>x</sub> X <sub>y</sub> (Ti,V,Cr,Mn); covalency increases as Cl 6 F
FMnO <sub>3</sub>	DF&94	640-660	T	ab initio CI; relaxed orb.; trends in MO <sub>x</sub> X <sub>y</sub> (Ti,V,Cr,Mn); covalency increases as Cl 6 F

### Manganese 1s (6.539 keV)

ClMnO <sub>3</sub>	DF&94	6.52-6.54	T	ab initio CI; relaxed orb.; MO <sub>x</sub> X <sub>y</sub> (Ti,V,Cr,Mn); coval. increases as Cl->F
FMnO <sub>3</sub>	DF&94	6.52-6.54	T	ab initio CI; relaxed orb.; MO <sub>x</sub> X <sub>y</sub> (Ti,V,Cr,Mn); coval. increases as Cl->F
Mn <sub>2</sub>	WRE89a	6.52-6.56	T	DVM-X $\alpha$ ; XANES; comp. of Co <sub>2</sub> , Mn <sub>2</sub> , Ni <sub>2</sub>

### Mercury 2p (12.3, 14.2 keV)

Cl <sub>2</sub> Hg	H31	12.2 – 14.0	P	1 <sup>st</sup> chemical state XAS ; photographic; compare Hg, HgCl <sub>2</sub>
	YK&96	12.2-13.3	P,T	T-dependent xafs; cumulants, Feff 6.0, force constants, anharmonicity

### Manganese 2p (645, 655)

Mn(C <sub>5</sub> H <sub>8</sub> O <sub>2</sub> ) <sup>+</sup>	AG&23	635-660	P	Mn(acac) ; RASPT2 calc., compare m =1,2,3
Mn(C <sub>5</sub> H <sub>8</sub> O <sub>2</sub> ) <sub>2</sub> <sup>+</sup>	AG&23	635-660	P	Mn(acac) <sub>2</sub> ; RASPT2 calc., compare m =1,2,3
Mn(C <sub>5</sub> H <sub>8</sub> O <sub>2</sub> ) <sub>3</sub> <sup>+</sup>	AG&23	635-660	P	Mn(acac) <sub>3</sub> ; RASPT2 calc., compare m =1,2,3

### Molybdenum 3d (230 eV)

C <sub>6</sub> MoO <sub>6</sub>	TD&92a	200-280	E	Mo(CO <sub>6</sub> ; comp. of 2p and 3d edges
---------------------------------	--------	---------	---	---

### Molybdenum 2p (2520,2625 eV)

C <sub>6</sub> O <sub>6</sub> Mo	TD91	2.50-2.80	P	Mo(CO) <sub>6</sub> ; XANES & EXAFS; less multipole in 2p->4d than 2p->3d
	TD&92a	2.50-2.80	P	comp. of 2p and 3d edges
	GD&95	2.52-2.64	P,T	TIY; ab initio CI; Mo d,p character of orbitals estimated
F <sub>6</sub> Mo	GH&94	2.52-2.63	P,T	comp. to crystal field multiplets; other MX <sub>6</sub> species; L <sub>3</sub> & L <sub>2</sub> edges differ
	GD&95	2.52-2.64	P,T	TIY; ab initio CI; Mo d,p character of orbitals estimated

### Molybdenum 1s (20,000 eV)

C <sub>6</sub> O <sub>6</sub> Mo	GD&95	2.52-2.64	P,T	Mo(CO) <sub>6</sub> ; TIY; ab initio CI; Mo d,p character of orbitals estimated
F <sub>6</sub> Mo	GD&95	2.52-2.64	P,T	TIY; ab initio CI; Mo d,p character of orbitals estimated

### Neon 1s (870 eV)

Ne <sub>n</sub>	FB&94	860-960	P	variable cluster size; Rydbergs, XANES and EXAFS
	BF&95a	860-960	P	EXAFS as f(cluster size); apparatus and beamline performance
	KB&97	860-920	P	near edge as f(cluster size)

Nickel 3p, 3s (78, 100 eV)

B <sub>18</sub> C <sub>4</sub> H <sub>22</sub> Ni	HLD91	40-180	E	Ni(B <sub>9</sub> H <sub>11</sub> C <sub>2</sub> ) <sub>2</sub> , Ni ballyl complex (Cp-analog)
C <sub>4</sub> NiO <sub>4</sub>	CSB90	60-110	E	Ni(CO) <sub>4</sub> ; comp. to CO
C <sub>10</sub> H <sub>10</sub> Ni	RH89b	50-200	E	Ni(Cp) <sub>2</sub> ; comp to other metallocenes
<u>Nickel 2p (860,880 eV)</u>				
C <sub>4</sub> NiO <sub>4</sub>	DFL92	855-865	T	Ni(NO) <sub>4</sub> ; absolute; ab initio-SCF-CI; comp. of 3d spectra of 5 TM compounds; supports MO-model for edge resonances
	FD&93	855-865	T	LCAO-SCF-CI; comp. of L-edges of organometallics
C <sub>6</sub> H <sub>10</sub> Ni	DFL92	855-865	T	Ni(C <sub>3</sub> H <sub>5</sub> ) <sub>4</sub> ; absolute; ab initio-SCF-CI; comp. of 3d spectra of 5 TM compounds; supports MO-model for edge resonances
C <sub>10</sub> H <sub>10</sub> Ni	RH93b	845-880	P	Ni(Cp) <sub>2</sub> ; total ion yield; comp. of NiCp <sub>2</sub> and FeCp <sub>2</sub>

Nickel 1s (8.333 keV)

(CO) <sub>4</sub> Ni	FDL93	5.98-6.04	T	Ni(CO) <sub>4</sub> ; absolute; ab initio SCF-CI; comp. to 2p; Ni, Fe, Cr cmpds
Ni <sub>2</sub>	WRE89a	8.32-8.36	T	DVM-X $\alpha$ ; comp. of Co <sub>2</sub> , Mn <sub>2</sub> , Ni <sub>2</sub> ; bond length effect (4.2-4.9 au)
Ni <sub>2</sub>	WRE89b	8.32-8.36	T	DV-X $\alpha$ ; XANES; discrete res.; comp. of Fe <sub>2</sub> , Ni <sub>2</sub> , Ni <sub>3</sub>
Ni <sub>3</sub>	WRE89b	8.32-8.36	T	DV-X $\alpha$ ; XANES; discrete res.; comp. of Fe <sub>2</sub> , Ni <sub>2</sub> , Ni <sub>3</sub>

Nitrogen 1s (410 eV)

<b>B<sub>3</sub>N<sub>3</sub>H<sub>6</sub></b>	DG&86	395-445	E	(borazine), comp. to Bz & cyclohexane, aromatic, two $\sigma^*$ res.
	VNP91	396-422	E	comp. of benzene, BN(s) and borazine; shape res. MO not R-related
	SC95	399	T	ADC local/delocal calc; Jahn-Teller localisation; comp. to B 1s, C <sub>3</sub> H <sub>3</sub> <sup>+</sup> absolute; 0.1-1 eV fwhm; low lying $\sigma^*(C-Br)$ below $\pi^*(CN)$
BrCN	OBI95	380-460	E,T	2-Br-pyrimidine; hi-res; comp of halogenated pyrimidines
BrC <sub>4</sub> H <sub>43</sub> N <sub>2</sub>	BO&10	396-415	P,T	5-Br-pyrimidine; hi-res; comp of halogenated pyrimidines
BrC <sub>4</sub> H <sub>43</sub> N <sub>2</sub>	BO&10	396-415	P,T	absolute
<b>CF<sub>3</sub>NO</b>	HIR89	390-440	E	(HCN), cont. res.
CHN	HB79a	395-435	E	cont. res., Z+1 analogy
	HB79b	395-435	E	$\sigma^*$ -res./bond length relationship
	SSH84a	420	T	$\sigma^*$ shape res.; pos. & shape as f(R); approx. cyl. well & ab initio
	SG&89	410-430	T	CNDO, systematic treatment of $\sigma^*$ energies
	LAL91	400-420	T	$\Delta$ SCF; core hole localisation; gen. rules for MO shifts in 2nd row
	ZZ&92	400-410	T	ab initio RPAE-STEX; comp of RCN (R=H,C <sub>n</sub> H <sub>2n-2</sub> , n=1,2,3,5,11); no $\sigma^*(C-C)$ in N 1s; supports building block model
	AC&94	390-430	T	HCONH <sub>2</sub> - formamide, comp. to (HCX, X=OH,F)
<b>CH<sub>3</sub>NO</b>	IH87	390-440	E	absolute; analysed as (CH <sub>3</sub> <sup>+</sup> , NO <sub>2</sub> <sup>-</sup> ); bond length corr.; 0.6 e- in N 2p
CH <sub>3</sub> NO <sub>2</sub>	VA&92	250-750	P	urea, comparison to polymers
<b>CH<sub>4</sub>N<sub>2</sub>O</b>	UH&95b	390-416	E	(NH <sub>2</sub> ) <sub>2</sub> CO, urea; absolute; modelling of polyurethane
<b>CH<sub>4</sub>N<sub>2</sub>O</b>	UH&95b	390-428	E,T	(CH <sub>3</sub> NH <sub>2</sub> - methylamine) res. at thresh.
CH <sub>5</sub> N	WB74b	395-435	E	$\sigma^*$ -res./bond length relationship
	SSH84a	410	T	$\sigma^*$ res. at thresh., comp. to (CH <sub>3</sub> ) <sub>x</sub> NH <sub>3-x</sub> , x=0-3
	SB85b	395-445	E	CNDO, systematic treatment of $\sigma^*$ energies
	LAL91	400-420	T	PIY; charge separation mass spec; decay dynamics
	TD&92b	400-450	P	absolute; selected E mass spec; no site-specific fragmentation
C <sub>2</sub> Cl <sub>3</sub> N	IO&99	390-440	P	CD <sub>3</sub> CN; relative; TIY, PIY; comp. of D/H; VARTMAN;
C <sub>2</sub> D <sub>3</sub> N	SY&99	395-440	P	anisotropic fragmentation at $\pi^*$
<b>C<sub>2</sub>F<sub>3</sub>N</b>	HS90	395-455	E	CF <sub>3</sub> CN, absolute, comp. to other triply bonded species

C <sub>2</sub> FeN <sub>2</sub> O <sub>4</sub>	SL&92	390-420	P	PEPIPICO; non-selective, step-wise fragmentation
C <sub>2</sub> H <sub>3</sub> N	HM&89	390-480	P	(CH <sub>3</sub> CN), absolute; total, partial ion yields; PIPICO, diss. IY; sel. frag.
	HTM89	390-440	E,P	comp. to solid, σ* res./bond length
	AC&94	390-430	T	ab initio RPAE-STEX; comp of RCN (R=H,C <sub>n</sub> H <sub>2n-2</sub> , n=1,2,3,5,11); no σ*(C-C) in N 1s; supports building block model
	SY&99	395-440	P	relative; TIY, PIY; D/H comp; VARTMAN; π* anisotropic frag.
	PS&01	390-426	T	STEX, extensive series of C-N compounds
	KS&06	399	P	(e,ion) coincidence, ion decay after resonant vs normal Auger
	KS&07	399	P	(e, ion) coincidence, PEPICO, PEPIPICO in AI and normal Auger
C <sub>2</sub> H <sub>3</sub> N	HTM89	390-440	E	(CH <sub>3</sub> NC), comp to CH <sub>3</sub> CN, vibrational ELS
C <sub>2</sub> H <sub>3</sub> NS	HTM89	390-440	E	(CH <sub>3</sub> SCN), comp to CH <sub>3</sub> NCS, vibrational ELS
C <sub>2</sub> H <sub>3</sub> NS	HTM89	390-440	E	(CH <sub>3</sub> NCS), comp to CH <sub>3</sub> SCN, vibrational ELS
C <sub>2</sub> H <sub>4</sub> NO <sub>2</sub>	PC&98	400-430	T	glycine; STEX; comp. of NEXAFS and circ. dichr. of amino acids
	GC&03	398-420	E,T	absolute, comp Gly, Gly-Gly; tri-gly(s); peptide bonds; GSCF3
	CG&04	282-304	E	comp. of Gly, Gly-gly, Gly <sub>3</sub> , gas-solid
	FP&09	398-413	P	comp. of Gly, Gly-gly
	PB&15	398-413	P	comp. of Gly, Gly-gly
	MG&16	399-412	P,T	comp Gly, Gly-gly
C <sub>2</sub> H <sub>5</sub> N <sub>3</sub> O <sub>2</sub>	UA&99	390-420	E	biuret; (NH <sub>2</sub> (CO)NH(CO)NH <sub>2</sub> ); absolute
	LC&07	390-420	E,T	malonamide; comp.of di-carbonyls; charge shifts for fingerprinting, GSCF3
C <sub>2</sub> H <sub>7</sub> N	SB85b	395-445	E	σ* res. at thresh., comp. of (CH <sub>3</sub> ) <sub>x</sub> NH <sub>3-x</sub> ,x=0-3
C <sub>2</sub> N <sub>2</sub>	HB79b	390-430	E	cont. res.
	SSH84a	420	T	σ*-res./bond length relationship
	SG&89	410-430	T	σ* shape res.; pos. & shape as f(R); approx. cyl. well & ab initio
C <sub>3</sub> H <sub>3</sub> N	HA&97	395-427	E,T	acrylonitrile; relative; Z+1 calc'n; π* interactions; comp. of CH <sub>2</sub> =CHCN, C <sub>2</sub> H <sub>2</sub> (CN) <sub>2</sub> , CH <sub>2</sub> =CHCH <sub>2</sub> CN
	IC&08	398-401	P,T	vibrational fine structure; rehybridization, local core hole effects. Full potential surface calculation
C <sub>3</sub> H <sub>3</sub> NO	IO&00	395-445	P	absolute; E-selected mass spec; low-lying π* <sub>N=C</sub>
C <sub>3</sub> H <sub>3</sub> NS	HH&96	392-427	P	thia-azole; absolute; E-selected mass spec; low-lying π* <sub>N=C</sub>
C <sub>3</sub> H <sub>3</sub> NO <sub>2</sub>	IO&00	395-445	P	methylcayano formate, CH <sub>3</sub> -OC(O)CN, absolute; E-selected mass spec; comp to C <sub>4</sub> H <sub>5</sub> NO <sub>2</sub> ; size dep..frag.
	TS&05	390-440	P, T	absolute, StoBE-DFT, N 1s and O 1s
C <sub>3</sub> H <sub>3</sub> N <sub>3</sub>	DR&89	395-420	P	(s-triazine); condensed films, comp. to pyrazine & pyridine; DES
	AGH93	390-430	E	absolute; comp. to solid
	PS&01	390-426	T	STEX, extensive series of C-N compounds
	DS&05	392-428	E,T	assignments revised; 405.3 ev peak attributed to (1s,π; π* <sup>2</sup> )
	VG&08	390-440	P,T	relative, transmission, double ion cell, DEMON calc, comp of 5 aza-rings
C <sub>3</sub> H <sub>3</sub> N <sub>3</sub> O <sub>2</sub>	BC&19	2402-415	P,T	2-nitroimidazole, NEXAFS, XPS, PIY; HF, DFT, MCSCF, TDDFT calc
C <sub>3</sub> H <sub>4</sub> N <sub>2</sub>	AGH93	390-430	E,P	imidazole; absolute; gas-EELS; comp. to sol.-NEXAFS
C <sub>3</sub> H <sub>4</sub> N <sub>2</sub>	DH&98	395-420	P	pyrazole, relative, 0.2 eV fwhm, Z+1 HONDO, pyrrole vs. pyrazole
C <sub>3</sub> H <sub>5</sub> N	AC&94	390-430	T	C <sub>2</sub> H <sub>5</sub> CN, ab initio RPAE-STEX; comp of RCN (R=H,C <sub>n</sub> H <sub>2n-2</sub> , n=1,2,3,5,11); no σ*(C-C) in N 1s; supports building block model
C <sub>3</sub> H <sub>6</sub> NO <sub>2</sub>	GH01	390-420	E	alanine; absolute; comp of amino acids
C <sub>3</sub> H <sub>6</sub> NO <sub>2</sub> S	PC&98	400-430	T	cysteine; (D,L) STEX; comp. of NEXAFS, circ. Dichr. of amino acids
C <sub>3</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub>	LC&07	280-320	E,T	malonamide; comp.of di-carbonyls; charge shifts for fingerprinting, GSCF3
C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub>	UH&95b	390-440	E	NH <sub>2</sub> CO <sub>2</sub> Et, absolute; modelling of polyurethane PEELS
C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub>	PC&98	400-430	T	alanine; (D,L-) STEX; comp. of NEXAFS, circ. Dichr. of amino acids
	GT&11	390-440	P, T	(alanine), gas, crystal, adsorbate comparison; conformers
C <sub>3</sub> H <sub>7</sub> NO <sub>3</sub>	PC&98	400-430	T	serine; (D,L-) STEX; comp. of NEXAFS, circ. Dichr. of amino acids

C <sub>3</sub> H <sub>9</sub> N	SB85b	395-445	E	N(Me) <sub>3</sub> ; σ* res. at thresh., comp. of (CH <sub>3</sub> ) <sub>x</sub> NH <sub>3-x</sub> ,x=0-3
	LAL91	400-420	T	CNDO, systematic treatment of σ* energies
	PS&01	390-426	T	STEX, extensive series of C-N compounds
C <sub>4</sub> ClH <sub>3</sub> N	BO&10	396-414	P,T	2-Cl-pyrimidine; hi-res; comp of halogenated pyrimidines
C <sub>4</sub> ClH <sub>3</sub> N	BO&10	396-414	P,T	5-Cl-pyrimidine; hi-res; comp of halogenated pyrimidines
C <sub>4</sub> H <sub>2</sub> N <sub>2</sub>	HA&97	395-427	E,T	dicyano-ethylene; relative; Z+1 calc'n; π* interactions; comp. of CH <sub>2</sub> =CHCN, C <sub>2</sub> H <sub>2</sub> (CN) <sub>2</sub> , CH <sub>2</sub> =CHCH <sub>2</sub> CN
C <sub>4</sub> H <sub>4</sub> FN <sub>3</sub> O	FP&11	397-414	P	(5-methylcytosine), tautomerism in cytosines
C <sub>4</sub> H <sub>4</sub> N <sub>2</sub>	PS&01	390-426	T	pyrimadine, STEX, extensive series of C-N compounds
C <sub>4</sub> H <sub>4</sub> N <sub>2</sub>	DR&89	395-420	P	pyrazine; condensed films, comp. to pyridine & triazene; DES
	PS&01	390-426	T	STEX, extensive series of C-N compounds
	VG&08	390-440	P,T	relative, transmission, double ion cell, DEMON calc, comp of 5 aza-rings
C <sub>4</sub> H <sub>2</sub> N <sub>2</sub>	HD&99	395-420	E,T	pyridazine; 0.2 eV fwhm; Z+1 calc; comp to pyridine; s-triazine
	PS&01	390-426	T	STEX, extensive series of C-N compounds
	VG&08	390-440	P,T	relative, transmission, double ion cell, DEMON calc, comp of 5 aza-rings
C <sub>4</sub> H <sub>4</sub> N <sub>2</sub>	PS&01	390-426	T	pyrimidine, STEX, extensive series of C-N compounds
	VC&06	390-420	P	TIY vs. vis-UV fluorescencence yield; state selective decay
	VG&08	390-440	P,T	relative, transmission, double ion cell, DEMON calc, comp of 5 aza-rings
C <sub>4</sub> H <sub>4</sub> N <sub>2</sub>	PS&01	396-414	P,T	(pyrimidine), STEX, extensive series of C-N compounds
	VC&06	280-320	P	TIY vs. vis-UV fluorescencence yield; state selective decay
	BO&10	283-300	P,T	hi-res; comp with 5- and 5- halogenated pyrimidines
C <sub>4</sub> H <sub>5</sub> N	PH&95	390-430	P,T	(1,2-pyrrole); comp. to polypyrrrole; π* 1 eV below in polymer; comp to other molecular solids; quasi-atomic calculation
	HH&96	392-427	P	comp. of pyrrole derivatives (N-Me, oxazole, thiazole); inductive, mesomeric efects
	NIH86	390-440	E	comp. to other heterocyclics
	DH&98	390-440	E,T	pyrazole, relative, 0.2 eV fwhm, Z+1 HONDO, pyrrole vs. pyrazole
	PS&01	390-426	T	STEX, extensive series of C-N compounds
	SU&09	398-418	P,T	TEY, relative, compared to ISEELS (DH&98), liquid, DFT; no changes on condensation or in water – inconsistent with dimer formation
C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub>	FP&10	396-412	P,T	(cytosine), tautomerism
C <sub>4</sub> H <sub>5</sub> N <sub>3</sub> O	FP&11	284-296	P	(5-fluorocytosine), tautomerism in cytosines
C <sub>4</sub> H <sub>5</sub> N	PS&01	390-426	T	(1,3-pyrrole); STEX, extensive series of C-N compounds
C <sub>4</sub> H <sub>5</sub> N	HA&97	395-427	E,T	allylcyanide; relative; Z+1 calc'n; π* interactions; comp. of CH <sub>2</sub> =CHCN, C <sub>2</sub> H <sub>2</sub> (CN) <sub>2</sub> , CH <sub>2</sub> =CHCH <sub>2</sub> CN
C <sub>4</sub> H <sub>5</sub> NO <sub>2</sub>	IO&99	390-440	P	MeO(CO)CH <sub>2</sub> CN; absolute; N1s, O1s → π* mass spect; site sel. frag.
	IO&00	395-445	P	absolute; E-selected mass spec; comp to C <sub>3</sub> H <sub>3</sub> NO <sub>2</sub> ; size dep..frag.
	TS&05	390-440	P, T	absolute, StoBE-DFT, N 1s and O 1s
C <sub>4</sub> H <sub>5</sub> N <sub>3</sub> O	FP&10	398-412	P,T	(uracil), tautomerism
C <sub>4</sub> H <sub>7</sub> N	AC&94	390-430	T	C <sub>3</sub> H <sub>7</sub> CN, ab initio RPAE-STEX; comp of RCN (R=H,C <sub>n</sub> H <sub>2n-2</sub> , n=1,2,3,5,11); no σ*(C-C) in N 1s; supports building block model
C <sub>4</sub> H <sub>7</sub> N	PS&01	390-426	T	(1-pyyroline), STEX, extensive series of C-N compounds
C <sub>4</sub> H <sub>7</sub> N	PS&01	390-426	T	(2-pyyroline), STEX, extensive series of C-N compounds
C <sub>4</sub> H <sub>7</sub> N	PS&01	390-426	T	(3-pyyroline), STEX, extensive series of C-N compounds
C <sub>4</sub> H <sub>7</sub> NO <sub>2</sub>	LC&07	390-420	E,T	Me(CO)N(CO)Me; di-acetamide; di-carbonyls; charge shifts, GSCF3
C <sub>4</sub> H <sub>7</sub> NO <sub>4</sub>	UH&99	395-435	E,T	ethyl allophanate; absolute; GSCF3; comp. of urethane species
C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> O <sub>4</sub>	CG&04	390-420	E	(glycyl-glycine), comp. of Gly, Gly-gly, Gly <sub>3</sub> , gas-solid
	FP&09	398-413	P	comp. of Gly, Gly-gly
	PB&15	398-413	P	comp. of Gly, Gly-gly
C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> O <sub>3</sub>	GC&03	398-420	E,T	absolute, comp Gly, Gly-Gly; tri-gly(s); peptide bonds; GSCF3
C <sub>4</sub> H <sub>9</sub> N	NIH86	390-440	E	(pyrrolidine), comp. to other heterocyclics
	PS&01	390-426	T	(1-pyyroline), STEX, extensive series of C-N compounds

<b>C<sub>5</sub>H<sub>2</sub>N<sub>4</sub></b>	AGH93	390-430	E,P	dicyano-imidazole; absolute; gas-EELS; comp. to sol.-NEXAFS
<b>C<sub>5</sub>H<sub>5</sub>N</b>	HS&85	390-440	E,P	(pyridine), gas, solid, monolayer comp.
	AV&85	396-423	P	absolute, $I(2\pi^*/1\pi^*)=1.3$ versus 6 (HS&85), comp. of C <sub>6</sub> H <sub>6</sub> , C <sub>6</sub> H <sub>5</sub> X
	DR&89	395-420	P	condensed films, comp. to pyrazine & triazene; DES
	ED&90	399	P	DES, dynamic screening effects; comp. of N <sub>2</sub> , N <sub>2</sub> O & azabenzenes
	H90a	390-440	E	comp. to reflection EELS of surf. adsorbed Py (on Ag)
	HD&99	395-420	E,T	0.2 eV fwhm; Z+1 calc; comp to pyridazine; s-triazine
	CPA01	390-430	T	STEX with screening; comp. to expt. (HS&85)
	KP&01	395-415	P,T	relative; high res – 150 meV; DFT; vibrations resolved; $\pi^*$ intensities
	PS&01	390-426	T	STEX, extensive series of C-N compounds
	FB&03b	398-400	P	partial ion yield, molecule - dicluster compared; 50 meV shift
	IH07	396-414	T	relative, Gaussian augmented plane wave (GAPW) - DFT; (-5 to +3 eV errors on 14 small molecules, compared to KP&01
	VG&08	390-440	P,T	relative, transmission, double ion cell, DEMON calc, comp of 5 aza-rings
	LG&09	398-400	P	relative, comparison of molecular and cluster $\pi^*$ , red-shift in cluster
<b>C<sub>5</sub>H<sub>5</sub>N<sub>5</sub>O</b>	PF&09	390-420	P,T	(gauanine) Tautomerism, thermal gas, DFT calc; Boltzmann-weighted
<b>C<sub>5</sub>H<sub>7</sub>N</b>	HH&96	390-430	P	N-methyl pyrrole; inductive, mesomeric effects
	PS&01	390-426	T	STEX, extensive series of C-N compounds
<b>C<sub>5</sub>H<sub>7</sub>N</b>	PS&01	390-426	T	(1,4-dihydropyridine), STEX, extensive series of C-N compounds
<b>C<sub>5</sub>H<sub>7</sub>N</b>	PS&01	390-426	T	(2,3-dihydropyridine), STEX, extensive series of C-N compounds
<b>C<sub>5</sub>H<sub>7</sub>N<sub>3</sub>O</b>	FP&11	397-414	P	(isocytosine), tautomerism in cytosines
<b>C<sub>5</sub>H<sub>7</sub>N<sub>5</sub></b>	PS&01	390-426	T	(2-amino, 4,5-imidazoledicarbonitrile), STEX, extensive C-N compounds
<b>C<sub>5</sub>H<sub>11</sub>N</b>	PS&01	390-426	T	(piperidine), STEX, extensive series of C-N compounds
<b>C<sub>5</sub>H<sub>10</sub>N<sub>2</sub></b>	HE&01	395-420	E	methyl-carbene; thermal decomposition of tetra-amino ethylene
<b>C<sub>5</sub>H<sub>11</sub>N</b>	NIH86	390-440	E	(piperidine), absolute, heterocycles
	PS&01	390-426	T	STEX, extensive series of C-N compounds
<b>C<sub>5</sub>H<sub>11</sub>NO<sub>2</sub></b>	PC&98	400-430	T	valine; (D,L-) STEX; comp. of NEXAFS, circ. Dichr. of amino acids
<b>C<sub>5</sub>H<sub>15</sub>NSi</b>	UH94b	390-440	E	Me <sub>3</sub> Si(NMe <sub>2</sub> ); comp. of Si-N cmpds; models for SiN <sub>x</sub> O <sub>y</sub> films
<b>C<sub>6</sub>H<sub>4</sub>N<sub>2</sub>S</b>	HD&91	390-430	E	Bz(N-S) ring; comp. of S-N heterocyles, aromaticity
<b>C<sub>6</sub>H<sub>4</sub>N<sub>2</sub>S<sub>2</sub></b>	HD&91	390-430	E	Bz(N-S) ring; comp. of S-N heterocyles, aromaticity
<b>C<sub>6</sub>H<sub>4</sub>N<sub>2</sub>S<sub>3</sub></b>	HD&91	390-430	E	Bz(N-S) ring; comp. of S-N heterocyles, aromaticity
<b>C<sub>6</sub>H<sub>5</sub>NO<sub>2</sub></b>	TUH96	390-430	E,T	nitrobenzene; absolute, EHMO, comp. to aniline, nitroanilines
<b>C<sub>6</sub>H<sub>6</sub>N<sub>2</sub>O<sub>2</sub></b>	TUH96	390-430	E,T	(1,2)-nitroaniline; absolute, EHMO, comp. to aniline, nitrobenzene
<b>C<sub>6</sub>H<sub>6</sub>N<sub>2</sub>O<sub>2</sub></b>	TUH96	390-430	E,T	(1,3)-nitroaniline; absolute, EHMO, comp. to aniline, nitrobenzene
<b>C<sub>6</sub>H<sub>6</sub>N<sub>2</sub>O<sub>2</sub></b>	TUH96	390-430	E,T	(1,4)-nitroaniline; absolute, EHMO, comp. to aniline, nitrobenzene
<b>C<sub>6</sub>H<sub>7</sub>N</b>	HUR93	390-430	E	aniline, comp. to dimethylaniline
	TUH96	390-430	E,T	absolute, EHMO, comp. to nitrobenzene, nitroanilines
	PY&97	395-425	T	STEX, comp to TUH96; ring substituent effects (Bz-X, X=F,OH,NH <sub>2</sub> )
	PP&00	399	T	MC-SCF Z+1 calc; vibrational structure, XPS better than NEXAFS
	CPA01	280-320	T	STEX with screening; comp. to expt. (HUR93)
<b>C<sub>6</sub>H<sub>12</sub>N<sub>2</sub></b>	RUH95	390-430	E	DABCO; absolute
<b>C<sub>6</sub>H<sub>9</sub>N<sub>3</sub>O<sub>3</sub></b>	UA&99	390-430	E	trimethyl-isocyanurate; absolute; polymer model
<b>C<sub>6</sub>H<sub>12</sub>N<sub>2</sub>Si</b>	UH&94b	390-420	E	bis(dimethylamino)dimethylsilane; exploring Si-N bond
<b>C<sub>6</sub>H<sub>16</sub>N<sub>2</sub>O<sub>5</sub></b>	GC&03	390-420	E	Gly-Gly-Gly, absolute, comp to Gly, Gly-Gly
<b>C<sub>6</sub>H<sub>14</sub>N<sub>4</sub>O<sub>2</sub></b>	LH&12	398-407	T	(arginine), gas-solid comparison
<b>C<sub>7</sub>F<sub>5</sub>N</b>	IOG97	390-440	P	C <sub>6</sub> F <sub>5</sub> CN; absolute; reflectron TOF; $\pi^*$ split; sym. resolved; comp. of (C <sub>7</sub> F <sub>5</sub> N, C <sub>6</sub> H <sub>5</sub> CN,p-CF <sub>3</sub> C <sub>6</sub> H <sub>4</sub> CN, p-CF <sub>3</sub> C <sub>6</sub> H <sub>4</sub> NCO)
	IO&99	390-430	P	TIY; comp of Cl's, N1s; no site selectivity; mass spec at $\pi^*$ <sub>ring</sub>
<b>C<sub>7</sub>H<sub>5</sub>N</b>	H92a	390-440	E,T	(benzonitrile), absolute; EHMO
	PS&01	390-426	T	STEX, extensive series of C-N compounds
<b>C<sub>7</sub>H<sub>7</sub>NO<sub>2</sub></b>	UH&95b	390-440	E	NH <sub>2</sub> CO <sub>2</sub> Ph, absolute

<b>C<sub>7</sub>H<sub>8</sub>N<sub>2</sub>O</b>	UH&95a	390-430	E	NH <sub>2</sub> CO <sub>2</sub> Ph,phenylurea; absolute; comp. to model polyurethanes
	UH&95b	390-440	E	absolute; ureas and urethanes similar at N 1s
<b>C<sub>7</sub>H<sub>8</sub>N<sub>2</sub>O</b>	UH&95a	390-420	E	phenylurea; absolute; modelling of polyurethane PEELS
<b>C<sub>7</sub>H<sub>9</sub>N</b>	UH96	390-430	E	N-methyl aniline; absolute
<b>C<sub>7</sub>H<sub>15</sub>N</b>	AC&94	390-430	T	C <sub>6</sub> H <sub>15</sub> CN, ab initio RPAE-STEX; comp of RCN (R=H,C <sub>n</sub> H <sub>2n-2</sub> , n=1,2,3,5,11); no σ*(C-C) in N 1s; supports building block model
<b>C<sub>7</sub>H<sub>18</sub>N<sub>3</sub>Si</b>	UH&94b	390-430	E	tris(dimethylamino)methylsilane; exploring Si-N bond
<b>C<sub>8</sub>F<sub>3</sub>H<sub>4</sub>NO</b>	IO&99	390-440	P	p-CF <sub>3</sub> C <sub>6</sub> H <sub>4</sub> NCO; TIY; N1s, O1s → π* frag.; no site selectivity
<b>C<sub>8</sub>H<sub>7</sub>N</b>	KB&18	420	P	indole, PEPICO, fragmentation kinetics, coincidence ang. dep.
<b>C<sub>8</sub>H<sub>9</sub>NO</b>	UH&95b	390-430	E	benzyl carbamate; absolute; modelling polyurethanes
<b>C<sub>8</sub>H<sub>9</sub>NO</b>	TC&16	2399-415	P,T	acetanilide; TIY; TD-LB94/6-31+G(d,p); comp to cis-Nbenzylacetamide
<b>C<sub>8</sub>H<sub>9</sub>NO<sub>2</sub></b>	GH01	390-430	E	phenylalanine, comp. of amino acids
<b>C<sub>8</sub>H<sub>11</sub>N</b>	HUR93	390-430	E	N,N-dimethylaniline
<b>C<sub>8</sub>H<sub>16</sub>N<sub>4</sub>O<sub>4</sub></b>	LK&20b	396-410	P,T	protonated tetra-glycine (G <sub>4</sub> P), NEXAMS, protonation site identification
<b>C<sub>8</sub>H<sub>24</sub>N<sub>4</sub>Si</b>	UH94b	390-440	E	Si(NMe <sub>2</sub> ) <sub>4</sub> ; comp. of Si-N cmpds; models for SiN <sub>x</sub> O <sub>y</sub> films
<b>C<sub>9</sub>H<sub>6</sub>N<sub>2</sub>O<sub>2</sub></b>	UHR99	390-420	E,T	2,4-TDI, absolute; isomeric effect
<b>C<sub>9</sub>H<sub>6</sub>N<sub>2</sub>O<sub>2</sub></b>	UHR99	390-420	E,T	2,6-TDI, absolute; isomeric effect
<b>C<sub>9</sub>H<sub>7</sub>N</b>	PS&01	390-426	T	(quinoline), STEX, extensive series of C-N compounds
<b>C<sub>9</sub>H<sub>7</sub>N</b>	PS&01	390-426	T	(isoquinoline), STEX, extensive series of C-N compounds
<b>C<sub>9</sub>H<sub>9</sub>N</b>	ZC&09	396-4105	P	(3-methyl indone); tautomers, comp aromatic amino acids
<b>C<sub>9</sub>H<sub>11</sub>NO<sub>2</sub></b>	UH&95b	390-440	E	Ph-NHCO <sub>2</sub> Et, absolute; modelling of polyurethane PEELS
<b>C<sub>9</sub>H<sub>11</sub>NO<sub>2</sub></b>	GW09	399-413	T	phenylalanine,DFT, comp to C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub> , C <sub>6</sub> H <sub>6</sub> , C <sub>8</sub> H <sub>10</sub> O <sub>2</sub> , C <sub>8</sub> H <sub>11</sub> N
	ZC&09	399-413	P	(3-methyl indone); tautomers, comp aromatic amino acids
<b>C<sub>9</sub>H<sub>11</sub>NO</b>	TC&16	399-414	P,T	cis-Nbenzylacetamide ; TIY; TD-LB94/6-31+G(d,p); comp to acetanilide
<b>C<sub>9</sub>H<sub>11</sub>NO<sub>3</sub></b>	ZC&09	399-413	P	(tyrosine), tautomers, comp aromatic amino acids
<b>C<sub>9</sub>H<sub>12</sub>NO</b>	LKC16	397-406	P, T	TEMPO, relative, ΔDFT-GGA, complex spectra
<b>C<sub>9</sub>H<sub>27</sub>NSi<sub>3</sub></b>	UH94b	390-440	E	N(SiMe <sub>3</sub> ) <sub>3</sub> ; comp. of Si-N cmpds; models for SiN <sub>x</sub> O <sub>y</sub> films
<b>C<sub>10</sub>H<sub>8</sub>N<sub>4</sub></b>	PS&01	390-426	T	(2,5-dimethyl-N,N'-dicyanoquinonediimine), STEX, extensive series of C-N compounds
<b>C<sub>10</sub>H<sub>11</sub>N<sub>2</sub>O<sub>2</sub></b>	LKC16	397-406	P, T	nit8, TEMPO, relative, ΔDFT-GGA, complex spectra
<b>C<sub>10</sub>H<sub>13</sub>N<sub>2</sub>O<sub>2</sub></b>	LKC16	397-406	P, T	nit9, TEMPO, relative, ΔDFT-GGA, complex spectra
<b>C<sub>10</sub>H<sub>27</sub>N</b>	PS&01	390-426	T	N('Bu) <sub>3</sub> , STEX, extensive series of C-N compounds
<b>C<sub>10</sub>H<sub>18</sub>N<sub>5</sub>O<sub>5</sub></b>	LK&20b	396-410	P,T	pentaglycine (G <sub>5</sub> ), NEXAMS, protonation site identification
<b>C<sub>10</sub>H<sub>19</sub>N<sub>2</sub>O<sub>2</sub></b>	LC&07	390-428	E,T	comp.of di-carbonyls; charge shifts for fingerprinting, GSCF3
<b>C<sub>10</sub>H<sub>20</sub>N<sub>2</sub></b>	LU&99	394-418	E	tBu-NC=CN-tBu; absolute; ligand rel. to cyclic diamino C:,Si:,Ge.
	HE&01	395-420	E	reference for thermal decomposition of tetra-amino ethylene
<b>C<sub>10</sub>H<sub>20</sub>N<sub>2</sub>Ge</b>	LU&99	396-412	E,T	c-Ge(RNCH=CHNR), comp.cyclic diamino C:, Si:, Ge: ; GSCF3 ab initio
<b>C<sub>10</sub>H<sub>20</sub>N<sub>2</sub>Si</b>	UH&98	396-412	E,T	c-Si(RNCH=CHNR), R=tBu, silylene; absolute; delocal. in Si-N-C=C
	LU&99	394-418	E,T	absolute; comparison of cyclic diamino C:, Si:, Ge: ; GSCF3 ab initio
<b>C<sub>10</sub>H<sub>22</sub>N<sub>2</sub></b>	LU&99	394-418	E	tBu-NCH <sub>2</sub> CH <sub>2</sub> N-tBu; absolute; ligand rel. to cyclic diamino C:,Si:,Ge.
<b>C<sub>10</sub>H<sub>22</sub>N<sub>4</sub></b>	HE&01	395-420	E	tetra-amino ethylene; used for thermal decomposition to form carbene
<b>C<sub>10</sub>H<sub>22</sub>N<sub>2</sub>Ge</b>	LU&99	396-412	E,T	c-Ge(RNCH <sub>2</sub> CH <sub>2</sub> NR), comp. cyclic diamino C:, Si:, Ge: ; GSCF3 ab initio
<b>C<sub>10</sub>H<sub>22</sub>N<sub>2</sub>Si</b>	UH&98	396-412	E,T	c-Si(RNCH <sub>2</sub> CH <sub>2</sub> NR), R=tBu, unsat. silylene; absolute;
	LU&99	394-418	E,T	absolute; comparison of cyclic diamino C:, Si:, Ge: ; GSCF3 ab initio
<b>C<sub>10</sub>H<sub>22</sub>N<sub>2</sub>Ge</b>	LU&99	396-412	E,T	c-H <sub>2</sub> Ge(RNCH=CHNR), cyc. diamino C:, Si:, Ge: comp ; GSCF3 ab initio
<b>C<sub>10</sub>H<sub>22</sub>N<sub>2</sub>Si</b>	UH&98	396-412	E,T	c-H <sub>2</sub> Si(RNCH=CHNR), R=tBu, silylene; absolute; no delocal.
	LU&99	394-418	E,T	absolute; comparison of cyclic diamino C:, Si:, Ge: ; GSCF3 ab initio
<b>C<sub>10</sub>H<sub>24</sub>N<sub>2</sub>Ge</b>	LU&99	396-412	E,T	c-H <sub>2</sub> Ge(RNCH <sub>2</sub> CH <sub>2</sub> NR), cyc. diamino C:, Si:, Ge: comp; GSCF3 ab initio
<b>C<sub>10</sub>H<sub>24</sub>N<sub>2</sub>Si</b>	UH&98	396-412	E,T	c-H <sub>2</sub> Si(RNCH <sub>2</sub> CH <sub>2</sub> NR), R=tBu, unsat. silylene; absolute;
	LU&99	394-418	E,T	absolute; comparison of cyclic diamino C:, Si:, Ge: ; GSCF3 ab initio
<b>C<sub>10</sub>H<sub>13</sub>NO<sub>2</sub></b>	UH&95b	390-440	E	Ph-N(CH <sub>3</sub> )-CO <sub>2</sub> Et, absolute; modelling of polyurethane PEELS
<b>C<sub>11</sub>H<sub>12</sub>N<sub>2</sub>O<sub>2</sub></b>	ZC&09	398-416	P	(tryptophan) tautomers, comp aromatic amino acids

<b>C<sub>11</sub>H<sub>14</sub>N<sub>2</sub>O<sub>4</sub></b>	UHR99	390-440	E	TDI-bis-methyl urethane; absolute
<b>C<sub>11</sub>H<sub>20</sub>N<sub>2</sub></b>	LU&99	396-412	E,T	c-C:(RNCH=CHNR), comparison of cyclic diamino C:, Si:, Ge: ; GSCF3 ab initio; saturated carbene
<b>C<sub>11</sub>H<sub>22</sub>N<sub>2</sub></b>	LU&99	396-412	E,T	c-C:(RNCH <sub>2</sub> CH <sub>2</sub> NR), comparison of cyclic diamino C:, Si:, Ge: ; GSCF3 ab initio; unsaturated carbene
<b>C<sub>11</sub>H<sub>24</sub>N<sub>2</sub></b>	LU&99	396-412	E,T	c-H <sub>2</sub> C:(RNCH <sub>2</sub> CH <sub>2</sub> NR), comparison of cyclic diamino C:, Si:, Ge: ; GSCF3 ab initio; protonated carbene
<b>C<sub>12</sub>H<sub>4</sub>N<sub>4</sub></b>	PS&01	390-426	T	(tetracyano-quinodimethane), STEX, extensive series of C-N compounds
<b>C<sub>12</sub>H<sub>15</sub>N<sub>2</sub>O<sub>2</sub>Re</b>	HS92	390-440	E	Cπ*Re(CO) <sub>2</sub> N <sub>2</sub> ; absolute; split N1s->π* (N <sub>a</sub> -N <sub>b</sub> chem. shift)
<b>C<sub>12</sub>H<sub>23</sub>N</b>	AC&94	390-430	T	C <sub>11</sub> H <sub>23</sub> N, ab initio RPAE-STEX; comp of RCN (R=H,C <sub>n</sub> H <sub>2n-2</sub> , n=1,2,3,5,11); no σ*(C-C) in N 1s; supports building block model
<b>C<sub>13</sub>H<sub>9</sub>N</b>	PS&01	390-426	T	(6,7-benzoquinoline), STEX, extensive series of C-N compounds
<b>C<sub>13</sub>H<sub>9</sub>N</b>	PS&01	390-426	T	(acridine), STEX, extensive series of C-N compounds
<b>C<sub>13</sub>H<sub>12</sub>N<sub>2</sub>O</b>	UH&95b	390-440	E	(Ph-NH) <sub>2</sub> C=O, absolute; modelling of polyurethane PEELS
	UA&99	390-430	E	tritylilisocyanurate; absolute, polymer model
<b>C<sub>14</sub>H<sub>14</sub>N<sub>12</sub>O<sub>3</sub></b>	WR&98	398-412	P,T	5'-d <sup>F</sup> UAG nuclic acid oligimer, 20K cryo-ion trap
<b>C<sub>14</sub>H<sub>25</sub>N<sub>5</sub>O<sub>4</sub></b>	LK&20b	396-410	P,T	proline- tetra-glycine (RG <sub>4</sub> ), NEXAMS, protonation site identification
<b>C<sub>14</sub>H<sub>29</sub>N<sub>7</sub>O<sub>6</sub></b>	LK&20b	396-410	P,T	arginine- tetra-glycine (RG <sub>4</sub> ), NEXAMS, protonation site identification
<b>C<sub>15</sub>H<sub>25</sub>N<sub>6</sub>O<sub>4</sub></b>	LK&20b	396-410	P,T	histidine- tetra-glycine (RG <sub>4</sub> ), NEXAMS, protonation site identification
<b>C<sub>15</sub>H<sub>26</sub>N<sub>5</sub>O<sub>6</sub></b>	LK&20b	396-410	P,T	lysine- tetra-glycine (RG <sub>4</sub> ), NEXAMS, protonation site identification
<b>C<sub>16</sub>H<sub>19</sub>N<sub>4</sub>O<sub>2</sub></b>	XX04	390-430	E	toluene ethyl urea, absolute
<b>C<sub>21</sub>H<sub>15</sub>N<sub>3</sub>O<sub>3</sub></b>	UHR92	390-440	E	(Bz-O) <sub>3</sub> C3N3 (tri-phenoxy-triazine); polyurethane modelling
	UA&99	390-430	E	absolute, polymer model
<b>C<sub>24</sub>H<sub>21</sub>N<sub>3</sub>O<sub>3</sub></b>	UA&99	390-430	E	tritylilisocyanurate; absolute, polymer model
<b>C<sub>27</sub>H<sub>35</sub>N<sub>5</sub>O<sub>7</sub>S</b>	DS&21	397-413	P,T	[LeuEnk+H], , ENK-Tyr-Gly-Gly-Phe); NEXAMS; DFT/ROCIS
<b>C<sub>28</sub>H<sub>37</sub>N<sub>5</sub>O</b>	DS&21	397-413	P,T	MetEnk+H], ENK = Tyr-Gly-Gly-Phe); mass spec; keto-enol; DFT/ROCIS
<b>C<sub>32</sub>H<sub>16</sub>N<sub>8</sub>Ni</b>	RSH93	50-450	E	Ni-phythalocyanine; compared to solid
<b>C<sub>34</sub>H<sub>24</sub>N<sub>11</sub>O<sub>16</sub>P<sub>2</sub></b>	WR&21	398-412	P,T	5' -d <sup>F</sup> (UAG) (nucleotide-phosphate trimer; PIT, NEXAMS
<b>C<sub>42</sub>H<sub>52</sub>FeN<sub>8</sub>O<sub>6</sub>S<sub>2</sub></b>	MC12	392-412	P	cytochrome c (12 kDa), NEXAMS
	MG&16	392-412	P	NEXAMS
<b>C<sub>80</sub>NSc<sub>3</sub><sup>m</sup></b>	MM&20	398-420	T	endohedral fullerene (m =-1, 0, +1 +2, +3, +4) (relative E-scale
<b>C<sub>131</sub>H<sub>229</sub>N<sub>39</sub>O<sub>31</sub><sup>+</sup></b>	EB&18	398-420	P	Melittin protein, NEXAMS, PIY
<b>C<sub>400</sub>N<sub>110</sub>O<sub>150</sub>S<sub>3</sub></b>	MN&15	393-413	P	ubiquitin protein (formula is approx); electrospray MS, and partial ion yield
<b>D<sub>3</sub>N</b>	ST&93	400-405	P,T	high res; ab initio; no resolved vib; comp. to NH <sub>3</sub> (no 3s vibronic); comp of H <sub>2</sub> O, NH <sub>3</sub> , CH <sub>4</sub> re Ryd/val char.
<b>F<sub>3</sub>N</b>	ZV72	396-415	P	pot. barr. effects
	BK74	396-415	P	pot. barr. effects
	VZ&74	398-425	P	pot. barr. effects
	BD&82	400-450	E,R	pot. barr. effect
	DR83	390-415	E	ion yield appearance pot., 1s->π* thresh. observed
	SBC84	400-450	E	discrete σ*(N-F), shake-up continua comp. to XPS satellite
	SSH84a	420	T	σ*-res./bond length relationship
	LAL91	400-420	T	CNDO, systematic treatment of σ* energies
	JC01	397-417	P	relative; comparison of NX <sub>3</sub> , PX <sub>3</sub> 1s edges; pot. barr. effects
<b>F<sub>4</sub>N<sub>2</sub></b>	HIR89	390-440	E	per-fluorohydrazine, comp to N <sub>2</sub> H <sub>4</sub> , NH <sub>3</sub>
<b>HN<sup>+</sup></b>	BI&19	390-435	P,T	PIY, XMolecule calc, compare N <sup>+</sup> , HN <sup>+</sup> , H <sub>2</sub> N <sup>+</sup> , H <sub>2</sub> N <sup>+</sup> nexafs
<b>H<sub>2</sub>N</b>	CC&82	405-415	T	ab initio calc. (CI)
<b>H<sub>2</sub>N<sup>+</sup></b>	BI&19	390-435	P,T	PIY, XMolecule calc, compare N <sup>+</sup> , HN <sup>+</sup> , H <sub>2</sub> N <sup>+</sup> , H <sub>2</sub> N <sup>+</sup> nexafs
<b>H<sub>3</sub>N</b>	WB74b	395-435	E	weak cont. features
	WB74g	395-425	T	Z+1 analogy
	WB74h	395-425	E	Z+1 analogy
	S75b	400-420	T	Z+1 analogy calc., comp. to expt. (WB74b)

(NH <sub>3</sub> cont'd)	DC76	400-420	T	absolute
	S76a	400-420	T	Z+1 analogy calc., comp. to expt. (WB74b)
	S76b	400-420	T	Z+1 analogy calc., comp. to expt. (WB74b)
	A80	400-415	P	relative, see SYD82
	AVZ82b	400-412	P	comp. to H <sub>2</sub> O, CH <sub>4</sub> , Ne, 3p splitting=0.6eV
	SYD82	400-415	T	ab initio, absolute, comp. to expt (A80)
	DR83	390-415	E	ion yield appearance pot.; 1s-> $\pi^*$ thresh. observed
	RR&83	395-435	P	H <sup>+</sup> IY from surface of condensed NH <sub>3</sub> , EY, extra peak at 420eV
	SSH84a	420	T	$\sigma^*$ -res./bond length relationship
	CH&85	400-410	T	Rydberg assignments comp. to 2nd & 3rd row hydrides
	SB85b	399-410	E	0.14eV FWHM, further Ryd. resolved & reassigned, as AVZ82b
	AVZ88	400-425	P	absolute; comp. of NH <sub>3</sub> , N <sub>2</sub> , Ne; res. effects; atomic 2p resonance
	H90a	395-425	E,R	absolute, comp. of N <sub>2</sub> , NH <sub>3</sub> , N <sub>2</sub> H <sub>4</sub> , Ne; $\sigma^*$ vs. Ryd
	MR&90	390-440	P	H <sup>+</sup> des. from Ru-adsorbed; comp. to AEY, TEY, gas (WB74b)
	RC&90	390-440	P	comp. of gas, solid; ion yields, H <sup>+</sup> ultrafast diss.
	LAL91	400-420	T	CNDO, systematic treatment of $\sigma^*$ energies
	S92	395-435	E,R	comp. of NH <sub>3</sub> , N <sub>2</sub> H <sub>4</sub> , N <sub>2</sub> ; $\sigma^*(N-N)$
	ST&93	400-405	P,T	high res; ab initio; no resolved vib; comp. to NH <sub>3</sub> (no 3s vibronic); comp of H <sub>2</sub> O, NH <sub>3</sub> , CH <sub>4</sub> re Ryd/val char.NH <sub>4</sub>
	KNP92	400-408	T	SCF-CI in (Z+1) approx.
	MH&95	420	P	Auger-ion-ion coincidence; KERDs; mapping NH <sub>3</sub> <sup>2+</sup> potential surface; simultaneous vs. sequential bond breaking
	JC01	397-417	P	relative; comparison of NX <sub>3</sub> , PX <sub>3</sub> 1s edges; pot. barr. Effects
	C05	404	T	DFT, small molecue BE and excitation energies
	LG&05	400-405	P	TIY, PEPICO, alignment modelled
	SG&05	400-407	P	TIY, PIY, vibrationally resolved, NH <sub>3</sub> <sup>2+</sup> yield strongly v dependent
	JV&07	399-407	P	partial luminescence yield, Balmer lines (H*), ultrafast decay
H <sub>3</sub> N <sup>+</sup>	BI&19	390-435	P,T	PIY, XMolecule calc, compare N <sup>+</sup> , HN <sup>+</sup> , H <sub>2</sub> N <sup>+</sup> , H <sub>2</sub> N <sup>+</sup> nexafs
H <sub>4</sub> N <sub>2</sub>	HIR89	390-440	E	hydrazine, comp to N <sub>2</sub> F <sub>4</sub> , NH <sub>3</sub>
	H90a	395-425	E,R	absolute, comp. of N <sub>2</sub> , NH <sub>3</sub> , N <sub>2</sub> H <sub>4</sub> , Ne; $\sigma^*$ vs. Ryd
	S92	395-435	E,R	comp. of NH <sub>3</sub> , N <sub>2</sub> H <sub>4</sub> , N <sub>2</sub> ; $\sigma^*(N-N)$
NO	GSM73	395-425	P	absorption saturation distortion
	MN74	397-412	P	photographic, Z+1 analogy, Rydberg analysis IP (409.9 eV)
	MN&74a	397-410	P	photographic, 0.05A res., Z+1 analogy
	MN&74b	397-410	P	photographic, 0.05A res., Z+1 analogy
	WB74c	395-438	E	cont. res., Z+1 analogy
	KMK79	395-425	T	ab initio calc., comp. to expt. (WBW74c), 2 e- transitions
	TKR80	399-401	E	<70meV FWHM res., vibnl struct.
	AVZ82a	398-400	P	comp. among N <sub>2</sub> , NO & O <sub>2</sub> , cont. to discrete shape res. shift
	WDD82	410-440	T	absolute cross-section calc., comp. to expt. (WB74c)
	DR83	390-415	E	ion yield appearance pot., 1s-> $\pi^*$ thresh. observed
	CF&84a	400	E	GOS, constant for $\pi^*$ in N <sub>2</sub> , NO, N <sub>2</sub> O, comp. to N <sub>2</sub> calc. (RO79)
	LT&84	414-440	P	cont. res. shape comp. to calc. (WDD82), $\beta$ -params
	SSH84a	420	T	$\sigma^*$ -res./bond length relationship
	LPL85	400-430	T	MS, quantum defect calc, R-dependence of $\sigma^*$ res.
	RL&85	400-430	P	comp. of multilayer PSID & ISSELS; comp. of CO, N <sub>2</sub> , NO, N <sub>2</sub> O
	RO85	400	T	$\pi^*$ GOS, quadrupole transition, constant for N <sub>2</sub> ,NO,N <sub>2</sub> O
	CA&87	400	E	Auger-loss coinc.; vibnl-time interference; cf. ETS boomerang model
	CF&87	400	E	GOS, constant for $\pi^*$ in N <sub>2</sub> , NO, N <sub>2</sub> O, comp. to N <sub>2</sub> calc (RO79)
	SG&89	410-430	T	$\sigma^*$ shape res.; pos. & shape as f(R); approx. cyl. well & ab initio
	PV&90	395-422	P	comp. to NO <sub>2</sub> <sup>-</sup> , NO <sub>3</sub> <sup>-</sup> (sol); $\delta(\pi-\sigma)$ correlated with R(NO)
	S90b	398-430	R,P	ionic fragmentation; ion KERD; ion (PIPICO) angular distribution

(NO cont'd)	MC&91	397-411	P	50 meV fwhm; $\pi^*$ - 2 vib'n'l series ( $2\Sigma^-$ , $2\Delta^-$ ); Ryd. vib'ns
	SS91	397-423	P	TEY; partial ion yields; KERD at $\pi^*$ ; $\beta$ -param.
	CT92	399	E	DES by (e,2e); $U_{CV} > 0$
	H92a	398-402	E	$^4\pi$ -state found at low impact energy
	KA&92a	395-435	P,T	symmetry resolved ion yield spectra, comp. to calc.
	S92	395-435	E,R,T	comp. of NH <sub>3</sub> , N <sub>2</sub> H <sub>4</sub> , N <sub>2</sub> ; $\sigma^*(N-N)$ ; MS-X $\alpha$ ; vib'n'l struct.; Ryd.
	ZZ&92	400-410	T	$\Delta$ SCF; core hole localisation; gen. rules for MO shifts in 2nd row
	MLH93	401-480	P	luminnescence spectra; rotational dist. of N <sub>2</sub> <sup>+</sup> at 401, 419, 480; no variation with E; interchannel coupling is origin of N <sub>2</sub> <sup>+</sup> above N 1s IP
	RD&93	396-420	P	74 meV fwhm; vibrational details of 3 $\pi^*$ states; Ryd; full analysis
	DRK94	398-402	P,R	SX700 high res. studies; vibrational structure in small mols.
	EH&96	398-412	P	PIY, TIY; QMS; state selective frag.; KERDs; threshold e- spectra - PCI shape; 160 meV natural linewidth; TPEPIPICO
	FM&96	410-500	E	Auger-ion coincidence; low-lying NO <sup>++</sup> states identified
	F97	399	T	de-excitation spectrum of $\pi^*$ predicted, comp to expt. (RD&93)
	WL98	398-403	T	HF-CI; comp to TKR80
	WP&98	298-402	P	resonant Auger; vibrationally resolved
	WF&00	399-401	P	vibrationally resolved $\pi^*$ ; C s filtered; separates $2\Delta$ , $2\Sigma^+$ states
	YH&00	398-402	P	TEY; resolution test of CSRF-SGM
	IOW01	400-410	T	potential energy surfaces for core excitation & doubles
	WF&01	399-401	P	vibrationally resolved $\pi^*$ ; CIS filtered; separates $2\Delta$ , $2\Sigma^+$ states
	YOW01	399-401	T	excitation energies and potential curves for $\pi^*$ states
	JW&02	412,420	P, T	fixed-in-space PES; COLTRIMS; circular dichroism at shape resonance, MS , RPAE calc
NO <sup>-</sup>	BRB04	400-410	T	generalized oscillatorstrength (GOS) for selected transitions
NO <sub>2</sub>	HA&04	410-425	P,T	multiple-specific shape resonance, PE ang. dist., partial wave analysis
	YHA05	418	P, R	ion angular dist; fixed-molecule PAD spectra, review
	SL&07	412	P	photoelectron angular distributions; inter-atomic Coulomb decay
	HM&08	412-420	P,T	vibrationally resolved PE X-sections; ang. dist.; shape resonance
	NAV88	395-422	P	comp. to KNO <sub>2</sub> , NaNO <sub>2</sub> (sol); $\delta(\pi-\sigma)$ correlated with R(NO)
	SCC77	400-412	P,T	photographic, Z+1 analogy calc., cont. shape res.
	SSH84a	420	T	$\sigma^*$ -res./bond length relationship - inconsistent
	BS87	380-430	E	high res.
	BS&88	390-460	E,R	IEELS, E <sub>0</sub> =3700eV, 0°, compare NO <sub>2</sub> SO <sub>2</sub>
	TL89	395-415	T,E	absolute, MCQD calc., stresses antibonding valence character
	ZS&90	390-455	E,T	absol.; identif. impurities in [SCC77]; MCQD calc.; split $\sigma^*(N-O)$
	ZZ&92	400-410	T	$\Delta$ SCF; core hole localisation; gen. rules for MO shifts in 2nd row
N <sub>2</sub>	GT&03b	398-426	P	angle resolved ion spectra; high-res; spectral assignments
	M38	350-450	P	photographic; <b>second gas phase XAS</b>
	NS&69	400-412	P	photographic, 0.03Å res., Z+1 analogy
	WSB70	390-420	E	ionic fragmentation (N <sup>+</sup> , N <sup>2+</sup> yields); <b>FIRST ISEELS SPECTRUM</b>
	WS72	390-425	E	absolute, ionic fragmentation
	C73	390-420	P,R	review
	WBW73	397-438	E	cont. res., Z+1 analogy
	GSM73	395-425	P	absorption saturation distortion
	CMT73	400-410	P	photographic, pressure dependence, upper bound to linewidth
	MN&74	397-412	P	photographic, Z+1 analogy
	VSZ74	390-425	P	Z+1 analogy, 0.3eV FWHM res.
	VZ&74	398-422	P	cont. res.
	DD75	400-410	T	X-alpha (MSM) calc., cont. shape res.
	R75	400-420	T	Z+1 analogy calc. comp. to expt.(NS&69)
	WS&75	.05-1.0	E	absolute, generalized oscillator strengths, Bethe surface

(N <sub>2</sub> cont' d)	DD76a	400-450	T	X-alpha (MSM) calc., cont. shape res.
	DD76b	400-450	T	X-alpha (MSM) calc., cont. shape res.
	DSD76	410-480	T	X-alpha (MSM) calc., shape res. PE ang. dist.
	BBP77	400-410	T	ab initio calc. with CI, comp. to expt. (WBW73)
	KLW77a	100-600	E	absolute, cont. res.
	KMR77	396-405	E	negative-ion K-shell-excited res.
	KM&77	397-430	T	vibnl structure, ab initio calc. comp. to expt. (NS&69, WBW73)
	KRT77	400-403	E	vibnl struct.
	RL77	395-425	T	absolute, comp. to expt. (KLW77a), cont. shape res.
	BP&78	390-450	P	photoelectric yield, absolute, cont. res.
	PB&78	390-450	P	absolute, cont. res.
	R78	400-402	E	vibnl struct., <70meV FWHM res.
	DD79	400-435	T	X-alpha (MSM) calc., cont. shape res.
	KDC79	400-402	T	ab initio calc. of vibnl structure, comp. to expt. (KRT77)
	KMN79	395-425	T	ab initio calc., comp. to expt. (KLW77a)
	RO79	400-402	T	absolute, comp. to expt (KLW77a), generalized oscillator strengths
	B80	390-450	P,R	review, (BP&78 data)
	DS&80	410-435	T	X-alpha (MSM) calc., shape res. Auger electron ang. dist.
	HB80a	380-430	E	vibnl struct., cont. res., comp. to theory (RO79)
	S80a	410-420	T,R	review of res. effects
	TKR80	405-410	E	<70meV FWHM res.
	W80	300-600	E	absolute, cont. shape res., vibnl struct.
	BH81	400-440	E,R	comp. of EELS and photoabsorption by SR
	AA&82	400-425	T	ab initio, multi-e- trans.; comp. to (HB80a), core hole localized
	AVZ82a	398-400	P	comp. among N <sub>2</sub> , NO & O <sub>2</sub> , cont. to discrete shape res. shift
	BD&82	400-420	E,R	vibnl struct., triplet π*, calibration (v=0, 400.88 eV)
	G82	400-440	R	shape res., related to valence cont. structure
	SK&82	399-402	E	dipole forbidden trans.; <sup>3</sup> π, vibration, 1,3 split=0.82(1) eV
	CF&83	401	E	generalized OS for (1s,π*), quadrupole trans.; f(opt)=.194
	DBH83	398-416	E	vibnl struct. resolved
	DR83	390-415	E	ion yield appearance pot., 1s->π* thresh. observed
	ES&83b	394-445	P	ion yields, comp to total e <sup>-</sup> ion spectra, DES at 401 eV
	GN&83	400-440	P,T	comp. of core & valence cont. shapes
	HH&83	395-430	P	N <sup>+</sup> yield from solid N <sub>2</sub> surfaces, comp. to gas, e <sup>-</sup> yield
	KK83	400-402	T	ab initio (Z+1) basis calc of (1s,π*) energy, comp. to expt (HB80a)
	UT83	360-390	E	decay of triplet (1s,π*) observed in Auger-ELS (e,2e)
	ZMP83	380-550	E	appearance pot.s, π* at 402.0
	AA&84	400-410	T	ab-initio, CI, non-dipole states, cf. AA&82
	CF&84a	400	E	GOS, constant for π* in N <sub>2</sub> , NO, N <sub>2</sub> O, comp. to theory (RO79)
	HS&84	385-430	E	apparatus paper for Auger-energy loss coincidence
	K84	399-402	E	<sup>3</sup> π; comp. to E( <sup>3</sup> π <sup>-1</sup> π) in CO, CO <sub>2</sub> , NNO & theory (KM&77)
	LM84	410-430	T	relaxed core, 1-e- calc., σ* res., comp. to expt (KLW77)
	LT&84	400-440	P	norm. at 432eV (BP&78), βs, comp. to (RL77), PE & Auger yield similar
	MRR84a	390-415	E	1s->π* res. in elastic scatt.; singlet 400.96, triplet 398.95 eV
	RRM84	398-404	E	1s->π* res. in elastic scattering
	SB84	401.10(2)	E	calibration standard (π* v=1)
	SSH84a	420	T	σ*-res./bond length relationship
	UT84	410-430	P	conjugate shake-up (core-excitation, val. ioniz.) enhancement
	B85	400-402	E	vibnl struct. of π*(0.055eV FWHM)
	BS85	400-415	T	absolute; pol.-propogator, allowed, forbidden, double excit.
	MR&85	399,401	E	ang. dist. of <sup>1</sup> π & <sup>3</sup> π elastic res., l=3 demonstrated
	RL&85	400-430	P	comp. of multilayer PSID & ISEELS; comp. of CO, N <sub>2</sub> , NO, N <sub>2</sub> O

(N <sub>2</sub> cont' d)				
RO85	400	T	$\pi^*$ GOS, quadrupole transition, constant for N <sub>2</sub> , NO, N <sub>2</sub> O	
UT85	401,416	E	autoionization & Auger decay by (e,2e)	
VA&85	400-440	P,R	comp. of BF <sub>3</sub> , N <sub>2</sub> , NO <sub>3</sub> <sup>-</sup> , shape resonances	
YPM85	410-436	T	ab initio, complex basis, coupled channels, comp. to (RL77, LM84)	
SS86b	395-435	P	N <sup>+</sup> , N <sub>2</sub> <sup>2+</sup> yields, partial spectra as function of ion kinetic energy	
CF&87	400	E	GOS, constant for $\pi^*$ in N <sub>2</sub> , NO, N <sub>2</sub> O, comp. to theory (RO79)	
EP&87	401	P	DES, Auger ion-coinc. with white light	
FR&87	420-500	P	shake-up satellite cross-sections; differs from CO	
K87	287-295	T	ab initio, CI, absolute dipole, comp. to expt	
MC&87	390-450	E	absolute OS, test of EELS-->OOS conversion	
PV87	395-430	T	MS-Xa; $\sigma^*$ due to neighbor, $\pi^*$ = atomic!; comp to (ZAV87)	
SS87a	395-435	P	PIPICO, partial ion yields, ion kinetic energies (yields)	
ZAV87	390-460	P	absolute, comp. to theory, 1s--> $\pi^*$ OS - 0.21(2)	
AVZ88	398-480	P	absolute; comp. of NH <sub>3</sub> , N <sub>2</sub> , Ne re osc. dist of discr/cont.; relates $\pi^*$ to atomic 2p resonance; f( $\pi^*$ )=0.12	
MF&88	400-440	P	ZEKE; XPS-sat & EELS/PA, higher Ryd., 2e & shake-up, PCI	
MLE88	400-402	P	TIY; DES; resolved vibnl struct. (0.2 eV FWHM); eval. of vib=n- interf. on DES (minor); disputes NO result (CA&87); see O <sub>2</sub> (CT88)	
SS88a	395-435	P	PEPICO, partial ion yields, ion kinetic energies (yields)	
SS88b	390-430	P	TEY; FIRST DEMO that ion ang. dist. at $\pi^*$ are anisotropic	
V88	410-450	T	shake-up X-sect.; comp. to surface PE (PRL 51 (83) 821)	
CMS89	398-425	P	high resol. (40 meV fwhm); new Ryd. series; vibns in 2e- excitn	
H89	380-440	E,R	review of electron-beam core excitation spectroscopies (Aussois)	
PK&89	385-435	P	dispersed-FL detn. (CIS); vibnlly-sensitive; $\sigma^*$ & cont. enhanced	
SG&89	410-430	T	$\sigma^*$ shape res.; pos. & shape as f(R); approx. cyl. well & ab initio	
SS89b	390-430	P	ion kinetic E; ion $\beta$ 's; small +ve $\beta$ value at $\sigma^*$	
SS89c	390-430	P	partial ion yield; KE dist'n; analysis of dissoc. paths	
SS&89	401	P	N <sup>+</sup> KERD; apparatus (grasshopper mono); $\pi^*$ $\beta$ (-0.7)	
YM&89	395-435	P	absolute, total ion yield; ion $\beta$ ; N <sup>2+</sup> KERD	
BS90	410-500	P,R	satellite X-sections; comp. to CO	
CS90	398-424	P	50 meV fwhm; $\pi^*$ , Ryd. vib'n; 2e-; Z+1 tested	
DQB90	399-403	E	$\sigma$ -resonance in <sup>1</sup> $\pi$ excitation; <sup>3</sup> $\pi$ - <sup>1</sup> $\pi$ branching ratio as f(Eo)	
ED&90	399	P	DES, dynamic screening effects; comp. of N <sub>2</sub> , N <sub>2</sub> O & azabenzenes	
H90a	395-425	E,R	absolute, comp. of N <sub>2</sub> , NH <sub>3</sub> , N <sub>2</sub> H <sub>4</sub> , Ne; $\sigma^*$ vs. Ryd	
HMS90	392-439	P	ZEKE; ZEK-ion coinc.; huge N <sub>2</sub> <sup>+</sup> signal rel. to non-ZEKE coinc.	
HS&90	400-402	P	80 meV fwhm; effect of slit width; SSRL-sph. grat. mono descr.	
LK&90	375-475	P	total ion ang. dist.; $\beta$ -s; comp. to theory (RO85)	
PV&90	395-415	P,T	XANES-MS calc.; comp. to expt [ZAV87]; $\delta$ (R) of $\sigma^*$ shape res.	
S90b	398-430	R,P	ionic fragmentation; ion KERDs; ang. dist.	
SU&90c	390-440	P	total ion yield; mol. orient. (N <sup>+</sup> +N <sup>2+</sup> ); $\beta$ : (-1 at $\pi^*$ , +1 at $\sigma^*$ )	
BB91	0-1000	E	GOS and sum rules; experimental methods reviewed	
L91	410-430	T	$\beta$ -param; comp. to expt. [YM&89]; frozen versus relaxed core	
LAL91	400-420	T	CNDO, systematic treatment of $\sigma^*$ energies	
MC&91	406-411	P	50 meV; Ryd. vib'n; comp.to CO; Z+1 breakdown (only intensities)	
SB91b	400-800	E,T	MS-Xa of edge; EXAFS of low-Z; comp. to HB80a	
BB92	41-850	E	generalised osc. str.; f <sub>opt</sub> ( $\pi^*$ )=0.19; comp to calc (CF&87, BNH92)	
BNH92	402	T	OOS&GOS - dipole&quad.; f <sub>opt</sub> ( $\pi^*$ )=0.20; GOS comp (CF&87, BB92)	
DM&92	400-403	P	high res. (80 meV); 2nd order	
ER&92	401-410	P	DES of $\pi^*$ , Ryd at high res.; interference effects	
K92	390-460	R	survey of numerical XANES	
KM&02a	405-425	P	total and partial luminescence yield, N <sup>+</sup> luminescence (excited frags.)	

(N <sub>2</sub> cont' d)	LD&92	400-440	P	ion yield, N <sup>+</sup> kinetic energy by retarding pot.
	MH&92b	399-422	P	ZEKE-PES; 200 meV fwhm; vibns at threshold; comp. to CO & abs.
	RF&92	400-402	P	40 meV fwhm; instrumentation
	S92	395-435	E,R,T	comp. of NH <sub>3</sub> , N <sub>2</sub> H <sub>4</sub> , N <sub>2</sub> ; σ*(N-N); high res.; vibn'l struct.; Ryd.
	SU&92a	395-445	P	total ion; symmetry-resolved states from N <sup>+</sup> ang. dist.; comp. to calc (RL77,BS85); challenges CS90 Rydberg assignments
	TWT92	400-403	P	60 meV fwhm; SSRL instrument description
	YM&92	399-403	P	95 meV fwhm
	YS92	398-404	P	photoion. ang. dist. at π*; instrument description
	BIB93	150-650	E	limiting shape of GOS (f <sup>(1)</sup> (E))
	M93	400-403	P	50 meV fwhm resolution
	ODF93	400-420	T	many body CI; ΔSCF; comp to NiN <sub>2</sub> ; Ni affects shakeup/relaxation
	RAZ93	400-445	P,T	MS-Feff reproduces σ* resonance
	RN&93	400-402	P,T	30 meV fwhm; vibrationally resolved core state decay; 120 < Γ < 132 meV; 2 step decay model OK; sma0x vibn'l-lifetime interference
	LK&94	405-410	P	ion anisotropy used to symmetry assign Rydbergs; (Z+1) fails!!; Ryd-derived IP = 409.922 eV
	DRK94	398-402	P,R	SX700 high res. studies; vibrational structure in small molecules
	LB&94b	399-433	P	10 <sup>4</sup> resolving power (< 40 meV) resolution
	ML&94a	395-425	P	FPICO (fluorescence coinc); parent and fragment exc. states
	NR&94	401-402	P	vibrationally resolved DES; small lifetime-vibrational interference; large potential curve overlap effects; comp. of CO, N <sub>2</sub> and O <sub>2</sub>
	S94	802	T	doubly K-excited & K-ionized states predicted; ΔSCF with opt. geom.
	AK&95c	400-402	P	SX700 pgm @ MAX; resolv. power >5000
	CC&95	395-410	P	SGM at SRBC performance test; high resolution
	F95	401	T	de-excitation spectrum of π*
	GV95	400-402	T	photodissoc. calc; comp. to vibrnly-resolved PEY, PSD of multilayer N <sub>2</sub> /Pt(111); desorption dominated by ultrafast, directly repulsive N <sub>2</sub> <sup>+</sup> states
	MBN95	410	T	core hole localisation is 78%; comp to CO <sub>2</sub> (60); C <sub>2</sub> H <sub>4</sub> (86%)
	NB95	400-412	T	coupled cluster ab initio; S-T splittings of Rydberg states
	QO&95	400-411	P	Elettra; high resolution (28 meV fwhm); 50% dip, v=7 visible
	RL&95	407-412	P	photoelectron-X-ray coinc.; peak at IP 0.5 eV BELOW ZEKE (due to PCI shift in ZEKE); PE-Auger coincidence
	S95	410-445	P	PE ang. dist. at σ*; (PE,ion) coinc; fragment ion ang. dist.; e- β
	SA&95c	395-420	P	fixed-in-space photoelectron angular distributions
	FH&96	398-412	P	high resolution (E/dE~6000); variable line spacing PGM
	GS&96	400-420	P	selectively excited X-ray emission; lifetime-vibrational interference
	K96a	390-425	P	partial ion yields; 60 meV fwhm; QMS
	KK&96a	395-450	P	absolute; high res. (80 meV); angle-res. XPS; part. X-sect.; βs; width=103(10) meV; comp. to calc; vib'n'l dep. of σ* (Δ=3eV v=0 to 2)
	KN&96	400-480	P	angle-resolved Auger; anisotropy in some channels
	NK&96a	407-413	P,T	2e- states near IP identified by resonant Auger; ultrafast decay; N <sub>2</sub> <sup>K*</sup> 6 N+N <sup>K*</sup> 6 N + N <sup>+</sup> + e ; (Z+1) calc for N <sup>K*</sup>
	NK&96b	410-560	P	Auger/AI decay; double excited states; ultrafast decay
	NM96	390-430	P,R	review; absorption; partial X-sect. (satellites); symmetry resolved
	RL&96	407-412	P	ZEKE, X-ray emission (FY); (ZEKE, FY) coincidence; eliminates PCI of regular ZEKE; 1-step model; 1 count/hour !!
	SST96	395-435	T	constant chemical potential LDA; π*, σ* res. rel. position;
	STS96	398-420	T	comp. of π-σ sep. in CO, C <sub>2</sub> H <sub>2</sub> , C <sub>2</sub> H <sub>4</sub> , N <sub>2</sub> , O <sub>2</sub>
	SCT96	420-440	T	analytical treatment of SR for diatomics (constant chemical potential); bond length determination; N <sub>2</sub> and O <sub>2</sub>
				core-valence double ionisation; <sup>1</sup> π, <sup>3</sup> π states; comp. of CO, H <sub>2</sub> CO, N <sub>2</sub>

(N <sub>2</sub> cont' d)				
	BN97	360-450	T	comparison of N <sub>2</sub> , quark-N <sub>2</sub> (+1/3N-N(-1/3); 1/3 charge shifts ~40 eV
	JA&97	400-403	P	relative; 32 meV; E/ΔE ~ 12500
	KA&97a	403-418	P	comp. of gas-sol; pol. dep.; bulk excitons by e- TOF; N <sub>2</sub> , IP=408.9(1)eV
	MS&97d	400-402	P	TIY, 80 meV fwhm; double toroid electron spectrometer
	NG&97	401-408	P	resonant X-ray emission
	SST97	395-440	T	analytical thoery of bond length - resonance correlation
	WZ&97	420	T	corrections to axial recoil for molecular rotation of core ion state
	ZZL97	397-428	T	MS-SCF calc; gs; Z+1; comp. to CMS89
	GTM98	401	P,T	Auger resonant Raman; time domain; detuning effects
	KM&98	400-403	P	line narrowing !; 80% dip between v=0, v=1 & Gaussian; partial Auger yield; 113 meV nominal peak width
	PF&98	419	P,T	ang. dist. PES at $\pi^*$ resonance; (pf) coherent interfer; comp to CO <sub>2</sub>
	S98	395-445	P	symmetry resolved ion yields; fixed-in-space photoelectron ang. dist.
	MM&99b	401	P,T	TIY, disp. Luminescence; vib'n-resolved $\pi^*$ ; int. coupling; vibronic CIS at $\pi^*$ ; vibration resolved; 160 mV total; participator decay
	PK&99a	400-403	P	relative; high res; $\pi^*$ AI as f(v); resonant Raman; detuning; vib. interfer.
	PK&99b	400-403	P,T	$\pi^*$ 115(4) & Ryd [3s 113(5), 3p 107(5), 4s 112(5) ] lifetime widths
	PV&99	400-415	P	RPA; $\sigma_g \rightarrow \sigma_u$ , $\sigma_u \rightarrow \sigma_g$ coupled; fixed-in-space $\beta$ ; comp. SA&95c
	CS&00	410-445	P,T	Auger partial yield (384 eV); 2e in discrete (406,407); PEY removes Ryd., $\sigma^*$ , single ioniz.
	NK&00	404-420	P,T	resonant Auger; vibrational excitation dependent; bond length effects
	PF&00	400-403	P,T	relative; molecule, cluster, solid comparison; (N <sub>2</sub> Ar) <sub>n</sub> mixed clusters; claims shape resonance changes in clusters
	PR00	390-440	P,T	TIY, PIY, PIPICO; lifetime-vibration effects; comp. of CO & N <sub>2</sub>
	SP&00	398-425	P	SB7 LURE beamline tests; ΔE/E > 8500
	SR&00	400-402	P	TIY; (PES, Auger) coincidence at $\pi^*$
	YH&00	399-403	P	TEY, resolution test of CSRF-SGM
	AD&01	399-401	E,T	threshold ejected electron spectra of <sup>1</sup> π, <sup>3</sup> π, DW calc.
	HK&01	390-445	P	$\sigma_g^{-1}$ , $\sigma_u^{-1}$ splitting 97(3) meV; partial PI X-sections; comp to theory
	I01	410-440	P,T	absolute, fixed-in-space photoelectron ang. dist.; shape resonances
	WJ&01	419	P,T	COLTRIMS detailed ionization analysis; shape resonance dynamics
	C02	401	T	cross-sections for inelastic scattering
	FG&02	400-402	P	resonant PES; bond length from interference quenching of v''=1 line
	K02	398-420	P,TR	symmetry resolved, high resolution; review
	MR&02	420	P	fixed-in-space ang. dist.; shape resonance
	SC02	410-450	T	RPAE, absolute; comp to KK&96a; interchannel coupling, vibrations
	FB&03a	404-425	P	angle resolved ion yield, state-selected spectra
	GT&03b	405-430	P	60 meV fwhm, $\pi^*$ vibrations; BL4B UVSOR-II commissioning
	MC&03	400-800	T	GOS near threshold, DWA calculations, comp to expt (DQB90)
	MGK03	404-410	P	angle-resolve phtoion-yield, symmetry resolved Rydbergs.
	K04	404-410	P,T	symmetry resolved Ryd states, gu split; comp to Ne, Ar, Kr, Xe matrices
	AR&05	409-411	P	X-ray emission threshold coincidence (XETECO); no-PCI threshold spectra; 0.1 eV u-g splitting observed; 40 meV fwhm
	HLS05	406-412	P	excited neutral (N*) detected at IP; PCI
	HA&06	430-700	P, T	beta, non-dipole exists but is SMALL, RPA calculation
	FB&07	397-404	E	500 < E <sub>0</sub> < 1000 eV, 90°; X-sect differ from SK&84, autoionization of <sup>3</sup> π detected by multi-coincidence (hijacked at Elettra!)
	KHS07	448	P	(Auger, ion) ; apparatus for E, θ correlations, evaluates K, θ resolution
	KK&07	398-425	P	absolute, super resolution ! (23 meV); natural width (113(2) meV)
	SK&07	405-413	P	PCI, TIY; (N*, N <sup>+</sup> ) coinc peak at threshold, polarization dep. Of autoionization electrons
	BF15	903	P,T	double core hole (DCH) PES&Auger; compare CO, CO <sub>2</sub> , N <sub>2</sub> , N <sub>2</sub> O

(N <sub>2</sub> cont' d)	PN&15	836,901	P	1-site, 2-site double core hole IP (ts-DCH), SR, not FEL, coincidences
	TKU15	836	T	(XH <sub>m</sub> -YH <sub>n</sub> ) X,Y = C,N,O,F; m,n = 0-3 – 2-site double core hole IPs
	NG&17	400-402	P,T	PE-Auger coincidence; core hole localization depends on measurement
	HV&20	390-410	P	TEY, 150 meV, VerSoX end-station test
	XW&22	399 – 403	E	<30 meV resolution, g-u sep = 67(7) meV $\Delta_{\text{vib}}= 29(5)$ meV; full deloc.
(N <sub>2</sub> ) <sub>n</sub>	R92	390-460	P	PIY,PEPICO, KER; clusters up to n=30; comp. to N <sub>2</sub> molecule
	FP&01	399-412	P	cluster-gas comparison, small shift in $\pi^*$ ; Ryd-exciton shift
N <sub>2</sub> Ni	DCT98	401	T	partial localized core hole; comp to N <sub>2</sub> /Ni(100) NEXAFS; XPS ang. effects
N <sub>2</sub> O	GSM73	395-425	P	absorption saturation distortion
	WB74a	395-440	E	cont. res., deviation from Z+1 analogy for terminal N
	GM&75	395-425	P	absorption saturation distortion
	SB76	395-420	T	geometry corrected, Z+1 analogy calc.
	BP&78	390-450	P	photoelectric yield, absolute
	HBW79	401,405	E	ionic fragmentation
	TKR80	400-407	E	<70meV FWHM res.
	B81	395-455	P,R	cont. res., XANES for structure determination
	B82a	401,405	E,R	ionic frag. of discrete autoionizing states, review (HBW79 data)
	DR83	390-415	E	ion yield appearance pot., 1s-> $\pi^*$ thresh. observed
	SK&83	390-410	E	dipole forbidden transition
	CF&84a	400	E	GOS, constant for $\pi^*$ in N <sub>2</sub> , NO, N <sub>2</sub> O, comp. to theory (RO79)
	SSH84a	420	T	$\sigma^*$ -res./bond length relationship - inconsistent with
	RL&85	400-430	P	comp. of multilayer PSID & ISEELS; comp. of CO, N <sub>2</sub> , NO, N <sub>2</sub> O
	RO85	400	T	$\pi^*$ GOS, quadrupole transition, constant for N <sub>2</sub> ,NO,N <sub>2</sub> O
	MN&86	380-460	P	total & partial ion yields, comp to HBW79
	SKR86	395-408	E	high res (65 meV), triplets observed, E( $^3\pi^-$ )=0.7,0.9eV)
	CF&87	400	E	GOS, constant for $\pi^*$ in N <sub>2</sub> , NO, N <sub>2</sub> O, comp. to N <sub>2</sub> calc (RO79)
	HK87	397-407	E	triplet states (1s <sub>C</sub> =0.98 eV, 1s <sub>T</sub> =0.65 eV)
	PL&87	390-430	T	shape-resonance bond length refutation
	GC&88	400-550	P,T	absolute; partials, $\beta$ s, N1s (C), N1s(T) comp. to expt (main line 420-450; chemical effects on $\beta$ at $\sigma^*$ res.
	H89	390-440	E,R	review of electron-beam core excitation spectroscopies (Aussois)
	LE&88	390-400	P,T	DES at (N <sub>T</sub> , $\pi^*$ ), (N <sub>C</sub> , $\pi^*$ ); spectator & participator lines
	SG&89	410-430	T	$\sigma^*$ shape res.; pos. & shape as f(R); approx. cyl. well & ab initio
	ED&90	399	P	DES, dynamic screening effects; comp. of N <sub>2</sub> , N <sub>2</sub> O & azabenzenes
	H90a	395-425	E,R	absolute, comp. of N <sub>2</sub> , NH <sub>3</sub> , N <sub>2</sub> H <sub>4</sub> , Ne; $\sigma^*$ vs. Ryd
	H90b	398-405	P	ionic frag. at N <sub>T</sub> ,N <sub>C</sub> -> $\pi^*$ ; comp. to O1s-> $\pi^*$
	HB&90	398-435	P	total ion; ZEKE; MS at N <sub>T</sub> ,N <sub>C</sub> -> $\pi^*$ and ZEKE peaks (very different)
	HM&90	400	P	M <sub>2+</sub> (Auger-selected) multiple ion coinc. (ERAEMKO)
	LLM90	390-450	P	total ion; PIPICO; PEPPIPICO; frag. dynamics; 1- vs. 2-step
	LAL91	400-420	T	CNDO, systematic treatment of $\sigma^*$ energies
	MC&91	399-412	P	50 meV fwhm; Ryd. vib'n; intensities unusual
	PBV91	390-430	T	MS; comp.to expt; dev. from $\delta(R)$
	SK&91	412-460	P,T	absolute; N <sub>C</sub> , N <sub>T</sub> ; ab initio calc; shape res. in partials
	SL&91b	423	P	multi-coincidence PEPPIPICO; 2-d display; continuum fragmentation
	K92	400-420	R	survey of numerical XANES
	KA&92b	395-440	P	symmetry resolved spectra using ion angular distributions
	ZZ&92	400-410	T	$\Delta$ SCF; core hole localisation; gen. rules for MO shifts in 2nd row
	BSS93	396-436	P	PEPICO-, PIY-, PIPICO-yield, $\beta$ ; comp. of $\beta$ for N <sub>2</sub> , NO, N <sub>2</sub> O, O <sub>2</sub>
	LL&93	390-450	P	PIY, TIY, PEPPIPICO at both $\pi^*$ ; $\sigma^*$ diss. dynamics
	ML&93	395-425	P	PE2PICO; frag.of N <sub>2</sub> O, CO <sub>2</sub> , Fe(CO) <sub>2</sub> (NO) <sub>2</sub>
	LH&94	395-445	P	(zeke, Auger) coinc; small threshold signal rel. to 'normal'; chemically sitr selective Auger

(N <sub>2</sub> O cont' d)	ML&94a	395-425	P	FPICO (fluorescence coinc); parent and fragment exc. states
	ML&94b	401,405	P	(Auger, ion, ion) coinc.; ERAMICO; apparatus design
	AK&95a	398-442	P,T	ab-initio ASCF-CI; symmetry resolved ion yields; Renner-Teller; Ryd.-val. mixing; $\sigma^*$ identified; large bending in $\pi^*$
	F95	399	T	de-excitation spectrum of $\pi^*$
	FS&95	401,405	P	(Auger, ion, ion) coinc.; ERAMICO; state-selective decay; clever pulsing!!
	AK&96a	339,405	P	angle-resolved PIPICO; test 3-body decay mech.; axial recoil breakdown
	FS&96	400-450	P	TIY; E-resolved PEPICO; frag. mech.; N <sub>T</sub> ,N <sub>C</sub> exchange prior to dissociation
	K96b	400-410	T	GSCF3; vibronic coupling
	NM96	390-430	P,R	review; absorption; partial X-sect. (satellites); symmetry resolved
	RJ96	390-440	P	relative; partial anion and cation yields; O <sup>-</sup> primary
	SL&96	400-420	P	fragmentation mechanisms
	MS&97d	401	P	resonant Auger; double toroid analyser (E, angle)
	CM&98	401,405	P	Auger,ion coinc.; partial ion yields as f(Auger); mapping. int. states
	MS&98a	401,405	P	Auger,ion coinc.; site selective fragmentation
	PV&99	400-415	P	Ryd [3d 106(10) ] lifetime width
	AR&05	408-414	P	X-ray emission threshold coincidence (XETECO); no-PCI threshold spectra; 40 meV fwhm; chem. Shifts & vibrations
	C07	398-420	T	density functional calc. mean error of only 0.26 eV
	DH&09	415	P	(N <sup>+</sup> , NO <sup>+</sup> ) KRD (e,ion, ion) site-selective fragmentation
	BF15	902	P,T	double core hole (DCH) PES&Auger; compare CO, CO <sub>2</sub> , N <sub>2</sub> , N <sub>2</sub> O
N <sub>2</sub> O <sub>2</sub>	PT&95	395-450	P,T	(NO) <sub>2</sub> ; multilayer NEXAFS; DFT calc; low-lying $\sigma^*(N-N)$ consistent with long bond (2.24 Å); 1.5 eV fwhm resol.
(N <sub>2</sub> O) <sub>n</sub>	R92	390-460	P	PIY,PEPICO, KER; clusters up to n=20; comp. to N <sub>2</sub> molecule; asymmetric charge fragmentation
	TT&05	401.1	P	PIY, TOF-PIMS, PEPICO, KERdissociation mechanisms, <n> up to 16

### Oxygen 1s (535 eV)

<b>BHO</b>	EH99	525-560	E,T	absolute; transient from H <sub>2</sub> S+B+SiO <sub>2</sub> ; comp of HBO, HBS, H <sub>3</sub> B <sub>3</sub> O <sub>3</sub>
	HE&01	525-560	E	absolute; transient ISEELS
<b>B<sub>3</sub>H<sub>3</sub>O<sub>3</sub></b>	EH99	530-560	E,T	absolute; from H <sub>2</sub> O+B; comp of HBO, HBS, H <sub>3</sub> B <sub>3</sub> O <sub>3</sub>
B <sub>5</sub> C <sub>19</sub> FeH <sub>17</sub> O <sub>2</sub> P	HLD91	520-560	E	Cp(CO) <sub>2</sub> FeB <sub>5</sub> H <sub>2</sub> PBz <sub>2</sub> , phosphaboranes
<b>BrC<sub>5</sub>MnO<sub>5</sub></b>	HSW89	525-570	E	Mn(CO) <sub>5</sub> Br, comp. to Mn(CO) <sub>10</sub>
	HWR90	525-560	E	absolute; comp. of TM carbonyls; f( $\pi^*$ ) as f(backbond)
<b>CCl<sub>2</sub>O</b>	HUR92	520-560	E,T	phosgene; absolute; comp. to EHT
	RY&92	520-560	E	comp. of small mol. analogs with PET polymer
CCuO	YA&97	534	T	Cu(CO); $\pi^*$ osc. str.; comp. of Cu-CO clusters
CCu <sub>17</sub> O	YA&97	534	T	Cu <sub>17</sub> (CO); $\pi^*$ osc. str.; comp. of Cu-CO clusters
	PA&96	530-580	T	absolute, STEX; comp. of CO, Cu <sub>17</sub> CO, Cu <sub>50</sub> Co; models of CO/Cu(100)
CCu <sub>50</sub> O	YA&97	534	T	Cu <sub>50</sub> (CO); $\pi^*$ osc. str.; comp. of Cu-CO clusters
	PA&96	530-580	T	absolute, STEX; comp. of CO, Cu <sub>17</sub> CO, Cu <sub>50</sub> Co; models of CO/Cu(100)
CD <sub>2</sub> O	RD&92	528-540	P	high res. isotope effects
CDH <sub>3</sub> O	AM&05	526-542	P	TIY, PIY, state-selective frag, isotope effects
<b>CHFO</b>	IH87	525-575	E	HCOF, formyl fluoride, comp. to HCOOH, HCONH <sub>2</sub>
	RI&88	525-575	E	C-F $\sigma^*$ res., absolute, perfluoro effect
	SLD95	534	T	absolute, DF-LCAO; OS for C1s, O1s → $\pi^*$ ; orbital mapping
	HC96	531	T	DFT; ${}^3\pi-{}^1\pi = 0.34$ eV
CH <sub>2</sub> O	HB80b	525-565	E	formaldehyde; cont. res., Z+1 analogy
	SSH84a	540	T	$\sigma^*$ -res./bond length relationship
	RI&88	525-575	E	C-F $\sigma^*$ res., absolute, perfluoro effect
	SBT88	529-537	T	absolute, ab initio, weak Ryd., comp to HB80b

CH <sub>2</sub> O cont' d)	SG&89	535-550	T	$\sigma^*$ shape res.; pos. & shape as f(R); approx. cyl. well & ab initio
	LAL91	530-550	T	CNDO, systematic treatment of $\sigma^*$ energies
	RD&92	528-540	P	high res. isotope effects
	S92	530-570	E,T,R	MS-X $\alpha$ ; comp. of CO, H <sub>2</sub> CO, CH <sub>3</sub> OH; $\sigma^*(C-O)$
	NB95	530-542	T	coupled cluster ab initio; S-T splittings of Rydberg states
	SLD95	534	T	absolute, DF-LCAO; OS for C1s, O1s $\rightarrow \pi^*$ ; orbital mapping
	HC96	531	T	DFT; $^3\pi^{-1}\pi = 0.41$ eV
	SCT96	550-570	T	core-valence double ionisation; $^1\pi$ , $^3\pi$ states; comp. of CO, H <sub>2</sub> CO, N <sub>2</sub>
	YA&96	520-560	T	absolute; STEX; comp. of R <sub>2</sub> CO; comp. to expt.
	YA&97	520-560	T	absolute; STEX; comp. of R <sub>2</sub> CO; comp. to expt.
	TPA98	525-570	T	absolute; DFT vs. STEX, compares CO and R <sub>2</sub> CO, R = H, Me
	TMG01	530-540	T	ADC2; comp. to RD&92
	TM&01b	528-557	T	relative, Green's function methods; vibrations; comp. to expt. (RD&92)
	SD&12	535-565	P,T	absolute, beta, RF-PAD, TD-DFT, shape resonance 2007
<b>CH<sub>2</sub>O<sub>2</sub></b>	IH87	525-575	E	(formic acid), $\sigma^*(C-O)$
<b>CH<sub>3</sub>NO</b>	IH87	525-575	E	HCONH <sub>2</sub> , formamide, comp. to HCOOH, HCOF
CH <sub>3</sub> NO <sub>2</sub>	VA&92	280-750	P	absolute; analysed as (CH <sub>3</sub> <sup>+</sup> , NO <sub>2</sub> <sup>-</sup> ); bond length corr.
<b>CH<sub>4</sub>N<sub>2</sub>O</b>	PV&93	530-550	T	quasi-atomic calc; short-range order (bond length) correlation
<b>CH<sub>4</sub>O</b>	UH&95b	528-550	E,T	(NH <sub>2</sub> ) <sub>2</sub> CO, urea; absolute; EHMO; modelling of polyurethane
	WB74b	525-570	E	(CH <sub>3</sub> OH - methanol) res. at thresh.
	SSH84a	540	T	$\sigma^*$ -res./bond length relationship
	YKS87	500-950	P	EXAFS; comp. of CO, CO <sub>2</sub> , COS, Me <sub>2</sub> CO, CH <sub>3</sub> OH, EtOEt, furan, C <sub>8</sub> H <sub>8</sub> O <sub>2</sub>
	IH88	525-570	E	absolute OS, used to test spectral additivity in methyl formate
	LAL91	530-550	T	CNDO, systematic treatment of $\sigma^*$ energies
	S92	530-570	E,T,R	MS-X $\alpha$ ; comp. of CO, H <sub>2</sub> CO, CH <sub>3</sub> OH; $\sigma^*(C-O)$
	HP&99	532-545	P	relative, TIY, PIY, PEPICO yields, site specific frag.; inter-atomic Auger
	SO&02	530-554	P	relative, anion PIY, OH <sup>-</sup> only in discrete C1s states
	AM&05	526-542	P	TIY, PIY, state-selective frag, isotope effects
	IH07	530-544	T	relative, Gaussian augmented plane wave (GAPW) - DFT; compared to dimer, (-5 to +3 eV errors on 14 small molecules
	KF&20	550	P	methanol; COLTRIM, PE ang. dist. from oriented molecules
<b>CH<sub>4</sub>O<sub>3</sub>S</b>	HH14	525-565	E	(methane sulfonic acid), references for PFSA (Nafion)
<b>CF<sub>2</sub>O</b>	RI&88	525-575	E	C-F $\sigma^*$ res., absolute, perfluoro effect
	SLD95	534	T	absolute, DF-LCAO; OS for C1s, O1s $\rightarrow \pi^*$ ; orbital mapping
	HC96	531	T	DFT; $^3\pi^{-1}\pi = 0.32$ eV
<b>CF<sub>3</sub>NO</b>	HIR89	525-575	E	absolute
	PV&93	530-550	T	quasi-atomic calc; short-range order (bond length) correlation
<b>CF<sub>4</sub>O</b>	IM&87	525-575	E	absolute OS low-lying $\sigma^*(O-F)$
CNiO	OD93	534-550	T	Ni(CO); ab initio SCF-CI; comp. of CO, NiCO; comp. to expt. (CSB89), NEXAFS of CO/Ni (PC&78); intensity ratios predicted; f( $\pi^*$ )=0.13
	SLD95	534	T	absolute, DF-LCAO; OS for C1s, O1s $\rightarrow \pi^*$ ; orbital mapping
<b>CO</b>	WSB70	520-550	E	comp. to C 1s, 1eV FWHM res.
	NM&71	525-545	P	photographic
	WBW73	527-578	E	cont. res.
	S74	525-545	T	Z+1 analogy, comp. to expt. (NM&71)
	DSD76	530-600	T	X-alpha (MSM) calc., shape res. photoelectron ang. dist.
	GMK77	532-536	T	ab initio calc. of vibnl struct. (1s to $\pi^*$ )
	KM&77	530-540	T	ab initio calc., vibnl struct., comp. to expt. (NM&71, WBW73)
	KMR77	528-537	T	negative-ion K-shell-excited res.
	IKN78	530-570	T	ab initio calc., comp. to expt. (WBW73)
	PC&78	535-575	T	ab initio calc., comp. to expt. (WB74a), cont. shape res.
	BB&79	500-600	P	photographic, absolute, pressure dependence

(CO cont'd)	DD79	535-585	T	X-alpha (MSM) calc., cont. shape res.
	KMN79	525-545	T	ab initio calc., osc.str.s
	DS&80	530-550	T	X-alpha (MSM) calc., shape res. Auger electron ang. dist.
	HB80a	525-565	E	cont. res., comp. to theory
	BD&82	530-540	E,R	calibration (534.21 eV)
	GN&83	540-560	P,T	comaprison of core & valence cont. shapes
	KK83	532-536	T	ab initio (Z+1)-basis calc. of E(1s, $\pi^*$ ) comp. to expt (HB80a)
	TS&83	540-630	P	absolute, cont. cross-sections, $\beta$ values
	UT83	530-540	E	search for triplet (1s, $\pi^*$ ), not seen at Eo=650eV
	ZMP83	520-580	E	appearance pot.s, $\pi^*$ at 536.2
	AA84	530-555	T	ab initio, CI, all one & two-electron transitions, osc.str.
	JH&84	529-539	P	e <sup>-</sup> yield, solid/gas/chemisorbed Ni(111), -1.7eV chemisorp. shift, M->C=O backbonding, 0.2eV FWHM, vibnl struct.
	SB84	534.21(9)	E	calibration standard ( $\pi^*$ )
	SSH84a	540	T	$\sigma^*$ -res./bond length relationship
	TL&84	535-690	P	Auger, PES X-sections, $\beta$ s, absolute
	BS85	530-540	T	polarisation-propogator, allowed, forbidden, double excitations, absolute, comp. to expt.
	CF&85	531-538	T	vibnl struct. calc., comp. to HB80a
	RL&85	520-580	P	comp. of multilayer PSID & ISEELS
	UT85	534	E	autoionization & Auger decay by (e,2e)
	YKS85b	500-1000	P	EXAFS, non-standard phase shifts indicated
	HI86	500-900	E	weak EXELFS, comp. to (YKS85b)
	KS&86	534	T	DV-Xalpha, 1s--> $\pi^*$ , comp. to IPES, NiCO, sensitive to R(Ni-C)
	YKS86	500-950	P	EXAFS, corrected for second order radiation
	FR&87	550-650	P	XPS satellite partial cross-sections
	MC&87	520-580	E	absolute OS, test of EELS-->OOS conversion
	YKS87	500-900	P	EXAFS, comp. to other O-X species
	HL&88	510-610	P	absolute OS, total & partial ion yields, PIPICO, breakdown patterns
	NE&88	550	P	PIPICO, ion kinetic energies at $\sigma^*$ , comp to val, Cls ionization
	CT89	534	E	DES by (e,2e); CO, CO <sub>2</sub> & COS similar O K-hole decay; atomic?
	SG&89	535-550	T	$\sigma^*$ shape res.; pos. & shape as f(R); approx. cyl. well & ab initio
	SY&89	520-570	P	O1s 2nd order, comp to EELS, discrete/cont. lower; cont. flatter
	CSB90	525-580	E	comp. to Ni(CO) <sub>4</sub>
	DX&90	532-543	P	85 meV fwhm; $\pi^*$ vib'n (weak but there !!)
	HWR90	525-560	E	absolute; comp. to TM carbonyls; f( $\pi^*$ ) as f(backbond)
	SBM90	540-640	T	RCHF calc, improved agreement with expt. [BB&79]
	FA91	530-540	T	absolute; XAS vs. XRF; comp. to expt. (HB78)
	JJ&91	530-800	T	MS calc; NEXAFS and EXAFS; CO and O <sub>2</sub>
	LAL91	530-550	T	CNDO, systematic treatment of $\sigma^*$ energies
	VBA91	500-900	T	CI effect on EXAFS; HF-SCF; low-Z EXAFS; comp. to (YKS87)
	DM&92	533-543	P	high. res. (140 meV); first $\pi^*$ vibrational structure; SX-700(II)
	RS&92a	530-560	P	clusters; PIPICO and TIY spectra
	S92	530-570	E,T,R	MS-X $\alpha$ ; comp. of CO, H <sub>2</sub> CO, CH <sub>3</sub> OH; $\sigma^*(C-O)$
	SK&92a	536-560	P	absolute cross-sections and $\beta$ from PES
	ZZ&92	530-540	T	$\Delta$ SCF; core hole localisation; gen. rules for MO shifts in 2nd row
	OD93	534-550	T	ab initio SCF-CI; comp. of CO, NiCO; comp. to expt. (CSB89), NEXAFS of CO/Ni (PC&78); intensity ratios predicted; f( $\pi^*$ )=0.13
	SH&93	525-555	P,T	symmetry resolved spectra using ion ang. dist.
	BSS94	530-560	P,T	ion- $\beta$ ; -0.8 at $\pi^*$ , +0.5 at $\sigma^*$ ; comp. to relaxed HF-calc.
	DRK94	533-537	P,R	SX700 high res. studies; vibrational structure in small mols.
	RH&94	540-1500	P,T	ZEKE and satellite partial cross-sections

(CO cont'd)	S94	823,1159	T	doubly K-excited, K-ionised states
	YND94	538-570	T	absolute; ab initio Z+1; multi-electron; comp. to expt. (HB90a)
	BM&95	530-540	P	HERMON at SRC; performance; $10^5$ resolving power
	CC&95	530-540	P	SGM at SRBC performance test; high resolution
	HA&95	543,551,571	P	(e,ion) PEPICO; PE ang. dist.; f-wave char. of $\sigma^*$ SR only in parallel
	NB95	530-542	T	coupled cluster abi initio; S-T splittings of Rydberg states
	SLD95	534	T	absolute, DF-LCAO; OS for C1s, O1s $\rightarrow \pi^*$ ; orbital mapping
	HC96	534	T	DFT; $^3\pi-^1\pi = 0.36$ eV
	NM96	520-560	P,R	PIPICO; review of coinc. tech.; cross-sections from HL&88
	PA&96	530-580	T	absolute, STEX; comp. of CO, Cu <sub>17</sub> CO, Cu <sub>50</sub> Co; models of CO/Cu(100)
	SCT96	550-570	T	core-valence double ionisation; $^1\pi$ , $^3\pi$ states; comp. of CO, H <sub>2</sub> CO, N <sub>2</sub>
	YA&96	520-560	T	absolute; STEX; comp. of R <sub>2</sub> CO; comp. to expt.
	GA97	530-590	T	absolute; STEX; resonant elastic X-ray scattering; nuclear-electronic coupling depends on detuning
	JA&97	534-544	P	high. res; $\pi^*$ vibrations – 10%; 2 <sup>nd</sup> order E/ $\Delta E > 10,000$
	NG&97	535-535	P,R	resonant X-ray emission (RIXS); ang. dep. at 3s, 3p, Ryd; v-dependent
	PN&97	532-537	P,T	relative; high resolution; vibrationally-resolved AI decay; ab initio calc; vibrational-lifetime interference
	SG&97a	534-545	P,T	resonant X-ray emission; screening shifts; ang. dep.; lifetime-vibrational interference; ab initio RIXS calc'n
	SG&97b	534-545	P,T	resonant X-ray emission; self-absorption; lifetime-vibrational interference
	YA&97	520-560	T	absolute; STEX; comp. of R <sub>2</sub> CO; comp. to expt.
	ZZL97	534-557	T	MS-SCF; comp. to DV-X $\alpha$ using Z+1 and g.s. approaches
	GTM98	534	P,T	Auger resonant Raman; time domain; detuning effects
	TPA98	525-570	T	absolute; DFT vs. STEX, compares CO and R <sub>2</sub> CO, R = H, Me
	BW&99	534	P	PEPICO; Auger-ion coinc; 2-step (C <sup>+</sup> , O <sup>+</sup> ) at $\pi^*$ ; wall coll. & KERD
	PD&99	532-543	P,T	65 meV fwhm; R( $\pi^*$ ) = 129.1 pm (8 pm longer); MC calc
	PV&99	530-540	P	$\pi^*$ 157(10) & Ryd 3p 138(10) lifetime width
	CR&00	540-560	P,T	fixed-in-space ang. dist; theory; double excitation; shape resonance
	IA&00	552	P,T	fixed-in-space; ng. Dist.; complete expt (10 ME, 8 phase); ab initio RCHF
	MA&00	545-560	P,T	fixed-in-space ang. dist; theory
	PR00	525-565	P,T	relative; molecule solid comparison; only Rydberg changes
	CPA01	530-570	T	STEX with screening; comp. to expt. (HB80)
	I01	556,561	P,T	absolute, fixed-in-space photoelectron ang. dist.; shape resonances
	KS01	540-1000	E	electron impact excited Auger-ion coincidence; comp to CO <sup>++</sup> PE curves
	HS&02	541-545	P	anion yield at threshold, high-res – vibn'l effects; PCI
	GM&04	525-575	P	TIY, PIPICO, PEPIPICO, absolute, partial ion & ion pair yields
	MTU04	542-557	P	vibrationally resolved PI X-sections – bond length dependence of SR
	C05	533	T	DFT, small molecue BE and excitation energies
	SC&05	540-600	P,T	absolute, beta-spectra, vibrational resolved PES, ab initio calc.
	YHA05	520	P, R	ion angular dist; fixed-molecule PAD spectra, review
	HK&07	530-560	P	relative, O <sup>-</sup> yield, ang. dist. from imaging time-of-flight; tracks absorption
	IH07	530-554	T	relative, Gaussian augmented plane wave (GAPW) - DFT; (-5 to +3 eV errors on 14 small molecules, comp to TPA98
	CC11	200-600	E	EELS in TEM; in situ catalysis
	CG&16	534-536	P,T	RIXS; (2e <sup>-</sup> , 1 hv) enhanced by avoided crossing
COPd	SLD95	534	T	absolute, DF-LCAO; OS for C1s, O1s $\rightarrow \pi^*$ ; orbital mapping
COPt	SLD95	534	T	absolute, DF-LCAO; OS for C1s, O1s $\rightarrow \pi^*$ ; orbital mapping
COS	WB74e	528-550	E	pot. barr. effects
	YKS86	500-950	P	EXAFS, corrected for second order radiation
	YKS87	500-900	P	EXAFS, comp. to other O-X species
	HI88b	500-900	E	EXELFS, comp to YKS87

(COS cont'd)	NH&88	530-560	R	comp. of all edges, ETS, (WB74e), $\sigma^*$ locations suggested
	CT89	534	E	DES by (e,2e); CO, $\text{CO}_2$ & COS similar O K-hole decay atomic?
	MG&99	530-550	P,T	TIY; STEX; res. emission; atomic lines – ultrafast decay; C1s, O1s, S2p
	MH&89	525-580	E,T	absolute, ab initio, comp. of $\text{CO}_2$ , COS & $\text{CS}_2$ - all edges
	SY&89	520-570	P	O1s 2nd order, comp to EELS, discrete/cont. lower; cont. flatter
	VBA91	500-900	T	CI effect on EXAFS; HF-SCF; comp. to (YKS87); forward foc. MS
	EK&97c	520-540	P	TIY, PIY; PE3PICO; fragmentation mechanisms
	MG&99	530-550	P,T	TIY, STEX, resonant emission; atomic like ultra-fast decay of $\sigma^*$
	GC&02	545-562	T	fixed-in-space ang. dist.; comp to expt.
	GA&05s	542-570	P, T	PAD, comp of S2p, C1s, O1s at selected energies, MS-X $\alpha$
	GA&05b	542-570	P, T	AR-PEPICO, comp of S2p, C1s, O1s at selected energies, MS-X $\alpha$
<b>CO<sub>2</sub></b>	WB74a	530-575	E	cont. res.
	L75b	525-560	P	absolute, distorted cont. shape
	VA&75	525-560	P	comp. to O <sub>2</sub> , $\text{C}_2\text{H}_5\text{OH}$
	BB&79	504-600	P	photographic, absolute, pressure dependence
	BDW79	.05-2.5	E	generalized osc.str.s, Bethe surface
	PC&81a	535-575	T	ab initio calc., comp. to expt. (WB74e), cont. shape res.
	DDH82	540-575	T	ab initio calc, comp. to expt (BB&79), shake-up
	LM82a	525-565	T	ab initio calc, comp. to expt (WB74a)
	LM82b	540-570	T	ab initio, comp. to expt. (WB74a, BB&79), cont. shape res.
	KK83	530-535	T	ab initio (Z+1) basis calc. of E(1s, $\pi^*$ ), comp. to expt (WB74a)
	ZMP83	520-580	E	appearance pot.s, $\pi^*$ at 539.0
	SA&84	520-950	P	absolute, 0.5eV FWHM, compared to WB74a, Z+1 analogy
	SSH84a	540	T	$\sigma^*$ -res./bond length relationship - anomalous
	TL&84	535-690	P	Auger, PES X-sections, $\beta$ s, absolute
	YKS84	500-1000	P	compare ion-yield, gas scintillation & absorption, EXAFS
	YKS85a	500-1000	P	expt.al app., EXAFS
	YKS85b	500-1000	P	EXAFS, non-standard phase shifts indicated
	HI86	500-900	E	smooth cont., very weak EXELFS (cf YKS85b)
	YKS86	500-950	P	EXAFS, corrected for second order radiation
	HS87	530-560	R	$\sigma_g^*$ , $\sigma_u^*$ identified
	MC&87	520-580	E	absolute OS, test of EELS-->OOS conversion
	PL&87	530-560	T	shape resonance – bond length refuted
	SAV87	10-1000	P,T	absolute, comp. to X-alpha
	YK87	500-900	P	EXAFS, analysis refined, both O-C & O-O detected
	YKS87	500-900	P	EXAFS, comp. to other O-X species
	HI88b	500-900	E	EXAFS identified, weaker than PA
	NH&88	530-560	R	comp with ETS, COS, $\text{CS}_2$ re $\sigma^*$ locations
	CT89	535	E	DES by (e,2e); CO, $\text{CO}_2$ & COS similar O K-hole decay atomic?
	LCS89	400-1000	E	EXAFS, q-dependence, comp. to PA; C-O backscatter phase derived
	MH&89	525-580	E,T	absolute, ab initio, comp. of $\text{CO}_2$ , COS & $\text{CS}_2$ - all edges
	SG&89	535-550	T	$\sigma^*$ shape res.; pos. & shape as f(R); approx. cyl. well & ab initio
	SY&89	520-570	P	O1s 2nd order, comp to EELS, discrete/cont. lower; cont. flatter
	HW&90	500-1000	E	EXELFS; excellent match to PA [YKS87]
	CT91	535	E	(e,2e) DES; comp. to Auger and theory [Phys. Rev. B 41 (90) 10510]
	FA91	530-540	T	absolute; XAS vs. XRF; comp. to expt. (WB74)
	LAL91	530-550	T	CNDO, systematic treatment of $\sigma^*$ energies
	VBA91	500-900	T	CI effect on EXAFS; HF-SCF; comp. to (YKS87); forward foc. MS
	S92	530-570	T,R	MS-X $\alpha$ , comp to W74a; $\sigma^*(\text{C-O})$
	SK&92a	536-570	P	absolute cross sections and $\beta$ 's from PES
	MB93	535.4	T	ab initio CI; GOS; OOS = 0.093; comp to EELS (0.12 MC&87) & PA (0.006 SA&84)

(CO <sub>2</sub> cont'd)	MB&93	534-540	T	GOS calculation, core hole localization
	L94	530,540	T	X-ray emission at $\pi^*$ , $\sigma^*$ ; compared to resonant AI
	BM&95	530-540	P	HERMON at SRC; 1e5 resolving power
	BSS95	530-580	P	total and partial ion yields, $\beta$ s; PIPICO
	HC&95	532-546	P	TIY, PIY; threshold e, ion,ion coinc.; no site-specific fragment.
	SK&95b	538-600	P	partial PE X-sections; $\beta$ s (main, satellite); coupling prevents main line X-section from detecting SR; strong conjugate shake-up
	HC&96	550 eV	P	triple coincidence; dissociation mechanisms
	SG&96a	530-570	P,T	absorption, resonant X-ray emission; STEX cacl.; 539 eV peak mostly 4s $\sigma_g$
	SG&96b	532-535	P,T	RIXS; dipole forbidden emission with sub-resonant $\pi^*$ energies (-2 eV detune); vibrinic coupling in SLOW, not-FAST non-resonant processes
	YA&96	520-560	T	absolute; STEX; comp. of R <sub>2</sub> CO; comp. to expt.
	CG&97	530-560	P,T	RIXS, symmetry breaking at $\pi^*$ due to Jahn-Teller; time-dependent and time-independent treatments compared
	NG&97	532-536	P,R	resonant X-ray emission (RIXS); ang. dep. at 3s, 3p, Ryd; v-dependent
	PK&97	532-545	P	relative; 130 meV fwhm; TEY; shoulders seen; 3s Ryd
	PL&87	530-560	T	shape-resonance bond length refutation
	YA&97	520-560	T	absolute; STEX; comp. of R <sub>2</sub> CO; $\pi^*$ OS; initial & final state effects
	GG&98a	530-565	P,T	use of X-ray emission as f(0) to assign XAS; 541 eV peak is $\sigma(s)$
	MK&98b	530-590	P	absolute; Beers' law absorption; vib'n'l res. XPS; main, satellite X-sect
	NK&98	550	P	core hole localization & symmetry breaking; vibrational resolved PES
	PF&98	559	P,T	ang. dist. PES at $\sigma^*$ resonance; incoherent (spd) sum
	S98	530-570	P	symmetry-resolved fast ion yield, PE ang dist; scattering path interference at shape resonance
	ET&00	520-580	E,T	methods; GOS at $\pi^*$ , Ryd; MC-GMS calc ; strong quadrupole GOS
	SU&00	534-538	P	C <sup>+</sup> /O <sup>+</sup> yield; 3s $\sigma_g$ enhanced in O <sup>+</sup> ; asymmetry; KERD, RT coupling
	TE&01b	520-580	E,T	GOS at $\pi^*$ , Ryd; MC-GMS calc indicate strong quadrupole GOS
	K02	530-560	P,T,R	symmetry resolved, high resolution; review
	OS&02	533-570	P	relative, Anion, cation PIY; only O <sup>-</sup> at (C1s <sup>-1</sup> , $\pi^*$ ); O <sup>-</sup> , C <sup>-</sup> at O1s edge
	OY&02	538-542	P	TIY, PIY, ang. Distr., fixed-in-space pol. dep; Rydberg assignments
	SM&02	535	P, T	COLTRIMS, ion-ion correlation, geometry deformation in (1s <sup>-1</sup> , $\pi^*$ )
	H02	544-574	P	total absorption compared to total and vibrationally resolved single hole
	BRB05	537-540	T	GOS; oscillations from Young-type interference; comp to ET&00
	YHA05	418	P, R	ion angular dist; fixed-molecule PAD spectra, review
	CC11	200-600	E	EELS in TEM; in situ catalysis
	HK&07	530-560	P	relative, O <sup>-</sup> yield, ang. dist. from imaging time-of-flight; tracks absorption
	KA&11	530-590	P	TIY, luminescence spectroscopy, O atom partial luminescence yield
				VUV-ion coincidence, C <sup>+</sup> , O <sup>+</sup> emitters dominate
	KAR12	542	P	XES – PI coincidence at O 1s edge
	SS&12	540	P	Auger-ion-ion coincidence, [Auger, metastable CO <sub>2</sub> <sup>2+</sup> ] coinc
	BF15	1173	P,T	double core hole (DCH) PES&Auger; compare CO, CO <sub>2</sub> , N <sub>2</sub> , N <sub>2</sub> O
	FH&20	526-550	T	coupled cluster calc; comp. to many solid species
	SK&22a	533-539	P	high accuracy E-caib (1s $\rightarrow\pi^*$ 535.334 eV), Ne, CO <sub>2</sub> -O1s, SF <sub>6</sub> -F1s
C <sub>2</sub>	MM&09	300-800	T	DWA cross-section calculation for EI
C <sub>2</sub> DH <sub>5</sub> O	AM&05	526-542	P	(CH <sub>3</sub> CH <sub>2</sub> OD), TIY, PIY, state-selective frag, isotope effects
C <sub>2</sub> D <sub>3</sub> H <sub>3</sub> O	AM&05	526-542	P	(CD <sub>3</sub> CH <sub>2</sub> OH), TIY, PIY, state-selective frag, isotope effects
C <sub>2</sub> F <sub>3</sub> HO <sub>2</sub>	RI&88	525-575	E	CF <sub>3</sub> COOH, absolute, comp. to acetic acid, perfluor effect
C <sub>2</sub> F <sub>3</sub> H <sub>3</sub> O <sub>3</sub> S	HH14	520-600	E	(Methyl trifluoromethanesulfonate), absolute, comp to Nafion
C <sub>2</sub> F <sub>6</sub> O <sub>2</sub>	H86b	525-575	E	CF <sub>3</sub> OCOF <sub>3</sub> , orbital mapping
	IM&87	525-575	E	low-lying $\sigma^*(O-O)$ , absolute
	HM&89	520-630	P	absolute; total, partial IYs; PIPICO, diss. IY; sel. frag.
	H90a	500-580	E,P	comp. of excitation (ISEELS) and ion branching ratios (TOF-PI)

<b>C<sub>2</sub>H<sub>4</sub>O</b>	RH91	525-560	E	absolute; comp. of peroxides and H <sub>2</sub> O; low-lying σ*(O-O)
	HB80b	525-565	E	(CH <sub>3</sub> CHO - acetaldehyde) cont. res.
	SSH84a	540	T	σ*-res./bond length relationship
	YA&96	520-560	T	absolute; STEX; comp. of R <sub>2</sub> CO; comp. to expt.
	YA&97	520-560	T	absolute; STEX; comp. of R <sub>2</sub> CO; π* OS; initial & final state effects
	TJ&99	525-565	P	relative; TIY; participator decay; 2 states in π*
<b>C<sub>2</sub>H<sub>4</sub>O</b>	SB91a	530-555	E	ethylene oxide
<b>C<sub>2</sub>H<sub>4</sub>O<sub>2</sub></b>	IH88	525-575	E	CH <sub>3</sub> COOH (acetic acid); absolute
	DF&08	525-575	E,T	valence-Rydberg mixed states; vibrational structure; ab initio, Z+1
<b>C<sub>2</sub>H<sub>4</sub>O<sub>2</sub></b>	IH88	525-575	E	HCOOCH <sub>3</sub> , methyl formate
	JT94b	520-565	P,T	ISEELS as f(resolution); DES by (e,2e); differs from DES of other R-CO
<b>C<sub>2</sub>H<sub>5</sub>NO<sub>2</sub></b>	PC&98	520-560	T	glycine; STEX; comp. of NEXAFS and circ. dichr. of amino acids
	GC&03	520-540	E,T	absolute, comp Gly, Gly-Gly; tri-gly(s); peptide bonds; GSCF3
	CG&04	525-555	E	comp. of Gly, Gly-gly, Gly <sub>3</sub> , gas-solid
	MG&16	399-412	P,T	comp Gly, Gly-gly
<b>C<sub>2</sub>H<sub>5</sub>N<sub>3</sub>O<sub>2</sub></b>	UA&99	520-560	E	biuret; (NH <sub>2</sub> (CO)NH(CO)NH <sub>2</sub> ); absolute
	LC&07	525-565	E,T	comp.of di-carbonyls; charge shifts for fingerprinting, GSCF3
<b>C<sub>2</sub>H<sub>6</sub>O</b>	WB74b	530-570	E	(CH <sub>3</sub> OCH <sub>3</sub> - dimethyl ether) res. at thresh.
	SSH84a	540	T	σ*-res./bond length relationship
	LAL91	530-550	T	CNDO, systematic treatment of σ* energies
<b>C<sub>2</sub>H<sub>6</sub>O</b>	VA&75	525-560	P	(CH <sub>3</sub> CH <sub>2</sub> OH - ethanol)
	YKS87	500-900	P	EXAFS, comp. to other O-X species
	SY&89	520-570	P	O1s 2nd order, lower discrete/cont. ratio, cont. flatter
	AM&05	526-542	P	(CD <sub>3</sub> CH <sub>2</sub> OH), TIY, PIY, state-selective frag, isotope effects
(C <sub>2</sub> H <sub>6</sub> O) <sub>n</sub>	TY&05	533-545	P	ethanol clusters TIY, PIY
C <sub>2</sub> H <sub>6</sub> OS	TB&88	525-555	E	(CH <sub>3</sub> ) <sub>2</sub> S=O, DMSO, comp. to S1s
<b>C<sub>2</sub>H<sub>6</sub>O<sub>2</sub></b>	HUR92	525-570	E	(CH <sub>3</sub> O) <sub>2</sub> CO methyl carbonate; comp. to polymer EELS
C <sub>2</sub> H <sub>6</sub> O <sub>2</sub>	EUH98	525-565	E	ethylene glycol; (CH <sub>2</sub> OH-CH <sub>2</sub> OH); absolute; comp to PEO
<b>C<sub>2</sub>H<sub>6</sub>O<sub>3</sub>S</b>	HH14	525-565	E	(CH <sub>3</sub> )SO <sub>3</sub> CH <sub>3</sub> , absolute, comp. to PFSA (Nafion) spectra
C <sub>2</sub> H <sub>8</sub> O <sub>2</sub>	IH07	530-544	T	methanol dimer, relative, Gaussian augmented plane wave (GAPW) - DFT; (-5 to +3 eV errors on 14 small molecules
C <sub>2</sub> N <sub>2</sub>	MM&09	300-800	T	DWA cross-section calculation for EI
C <sub>3</sub> ClH <sub>5</sub> O	LDN07	528-548	P	epichlorohyrin – CH <sub>3</sub> (CH-O-CH <sub>2</sub> ); TIY, PEPICO, site selective
<b>C<sub>3</sub>F<sub>6</sub>O</b>	RI&88	525-575	E	(perfluoroacetone), C-F σ* res., absolute, perfluoro effect
<b>C<sub>3</sub>H<sub>2</sub>O<sub>2</sub></b>	IH88	525-575	E	propionic acid, comp. to solid, absolute, group analysis
C <sub>3</sub> H <sub>3</sub> NO <sub>2</sub>	IO&00	525-560	P	absolute; E-selected mass spec; comp to C <sub>4</sub> H <sub>5</sub> NO <sub>2</sub> ; size dep..frag.
	TS&05	520-570	P, T	absolute, StoBE-DFT, N 1s and O 1s
C <sub>3</sub> H <sub>3</sub> N <sub>3</sub> O <sub>2</sub>	BC&19	536-544	P,T	2-nitroimidazole, NEXAFS, XPS, PIY; HF, DFT, MCSCF, TDDFT calc
C <sub>3</sub> H <sub>4</sub> O	IH88	525-575	E	propionic alcohol, comp. to solid, absolute, group analysis
C <sub>3</sub> H <sub>4</sub> O	DF&03	520-560	E	CH <sub>2</sub> =CH-CHO, acrolein; π* delocalisation; ab initio GAMES
<b>C<sub>3</sub>H<sub>4</sub>O<sub>2</sub></b>	IH88	525-575	E	acrylic acid, comp. to solid, absolute, group analysis
<b>C<sub>3</sub>H<sub>6</sub>NO<sub>2</sub></b>	GH01	525-565	E	alanine; absolute; comp of amino acids
C <sub>3</sub> H <sub>6</sub> NO <sub>2</sub> S	PC&98	530-560	T	cysteine; (D,L-) STEX; comp. of NEXAFS, circ. dichr. of amino acids
<b>C<sub>3</sub>H<sub>6</sub>N<sub>2</sub>O<sub>2</sub></b>	LC&07	525-565	E,T	malonamide; comp.of di-carbonyls; charge shifts for fingerprinting, GSCF3
<b>C<sub>3</sub>H<sub>6</sub>O</b>	HB80b	525-565	E	(acetone) cont. res.
	SSH84a	540	T	σ*-res./bond length relationship
	NM&87	500-600	P	total ion yield; TOF-MS; slight selectivity
	YKS87	500-900	P	EXAFS, comp. to other O-X species
	RI&88	525-575	E	ref for C-F σ* res., absolute, perfluoro effect
	SY&89	520-570	P	O1s 2nd order, comp to EELS, discrete/cont. lower; cont. flatter
	YA&97	520-560	T	absolute; STEX; comp. of R <sub>2</sub> CO; π* OS; initial & final state effects
	TPA98	525-570	T	absolute; DFT vs. STEX, compares CO and R <sub>2</sub> CO, R = H, Me

C <sub>3</sub> H <sub>6</sub> O (cont'd)	TJ&99a	528-565	P,T	absolute; resonant Auger; STEX calc.
	TJ&99b	528-565	P	relative, TIY
	SS00	528-565	P	TIY, PIY; weak site or state selective fragmentation
	IH07	530-544	T	relative, Gaussian augmented plane wave (GAPW) - DFT; (-5 to +3 eV errors on 14 small molecules
C <sub>3</sub> H <sub>6</sub> O	YA&96	520-560	T	ethylaldehyde; absolute; STEX; comp. of R <sub>2</sub> CO; comp. to expt.
	YA&97	520-560	T	absolute; STEX; R <sub>2</sub> CO comp; π* OS; initial,final state effects
	TJ&99a	520-560	P,T	absolute, resonant Auger, STEX
	TJ&99b	528-565	P	relative, TIY
C <sub>3</sub> H <sub>6</sub> O	PL&07	528-542	P, T	methyloxirane CH <sub>3</sub> -[CHOCH <sub>2</sub> ]; TIY; XPS
<b>C<sub>3</sub>H<sub>6</sub>O</b>	IH88	525-575	E	acrylic alcohol, comp. to solid, absolute, group analysis
C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	IH88	525-575	E	propanoic acid, comp. to solid, absolute, group analysis
<b>C<sub>3</sub>H<sub>6</sub>O<sub>3</sub></b>	HW&91	525-570	E	dimethylcarbonate; absolute
<b>C<sub>3</sub>H<sub>6</sub>O<sub>3</sub></b>	H01	525-565	E	lactic acid; Me(CHOH(COOH); absolute
<b>C<sub>3</sub>H<sub>7</sub>NO<sub>2</sub></b>	UH&95b	525-575	E	NH <sub>2</sub> CO <sub>2</sub> Et, absolute; modelling of polyurethane PEELS
C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub>	PC&98	530-560	T	alanine; (D-,L-); STEX; comp. of NEXAFS, circ. Dichr. of amino acids
	GT&11	528-546	T	gas, crystal, adsorbate comparison; conformers
C <sub>3</sub> H <sub>7</sub> NO <sub>3</sub>	PC&98	530-560	T	serine; (D-,L-); STEX; comp. of NEXAFS, circ. Dichr. of amino acids
<b>C<sub>3</sub>H<sub>8</sub>O</b>	IH88	525-575	E	n-propanol, absolute, group analysis
	TH&98	532-543	P	threshold e-; TIY; TPEPICO; triple coinc; isomer study
C <sub>3</sub> H <sub>8</sub> O	TH&98	532-543	P	(isoproponol); threshold e-; TIY; TPEPICO; triple coinc; isomer study
C <sub>3</sub> H <sub>8</sub> O <sub>2</sub>	EUH98	525-565	E	1,2-propane diol; absolute; comp to PPO
<b>C<sub>4</sub>H<sub>4</sub>O<sub>3</sub>S</b>	HH14	525-565	E	(methane sulfonic acid), references for PFSA (Nafion)
<b>C<sub>4</sub>H<sub>4</sub>O</b>	NIH86	525-575	E	(furan), absolute; compared to tetrahydro-furan, other heterocycles
C <sub>4</sub> H <sub>4</sub> FN <sub>3</sub> O	FP&11	530-540	P	(5-methylcytosine), tautomerism in cytosines
C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub>	FP&10	530-545	P,T	(cytosine), tautomerism
C <sub>4</sub> H <sub>5</sub> NO <sub>2</sub>	IO&99	525-575	P	MeO(CO)CH <sub>2</sub> CN; absolute; N1s, O1s → π* mass spect; site sel. frag.
	IO&00	525-560	P	absolute; E-selected mass spec; comp to C <sub>3</sub> H <sub>3</sub> NO <sub>2</sub> ; size dep..frag.
	TS&05	520-570	P, T	absolute, StoBE-DFT, N 1s and O 1s
				(uracil), tautomerism
C <sub>4</sub> H <sub>5</sub> N <sub>3</sub> O	FP&10	530-545	P,T	
<b>C<sub>4</sub>H<sub>6</sub>O<sub>3</sub></b>	LC&07	525-565	E,T	acetic anhydride; di-carbonyls; charge shifts for fingerprinting, GSCF3
<b>C<sub>4</sub>H<sub>6</sub>O<sub>5</sub></b>	LCH03	525-565	E,T	MeO(CO)O(CO)OMe; di-carbonyls; charge shifts, GSCF3
	LC&07	525-565	E,T	MeO(CO)O(CO)OMe; di-carbonyls; charge shifts, GSCF3
<b>C<sub>4</sub>H<sub>7</sub>NO<sub>2</sub></b>	LC&07	525-565	E,T	Me(CO)N(CO)Me; di-acetamide; di-carbonyls; charge shifts, GSCF3
<b>C<sub>4</sub>H<sub>7</sub>NO<sub>2</sub></b>	UA&99	525-565	E	ethyl allophanate (NH <sub>2</sub> (CO)O(CO)OEt); absolute; polymer model
	UH&99	525-565	E,T	ethyl allophanate; absolute; GSCF3; comp. of urethane species
<b>C<sub>4</sub>H<sub>8</sub>N<sub>2</sub>O<sub>3</sub></b>	GC&03	520-540	E,T	absolute, comp Gly, Gly-Gly; tri-gly(s); peptide bonds; GSCF3
	CG&04	525-555	E	(glycyl-glycine), comp. of Gly, Gly-gly, Gly <sub>3</sub> , gas-solid
<b>C<sub>4</sub>H<sub>8</sub>O</b>	NIH86	525-575	E	(tetrahydrofuran), compared to furan, other heterocycles
	YKS87	500-900	P	EXAFS, comp. to other O-X species
	SY&89	520-570	P	O1s 2nd order, comp to EELS, discrete/cont. lower; cont. flatter
C <sub>4</sub> H <sub>8</sub> O	YA&96	520-560	T	propaldehyde; absolute; STEX; comp. of R <sub>2</sub> CO; comp. to expt.
	YA&97	520-560	T	absolute; STEX; R <sub>2</sub> CO comp; π* OS; initial,final state effects
C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	YKS87	500-900	P	(dioxane), EXAFS, comp. to other O-X species
	SY&89	520-570	P	O1s 2nd order, comp to EELS, discrete/cont. lower; cont. flatter
C <sub>4</sub> H <sub>9</sub> F <sub>3</sub> O <sub>3</sub> SSi	UH94a	525-560	E	Me <sub>3</sub> SiOSO <sub>2</sub> CF <sub>3</sub> ; comp of SI-O-X species re inductive, resonance effects
<b>C<sub>4</sub>H<sub>10</sub>O</b>	IM&87	525-575	E	t-butanol, absolute, comp. to t-butyl peroxide
<b>C<sub>4</sub>H<sub>10</sub>O</b>	YKS87	500-900	P	(C <sub>2</sub> H <sub>5</sub> OC <sub>2</sub> H <sub>5</sub> , di-ethyl ether), EXAFS, comp. to other O-X species
	SY&89	520-570	P	O1s 2nd order, comp to EELS, discrete/cont. lower; cont. flatter
	UH&95b	528-550	E,T	absolute; EHMO; comp. to polyurethanes
<b>C<sub>4</sub>H<sub>12</sub>OSi</b>	UH94a	525-560	E	Me <sub>3</sub> Si(OMe); comp of SI-O-X species re inductive, resonance effects

<b>C<sub>4</sub>NiO<sub>4</sub></b>	CSB90a	525-580	E	Ni(CO) <sub>4</sub> ; comp. to CO
	HWR90	525-560	E	absolute; comp. of TM carbonyls; f( $\pi^*$ ) as f(backbond)
	SLD95	534	T	absolute, DF-LCAO; OS for C1s, O1s $\rightarrow \pi^*$ ; orbital mapping
<b>C<sub>5</sub>FeO<sub>5</sub></b>	MSN89	500-650	P	total, partial ion yields; comp to CO, Fe <sub>2</sub> (CO) <sub>9</sub>
	HWR90	525-560	E	absolute; comp. of TM carbonyls; f( $\pi^*$ ) as f(backbond)
	WRH92	525-570	E	absolute, comp. of organo-iron complexes, ligand interaction effects
	SLD95	534	T	absolute, DF-LCAO; OS for C1s, O1s $\rightarrow \pi^*$ ; orbital mapping
<b>C<sub>5</sub>H<sub>5</sub>N<sub>5</sub>O</b>	PF&09	528-548	P,T	(gauanine) Tautomerism, thermal gas, DFT calc; Boltzmann-weighted
<b>C<sub>4</sub>H<sub>5</sub>N<sub>3</sub>O</b>	FP&11	530-540	P	(5-fluorocytosine), tautomerism in cytosines
<b>C<sub>5</sub>H<sub>7</sub>N<sub>3</sub>O</b>	FP&11	530-540	P	(isocytosine), tautomerism in cytosines
<b>C<sub>5</sub>H<sub>8</sub>MnO<sub>2</sub><sup>+</sup></b>	AG&23	528-540	P	Mn(acac); RASPT2 calc., compare m = 1,2,3
<b>C<sub>5</sub>HMnO<sub>5</sub></b>	RH89	525-560	E	HMn(CO) <sub>5</sub>
	SLD95	534	T	absolute, DF-LCAO; OS for C1s, O1s $\rightarrow \pi^*$ ; orbital mapping
<b>C<sub>5</sub>H<sub>8</sub>O<sub>2</sub></b>	LC&07	525-565	E,T	Me(CO)Me(CO)Me; di-carbonyls; charge shifts, GSCF3
<b>C<sub>5</sub>H<sub>8</sub>O<sub>4</sub></b>	LC&07	525-565	E,T	MeO(CO)Me(CO)OMe; di-carbonyls; charge shifts, GSCF3
<b>C<sub>5</sub>H<sub>8</sub>O</b>	HI88	525-575	E	(1,3-dihydropyran)
<b>C<sub>5</sub>H<sub>8</sub>O<sub>2</sub></b>	CH98	534	T	malonaldehyde (CH <sub>3</sub> COC=C(OH)CH <sub>3</sub> ); DFT; 0.2 eV keto-enol $\pi^*$ shift
<b>C<sub>5</sub>H<sub>8</sub>O<sub>2</sub></b>	CH98	534	T	acetylacetone (CH <sub>3</sub> COCH <sub>2</sub> (CO)CH <sub>3</sub> ); DFT; 0.2 eV keto-enol $\pi^*$ shift
	YY&99	510-570	P	TIY, PIY, site selective fragmentation; enhanced Me <sup>+</sup> , MeCO <sup>+</sup>
	LC&07	525-565	E,T	absolute, GSCF3, comp of dicarbonyls
<b>C<sub>5</sub>H<sub>10</sub>O</b>	NIH86	525-575	E	(tetrahydropyran), absolute, heterocycles
<b>C<sub>5</sub>H<sub>10</sub>O</b>	YA&96	520-560	T	diethylketone; absolute; STEX; comp. of R <sub>2</sub> CO; comp. to expt.
	YA&97	520-560	T	absolute; STEX; R <sub>2</sub> CO comp; $\pi^*$ OS; initial,final state effects
<b>C<sub>5</sub>H<sub>11</sub>NO<sub>2</sub></b>	PC&98	520-560	T	valine; (D,L-) STEX; comp. of NEXAFS, circ. Dichr. of amino acids
<b>C<sub>5</sub>H<sub>14</sub>O</b>	UHR95	520-560	E	sec-butyl ethyl ether; absolute
<b>C<sub>5</sub>H<sub>14</sub>OSi</b>	TC&02	525-565	E	Me <sub>3</sub> SiOEt; absolute; comp. to vinyl silanes
<b>C<sub>6</sub>CrO<sub>6</sub></b>	CSB90	525-575	E	comp. of M(CO) <sub>6</sub> , M=Cr,Mo,W
	SLD95	534	T	absolute, DF-LCAO; OS for C1s, O1s $\rightarrow \pi^*$ ; orbital mapping
<b>C<sub>6</sub>H<sub>4</sub>O<sub>2</sub></b>	FH92	520-570	E,T	benzoquinone, absolute, EHMO; quinoid effect
<b>C<sub>6</sub>H<sub>5</sub>NO<sub>2</sub></b>	TUH96	525-565	E	nitrobenzene; absolute; EHMO, comp. to nitroanilines
<b>C<sub>6</sub>H<sub>6</sub>N<sub>2</sub>O<sub>2</sub></b>	TUH96	525-565	E,T	(1,2)-nitroaniline; absolute, EHMO, comp. to aniline, nitrobenzene
<b>C<sub>6</sub>H<sub>6</sub>N<sub>2</sub>O<sub>2</sub></b>	TUH96	525-565	E,T	(1,3)-nitroaniline; absolute, EHMO, comp. to aniline, nitrobenzene
<b>C<sub>6</sub>H<sub>6</sub>N<sub>2</sub>O<sub>2</sub></b>	TUH96	525-565	E,T	(1,4)-nitroaniline; absolute, EHMO, comp. to aniline, nitrobenzene
<b>C<sub>6</sub>H<sub>6</sub>O</b>	FH92	520-570	E,T	phenol, absolute, EHMO; quinoid effect
	PY&97	530-560	T	STEX, comp to FH92; substituent effects (X=F,OH, NH <sub>2</sub> )
	PP&00	534	T	MC-SCF Z+1 calc; vibrational structure, XPS better than NEXAFS
	LL&14a	530-560	P	TIY, PIY
<b>C<sub>6</sub>H<sub>6</sub>O<sub>2</sub></b>	FH92	520-570	E,T	hydroquinone, absolute, EHMO; quinoid effect
<b>C<sub>6</sub>H<sub>8</sub>O</b>	UHR99	520-570	E	2-cyclohexene-1-one; absolute; conjugation test
<b>C<sub>6</sub>H<sub>8</sub>O<sub>2</sub></b>	FH94	520-570	E,T	1,2-cyclohexanedione, absolute, conjugation of $\pi^*(CO)$
<b>C<sub>6</sub>H<sub>8</sub>O<sub>2</sub></b>	FH94	520-570	E,T	1,3-cyclohexanedione, absolute, conjugation of $\pi^*(CO)$
<b>C<sub>6</sub>H<sub>8</sub>O<sub>2</sub></b>	FH94	520-570	E,T	1,4-cyclohexanedione, absolute, conjugation of $\pi^*(CO)$
<b>C<sub>6</sub>H<sub>9</sub>N<sub>3</sub>O<sub>3</sub></b>	UA&99	520-570	E	trimethyl-isocyanurate; absolute; polymer model
<b>C<sub>6</sub>H<sub>10</sub>O</b>	FH94	520-570	E,T	(cyclohexanone); absolute; comp. to o,m,p-cyclohexanenedione
<b>C<sub>6</sub>H<sub>14</sub>N<sub>4</sub>O<sub>2</sub></b>	LH&12	531-538	T	(arginine), gas-solid comparison
<b>C<sub>6</sub>H<sub>10</sub>O</b>	UHR99	520-570	E	4-hexene-3-one; absolute; conjugation test
<b>C<sub>6</sub>H<sub>14</sub>O</b>	UH&95a	525-575	E	i-Pr-ether; absolute; model for poly-ol of polyurethanes
	UH&95b	525-575	E	absolute; comp. to diethylether
<b>C<sub>6</sub>H<sub>16</sub>OSi</b>	UH94a	525-560	E	Et <sub>3</sub> SiOH; comp of SI-O-X species re inductive, resonance effects
<b>C<sub>6</sub>H<sub>18</sub>OSi<sub>2</sub></b>	UH94a	525-560	E	Me <sub>3</sub> SiOSiMe <sub>3</sub> ; comp of SI-O-X species re inductive, resonance effects
<b>C<sub>6</sub>H<sub>18</sub>O<sub>3</sub>Si<sub>3</sub></b>	UH94a	525-560	E	c-(SiMe <sub>2</sub> O) <sub>3</sub> ; comp of SI-O-X species re inductive, resonance effects

<b>C<sub>6</sub>MoO<sub>6</sub></b>	CSB90	525-575	E	comp. of M(CO) <sub>6</sub> , M=Cr,Mo,W
	SLD95	534	T	DF-LCAO; absolute osc. str for C1s, O1s → π*; orbital mapping
<b>C<sub>6</sub>O<sub>6</sub>V</b>	TD&92	525-575	P,E	V(CO) <sub>6</sub> , absolute
<b>C<sub>6</sub>O<sub>6</sub>W</b>	CSB90	525-575	E	comp. of M(CO) <sub>6</sub> , M=Cr,Mo,W
<b>C<sub>7</sub>CoH<sub>5</sub>O<sub>2</sub></b>	HWR90	525-560	E	CoCp(CO) <sub>2</sub> ; absolute; comp. of TM carbonyls; f(π*) as f(backbond)
	RWH91	520-700	E	absolute; comp. to other mixed-Cp, CO species
<b>C<sub>7</sub>FeH<sub>6</sub>O<sub>3</sub></b>	WRH92	525-570	E	RFe(CO) <sub>3</sub> , R=butadiene; absol; organo-irons; ligand interactions
<b>C<sub>7</sub>H<sub>6</sub>O</b>	HUR92	525-570	E	benzaldehyde; comp. to polymer EELS
	RY&92	520-560	E	comp. of small mol. analogs with PET polymer
<b>C<sub>7</sub>H<sub>6</sub>O<sub>2</sub></b>	ITH17	525-545	T	benzoic acid, StoBE-DeMon calc; triplet states
<b>C<sub>7</sub>H<sub>7</sub>NO<sub>2</sub></b>	UH&95b	525-575	E	NH <sub>2</sub> CO <sub>2</sub> Ph, absolute; modelling of polyurethane PEELS
<b>C<sub>7</sub>H<sub>8</sub>O</b>	UHR97	530-560	E	anisole (Ph-OMe); absolute
<b>C<sub>7</sub>H<sub>8</sub>O</b>	AM&05	526-542	P	(CD <sub>3</sub> CH <sub>2</sub> OH), TIY, PIY, state-selective frag, isotope effects
<b>C<sub>7</sub>H<sub>8</sub>N<sub>2</sub>O</b>	UH&95a	525-560	E	phenylurea; absolute; comp. to PEELS of polyurethane models
	UH&95b	525-560	E	absolute; urea and urethanes differ at O 1s
<b>C<sub>7</sub>H<sub>12</sub>O<sub>2</sub></b>	LUH97	525-560	E	butyl acrylate; absolute; polymer model
<b>C<sub>7</sub>H<sub>14</sub>O</b>	YA&96	520-560	T	dipropylketone; absolute; STEX; comp. of R <sub>2</sub> CO; comp. to expt.
	YA&97	520-560	T	absolute; STEX; R <sub>2</sub> CO comp; π* OS; initial,final state
<b>C<sub>8</sub>Cl<sub>2</sub>H<sub>4</sub>O<sub>2</sub></b>	HUR92	525-570	E	terphthalyl chloride; comp. to polymer EELS
	RY&92	520-560	E	comp. of small mol. analogs with PET polymer
<b>C<sub>8</sub>Co<sub>2</sub>O<sub>8</sub></b>	HWR90	525-560	E	Co <sub>2</sub> (CO) <sub>8</sub> ; absolute; comp. of TM carbonyls; f(π*) as f(backbond)
	RWH91	520-700	E	absolute; comp. to mixed-Cp, CO species
<b>C<sub>8</sub>F<sub>3</sub>C<sub>6</sub>H<sub>4</sub>NO</b>	IO&99	520-565	P	p-CF <sub>3</sub> C <sub>6</sub> H <sub>4</sub> NCO; TIY; N1s, O1s → π* frag.; no site selectivity
<b>C<sub>8</sub>H<sub>6</sub>O<sub>2</sub></b>	HUR92	525-570	E	terphthaldehyde; comp. to polymer EELS
	RY&92	520-560	E	comp. of small mol. analogs with PET polymer
<b>C<sub>8</sub>H<sub>8</sub>O</b>	HH13	520-560	E	(phenyl-methyl-ketone), absolute
<b>C<sub>8</sub>H<sub>8</sub>O<sub>2</sub></b>	ITH17	525-545	T	methyl benzoate, StoBE-DeMon calc; triplet states
<b>C<sub>8</sub>H<sub>9</sub>NO</b>	UH&95a	520-560	E	benzyl carbamate; absolute; comp to PEELS of model polyurethanes
	UH&95b	520-560	E	absolute; O 1s useful to distinguish urea/urethane
<b>C<sub>8</sub>H<sub>9</sub>NO</b>	TC&16	2399-415	P,T	acetanilide; TIY; TD-LB94/6-31+G(d,p); comp to cis-Nbenzylacetamide
<b>C<sub>8</sub>H<sub>9</sub>NO<sub>2</sub></b>	GH01	520-560	E	phenylalanine, comp. of amino acids
<b>C<sub>8</sub>H<sub>12</sub>O<sub>3</sub>Si</b>	TC&02	520-560	E	(CH <sub>2</sub> =CH)Si(OAc) <sub>3</sub> ; absolute; vinyl silanes
<b>C<sub>8</sub>H<sub>18</sub>O<sub>3</sub>Si</b>	TC&02	280-320	E	(CH <sub>2</sub> =CH)Si(OEt) <sub>3</sub> ; absolute
<b>C<sub>8</sub>H<sub>16</sub>O</b>	UHR92	525-575	E	sec-But-ether, absolute; modelling of polyurethane PEELS
<b>C<sub>8</sub>H<sub>18</sub>O<sub>2</sub></b>	IM&87	525-575	E	t-Bu-O-O-t-Bu, absolute, low lying σ*(O-O)
	RH91	525-560	E	absolute; comp. of peroxides and H <sub>2</sub> O; low-lying σ*(O-O)
<b>C<sub>8</sub>H<sub>24</sub>O<sub>4</sub>Si<sub>4</sub></b>	UH94a	525-560	E	c-(SiMe <sub>2</sub> O) <sub>4</sub> ; comp of SI-O-X species re inductive, resonance effects
<b>C<sub>9</sub>CrH<sub>6</sub>O<sub>3</sub></b>	W92	520-560	E	BzCr(CO) <sub>3</sub> , absolute
	WHR92	520-560	E	BzCr(CO) <sub>3</sub> , absolute
<b>C<sub>9</sub>FeH<sub>8</sub>O<sub>3</sub></b>	WRH92	520-560	E	CxFe(CO) <sub>3</sub> ; comp. of Fe(CO) <sub>5</sub> , RFe(CO) <sub>3</sub> , Fe(Cp) <sub>2</sub> ; mix. lig. effect
<b>C<sub>9</sub>Fe<sub>2</sub>O<sub>9</sub></b>	MSN89	500-650	P	total, partial ion yields; comp to CO, Fe(CO) <sub>5</sub>
	WRH92	520-560	E	CxFe(CO) <sub>3</sub> ; comp. of Fe(CO) <sub>5</sub> , RFe(CO) <sub>3</sub> , Fe(Cp) <sub>2</sub> ; mix. lig. effect
<b>C<sub>9</sub>H<sub>5</sub>O<sub>4</sub>V</b>	WHR92	525-550	E	cyclopentadienyl vanadium tetracarbonyl
<b>C<sub>9</sub>H<sub>6</sub>N<sub>2</sub>O<sub>2</sub></b>	UHR99	520-560	E,T	2,4-TDI, absolute; isomeric effect
<b>C<sub>9</sub>H<sub>6</sub>N<sub>2</sub>O<sub>2</sub></b>	UHR99	520-560	E,T	2,6-TDI, absolute; isomeric effect
<b>C<sub>9</sub>H<sub>7</sub>MnO<sub>3</sub></b>	W92	520-560	E	Me-CpMn(CO) <sub>3</sub> , absolute
<b>C<sub>9</sub>H<sub>8</sub>O<sub>2</sub></b>	LUH97	520-560	E	vinyl benzoate; absolute; model for PET X-ray damage
<b>C<sub>9</sub>H<sub>9</sub>N</b>	ZC&09	528-544	P	(3-methyl indone); tautomers, comp aromatic amino acids
<b>C<sub>9</sub>H<sub>10</sub>O<sub>2</sub></b>	HUR92	525-570	E	Ethylbenzoate; comp. to polymer EELS
	H92b	520-565	E,R	comp. to polymer EELS
	RY&92	520-560	E	comp. of small mol. analogs with PET polymer
<b>C<sub>9</sub>H<sub>11</sub>NO</b>	TC&16	528-542	P,T	cis-N-benzylacetamide ; TIY; TD-LB94/6-31+G(d,p); comp to acetanilide

<b>C<sub>9</sub>H<sub>11</sub>NO<sub>2</sub></b>	UH&95b	525-575	E	Ph-NHCO <sub>2</sub> Et, absolute; modelling of polyurethane PEELS
C <sub>9</sub> H <sub>11</sub> NO <sub>2</sub>	GW09	528-542	T	phenylalanine,DFT, comp to C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub> , C <sub>6</sub> H <sub>6</sub> , C <sub>8</sub> H <sub>10</sub> O <sub>2</sub> , C <sub>8</sub> H <sub>11</sub> N
	ZC&09	528-544	P	tautomers, comp aromatic amino acids
C <sub>9</sub> H <sub>11</sub> NO <sub>3</sub>	ZC&09	528-544	P	(tyrosine), tautomers, comp aromatic amino acids
C <sub>9</sub> H <sub>11</sub> NO <sub>5</sub> P	LC&25	528-545	P,T	protonated phosphotyrosine, NEXAMS, TIY, PIY; conformer calc
<b>C<sub>10</sub>ClCo<sub>3</sub>O<sub>9</sub></b>	HM&93	525-560	E,P	Cl-C-[Co(CO) <sub>3</sub> ] <sub>3</sub> , abs.; gas(E,P-ions), sol(P); PIPICO, TOF-MS
C <sub>10</sub> CrH <sub>8</sub> O <sub>3</sub>	W92	520-560	E	CH <sub>3</sub> -BzCr(CO) <sub>3</sub> , absolute
	WHR92	520-560	E	absolute
<b>C<sub>10</sub>H<sub>10</sub>O<sub>4</sub></b>	UH&96	525-545	E,T	p-dimethylphthalate (MeO <sub>2</sub> C-C <sub>6</sub> H <sub>4</sub> -CO <sub>2</sub> Me); ab initio; isomer effects; comp. to polymer
	RH&97	525-555	E,P,T	absolute; comp. to solid; NEXAFS, PEELS, STXM of PET; radiation damage quantified
	UT&97	525-555	E,T	absolute; ab initio; comp. to oligimer NEXAFS
<b>C<sub>10</sub>H<sub>10</sub>O<sub>4</sub></b>	UH&96	525-545	E,T	o-dimethylphthalate (MeO <sub>2</sub> C-C <sub>6</sub> H <sub>4</sub> -CO <sub>2</sub> Me); ab initio; isomer effects in o-, m-, p-phthalates; comp. to polymer
	UT&97	525-555	E,T	absolute; ab initio; comp. to oligimer NEXAFS
<b>C<sub>10</sub>H<sub>10</sub>O<sub>4</sub></b>	UH&96	525-545	E,T	m-dimethylphthalate (MeO <sub>2</sub> C-C <sub>6</sub> H <sub>4</sub> -CO <sub>2</sub> Me); ab initio; isomer effects in o-, m-, p-phthalates; comp. to polymer
	UT&97	525-555	E,T	absolute; ab initio; comp. to oligimer NEXAFS
C <sub>9</sub> H <sub>12</sub> NO	LKC16	527-540	P, T	TEMPO, relative, ΔDFT-GGA, complex spectra
C <sub>10</sub> H <sub>11</sub> N <sub>2</sub> O <sub>2</sub>	LKC16	527-540	P, T	nit8, TEMPO, relative, ΔDFT-GGA, complex spectra
<b>C<sub>10</sub>H<sub>12</sub>N</b>	UH98	525-575	E	1234-tetrahydro-1-naphthyl-amine, absolute
<b>C<sub>10</sub>H<sub>13</sub>NO<sub>2</sub></b>	UH&95b	525-575	E	Ph-N(CH <sub>3</sub> )-CO <sub>2</sub> Et, absolute; modelling of polyurethane PEELS
C <sub>10</sub> H <sub>13</sub> N <sub>2</sub> O <sub>2</sub>	LKC16	527-540	P, T	nit9, TEMPO, relative, ΔDFT-GGA, complex spectra
C <sub>10</sub> H <sub>16</sub> MnO <sub>4</sub> <sup>+</sup>	AG&23	528-540	P	Mn(acac) <sub>2</sub> ; RASPT2 calc., compare m =1,2,3
<b>C<sub>10</sub>H<sub>19</sub>O<sub>4</sub></b>	LC&07	525-565	E,T	<sup>t</sup> BuO(CO)NH(CO)O <sup>t</sup> Bu; di-carbonyls; charge shifts, GSCF3
<b>C<sub>10</sub>Mn<sub>2</sub>O<sub>10</sub></b>	HSW89	525-570	E	Mn <sub>2</sub> (CO) <sub>10</sub> , absolute, comp to CO, Mn(CO) <sub>5</sub> Br
<b>C<sub>11</sub>Co<sub>3</sub>H<sub>3</sub>O<sub>10</sub></b>	HM&93	525-560	E,P	CH <sub>3</sub> O-C-[Co(CO) <sub>3</sub> ] <sub>3</sub> , abs.; gas(E), sol(P)
<b>C<sub>11</sub>FeH<sub>8</sub>O<sub>3</sub></b>	WRH92	525-570	E	RFe(CO) <sub>3</sub> , R=COT; absolute, organo-irons; ligand interactions
C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>	ZC&09	528-542	P	(tryptophan) tautomers, comp aromatic amino acids
<b>C<sub>11</sub>H<sub>14</sub>N<sub>2</sub>O<sub>4</sub></b>	UHR99	525-570	E	TDI-bis-methyl urethane; absolute
<b>C<sub>12</sub>H<sub>10</sub>O<sub>3</sub></b>	HUR92	525-570	E	(BzO) <sub>2</sub> CO phenyl carbonate; comp. to polymer EELS
C <sub>12</sub> H <sub>18</sub> O	LL&14B	530-545	T	diphenylether, TIY, TD-DFT (Q-CHEM-4.1)
<b>C<sub>12</sub>H<sub>15</sub>N<sub>2</sub>O<sub>2</sub>Re</b>	HS92	520-560	E	Cp*Re(CO) <sub>2</sub> N <sub>2</sub> , absolute
C <sub>12</sub> O <sub>12</sub> Ru <sub>3</sub>	SF&90	520-560	P	relative, TEY; comp. to free CO; relaxation d(R) effects
<b>C<sub>13</sub>H<sub>12</sub>N<sub>2</sub>O</b>	UH&95b	525-575	E	Ph-NH <sub>2</sub> C=O; absolute; modelling of polyurethane PEELS
C <sub>13</sub> H <sub>15</sub> MnO <sub>3</sub>	WRH89	520-570	E	Cp*Mn(CO) <sub>3</sub> ; absolute
C <sub>14</sub> H <sub>10</sub> O <sub>3</sub>	LUH97	520-560	E	benzoic anhydride; absolute; polymer model
C <sub>15</sub> H <sub>24</sub> MnO <sub>6</sub> <sup>+</sup>	AG&23	528-540	P	Mn(acac) <sub>3</sub> ; RASPT2 calc., compare m =1,2,3
<b>C<sub>15</sub>H<sub>24</sub>O</b>	LUH97	520-560	E	butylated hydroxy toluene; absolute; polymer model
<b>C<sub>16</sub>H<sub>19</sub>N<sub>4</sub>O<sub>2</sub></b>	XX04	530-560	E	toluene ethyl urea, absolute
C <sub>18</sub> H <sub>14</sub> O <sub>2</sub>	LL&14B	530-550	P,T	1,3-diphenoxylbenzene, TIY, TD-DFT (Q-CHEM-4.1)
C <sub>19</sub> H <sub>22</sub> O <sub>3</sub>	AP&20	533-544	P	avobenzone, PEPICO, fragmentation, PES-derived
C <sub>18</sub> H <sub>15</sub> PO	GZ&20	529-537	P,T	triphenylphosphine (TP); OLED, XPS
<b>C<sub>18</sub>H<sub>16</sub>OSi</b>	UT&97	520-560	E	triphenylsilanol; absolute; Si-Si, Si-O-R systems
<b>C<sub>21</sub>H<sub>15</sub>N<sub>3</sub>O<sub>3</sub></b>	UHR92	520-560	E	(Bz-O)C <sub>3</sub> N <sub>3</sub> , triphenoxy-triazine; polyurethane modelling
	UA&99	520-560	E	tritylolyisocyanurate; absolute, polymer model
<b>C<sub>24</sub>H<sub>21</sub>N<sub>3</sub>O<sub>3</sub></b>	UA&99	520-560	E	tritylolyisocyanurate; absolute, polymer model
C <sub>27</sub> H <sub>35</sub> N <sub>5</sub> O <sub>7</sub> S	DS&21	530-545	P,T	[LeuEnk+H], , ENK-Tyr-Gly-Gly-Phe); NEXAFS mass spec; DFT/ROCI S
C <sub>28</sub> H <sub>37</sub> N <sub>5</sub> O	DS&21	530-545	P,T	MetEnk+H], ENK = Tyr-Gly-Gly-Phe); NEXAFS mass spec; DFT/ROCI S
C <sub>32</sub> H <sub>28</sub> P <sub>2</sub> O <sub>2</sub>	GZ&20	529-537	P,T	2,8-bis- (diphenylphosphoryl)-dibenzo[b,d]thiophene (PPT); OLED, XPS

C <sub>42</sub> H <sub>52</sub> FeN <sub>8</sub> O <sub>6</sub> S <sub>2</sub>	MC12	526-544	P	cytochrome c (12 kDa), NEXAMS
	MG&16	526-544	P	NEXAMS
C <sub>131</sub> H <sub>229</sub> N <sub>39</sub> O <sub>31</sub> <sup>+</sup>	EB&18	526-544	P	Melittin protein, NEXAMS, PIY
Cl <sub>3</sub> OP	SB85d	525-600	E	pot. barr. effects
ClO <sub>2</sub>	FPR06	525-560	P	PIY, TIY; ionization yield; PEPICO, PIPICO
DO	SRA02	525-528	P	high res.; comp. of vib'n &Ryd of OH,OD; v. low E (526eV)
D <sub>2</sub> O	RR&83	525-575	P	D <sup>+</sup> yields from sol; gas, solid, EY comp; extra peak at 560eV
	KP94b	530-540	T	ab initio DSCF-CI; vibrational analysis; comp. of H <sub>2</sub> O/D <sub>2</sub> O
<b>F<sub>2</sub>O</b>	IM&87	530-570	E	absolute; comp. to H <sub>2</sub> O; conj. val.- Ryd. obsv'd; strong σ*(O-O)
F <sub>3</sub> OP	SB85d	525-600	E	pot. barr. Effects
HO	SRA02	525-528	P	high res.; comp. of vib'n &Ryd of OH,OD; v. low E (526eV)
<b>H<sub>2</sub>O</b>	WB74b	530-575	E	weak cont. features
	WB74g	530-540	E	Z+1 analogy (H <sub>2</sub> F radical)
	WB74h	530-545	E	Z+1 analogy
	ASW75	530-545	T	ab initio calc., comp. to expt. (WB74b)
	S75b	530-545	T	Z+1 analogy calc., comp. to expt. (WB74b)
	DC76	530-540	T	ab initio calc.
	WFM77	530-550	E	alternate assignment of WB74c
	A80	530-550	P	relative, see SYD82
	DK&82	530-580	T	ab initio calc., comp. to expt (WB74b)
	AVZ82b	532-540	P	comp. to NH <sub>3</sub> ,CH <sub>4</sub> ,Ne, 3p splitting=0.8eV
	SYD82	530-550	P	ab initio, absolute, comp. to expt (A80)
	R83	530-580	T	gas(WB74b), solid, chemisorbed spectra & diss. IY comp.
	RL&83	500-800	P	(D <sub>2</sub> O, H <sub>2</sub> O) (s), comp. to gas (WB74b), O Auger yield,, residual Rydbergs, EXAFS, O <sup>+</sup> yield follows O <sub>K</sub> -cont.
	SSH84a	540	T	σ*-res./bond length relationship
	CH&85	530-540	T	Rydberg assignments comp. to 2nd & 3rd row hydrides
	IM&87	530-570	E	absolute OS, comp. to F <sub>2</sub> O, valence-Rydberg mixing
	CAC89	500-550	T	vibronic effects in decay; Auger, PE, fluorescence comp.; vib'n-core lifetime coupling critical
	MD89	540-590	T	absolute, partial PI; ab initio; comp. to expt [IM&87]
	CP&90	500-1000	P	ion desorption (Ru(001); comp. to gas; coupled decay-dissoc. in H <sup>+</sup>
	MR&90	520-570	P	ion desorption (H <sup>+</sup> ); comp. to AEY, gas EELS (WB74b)
	RC&90	520-570	P	comp. of gas, solid; ion yields, H <sup>+</sup> ultrafast diss.
	LAL91	530-550	T	CNDO, systematic treatment of σ* energies
	RH91	525-560	E	absolute; comp. of peroxides and H <sub>2</sub> O; low-lying σ*(O-O)
	KL&92	530-544	P	ion yield, symmetry resolved b values
	KNP92	530-540	T	SCF-CI in (Z+1) approx.
	S92	525-565	E,R	σ*(O-H), comp. of X-H species
	SS92c	529-540	T	relaxed core HF; comp. to DSCF; TV, f computed; comp. to RF&93
	ZZ&92	530-540	T	DSCF; core hole localisation; gen. rules for MO shifts in 2nd row
	IS&93	510-610	P	partial ion yields (H <sup>+</sup> , OH <sup>+</sup> , O <sup>+</sup> , O <sup>++</sup> ); comp. to PSID of 10 L H <sub>2</sub> O/Si(100)
	M93	532-542	P	partial ion yields (H <sup>+</sup> , OH <sup>+</sup> , O <sup>+</sup> , O <sup>++</sup> )
	ST&93	533-540	P,T	(120 mV); ab initio SCF(ADC); no resolved vib; comp of H <sub>2</sub> O, NH <sub>3</sub> , CH <sub>4</sub> re Ryd/val char.NH <sub>4</sub> ; ultrafast dissociation; abs. osc. str. calc.
	KP94b	530-540	T	ab initio DSCF-CI; vibn=l analysis; comp. of H <sub>2</sub> O/D <sub>2</sub> O; comp. (ST&93)
	LB&94b	532-542	P	partial IY; test of new PGM on HASYLAB undulator
	SI&95	520-620	P	PIY(O <sup>+</sup> , O <sup>2+</sup> , O <sup>3+</sup> ); comp. to PSID for H <sub>2</sub> O/Si(100); no ultrafast H <sup>+</sup> ; first PIPICO at a surface (O <sup>+</sup> ,H <sup>+</sup> )
	HP&98	532-534	P	reosnant Auger coinc. with OH <sup>+</sup> , H <sub>2</sub> O <sup>+</sup> , ultrafast decay
	PH&99	531-542	P	TIY, PIY, PE3PICO; H <sup>2+</sup> from 2b <sub>2</sub> ; H <sup>o</sup> at 4a <sub>1</sub> ; ultrafast; 170 meV
	PK&99c	532-540	P	reosnant Auger; non-linear dispersion; potential curves; no ultrafast

(H <sub>2</sub> O cont'd)	RB99	530-534	T	absolute; GOS; 4a <sub>1</sub> GOS shows structure
	WR&01	530-550	P	TIY, TEY; comp of liq, gas, sol; surface / bulk on droplets; EXAFS
	HN02	531-541	P,R	PIY, H <sub>2</sub> <sup>+</sup> formation at 2b <sub>2</sub> ; (from PH&99)
	HP&01	534	P	resonant Auger, ultra-fast decay
	SS&03	528-550	P	TIY, partial ion yields, O <sup>-</sup> yield; deduce O <sup>*</sup> H <sup>-</sup> decays radiatively
	C05	534	T	DFT, small molecule BE and excitation energies
	KC&06	533-542	P	TIY, Lyman- $\alpha$ yield. Ultrafast decay to from H*
	IH07	530-544	T	relative, Gaussian augmented plane wave (GAPW) - DFT; (-5 to +3 eV errors on 14 small molecules , comp. to ML&02
	FP11	534	P	resonant Auger decay, core hole dynamics
	FH&16	530-550	P,T,R	review of X-eat spectroscopy of gas, liquid and solid water
	YI&17	28-540	P,T	X-ray emission; effect of cations & anions, MD-calc
	NF&19	530-540	P,T	phase dependence of structure deduced from O 1s spectra
H <sub>2</sub> O <sup>+</sup>	SK&22b	525-570	T	hydronium cation; PIY, FLAGs, compared to H <sub>3</sub> O <sup>+</sup>
(H <sub>2</sub> O) <sub>n</sub>	BF&99	532-542	P	spectra as function of <cluster size>; 20 up to 200; PIY spectra
	TM&01a	532-539	P	XAS, XPS of expanded liquid (clusters) and Ar-seeded (more condensed)
H <sub>2</sub> O <sub>2</sub>	RH91	525-560	E	absolute; comp. of peroxides and H <sub>2</sub> O; low-lying σ*(O-O)
	TV93	530-540	T	ab initio-SCF-EICVOM; pre-edge res. (π*, σ* <sub>O-O</sub> ,σ* <sub>S-S</sub> ); comp. RH91
H <sub>3</sub> O <sup>+</sup>	SK&22b	525-570	P,T	hydronium cation; PIY, FLAGs, compared to H <sub>2</sub> O <sup>+</sup>
H <sub>4</sub> O <sub>2</sub>	IH07	530-544	T	water dimer, acceptor & donor, relative, Gaussian augmented plane wave (GAPW) - DFT; (-5 to +3 eV errors on 14 small molecules
(Na <sub>2</sub> SO <sub>4</sub> .10H <sub>2</sub> O) <sub>n</sub>	ABL13	525-555	P	size selected nanoparticles; aerodynamic lenses * diff. pump
NO	WB74c	525-568	E	cont. res.
	KMK79	525-545	T	ab initio calc., comp. to expt. (WB74c), cont. shape res.
	AVZ82a	525-535	P	comp. among N <sub>2</sub> , NO & O <sub>2</sub> , cont. to discrete shape res. shift
	WDD82	545-570	T	absolute cross-section calc., comp. to expt. (WB74c)
	SSH84a	540	T	σ*-res./bond length relationship
	RL&85	520-560	P	comp. of multilayer PSID & ISEELS
	NAV88	528-552	P	comp. to KNO <sub>2</sub> , NaNO <sub>2</sub> (sol); dp-s correlated with R(NO)
	SG&89	535-550	T	σ* shape res.; pos. & shape as f(R); approx. cyl. well & ab initio
	PV&90	535-555	P	comp. to NO <sub>3</sub> <sup>-</sup> , NO <sub>2</sub> <sup>-</sup> , d(p-s) as f(R); MO splitting
	S90b	525-560	R,P	ionic fragmentation; KERD; ang. dist.
	ZS&90	520-580	E,T	absolute, ident. impurities in [SCC77]; MCQD calc.; split σ*(N-O)
	SS91	526-556	P	TEY; partial ion yields; KER at π*; ion b-param
	CT92	532	E	DES by (e,2e); U <sub>C-V</sub> at N>0
	KA&92a	525-565	P,T	symmetry-resolved ion yield; comp. to ab initio; (Z+1) breakdown
	ZZ&92	530-540	T	DSCF; gen. rules for MO shifts in 2nd row
	PV&93	530-550	T	quasi-atomic calc; short-range order (bond length) correlation
	RD&93	530-544	P	120 meV fwhm; vibrational details of 3 π* states; Ryd; full analysis
L94	530,540	T	X-ray emission at π*, σ*; compared to resonant AI	
	AK&95a	530-560	P,T	ab-initio DSCF-CI; symmetry resolved ion yields; Renner-Teller; Ryd.-val. mixing; σ* identified; large bending in π*
	F97	532	T	de-excitation spectrum of π* predicted, comp to expt. (RD&93)
	WL98	528-536	T	HF-Cl; comp to TKR8
	WP&98	530-537	P	resonant Auger; vibrationally resolved
	PD&99	531-544	P,T	resonant Auger, vibrationally resolved
	IOW01	530-540	T	potential energy surfaces for core excitation & doubles
	YOW01	533-535	T	excitation energies and potential curves for π* states
	BRB04	533-540	T	generalized oscillatorstrength (GOS) for selected transitions
	YHA05	520	P, R	ion angular dist; fixed-molecule PAD spectra, review
	FH&20	526-550	T	coupled cluster calc; comp. to many solid species

NO <sub>2</sub>	SCC77	530-541	P,T	photographic, Z+1 analogy calc.
	SSH84a	540	T	$\sigma^*$ -res./bond length relationship, anomalous
	BS87	530-570	E	high res.
	BS&88	520-580	E,R	IEELS, E <sub>0</sub> =3700eV, 0°, compare NO <sub>2</sub> SO <sub>2</sub>
	JC02	525-555	P,T	relative, Gaussian94 calc (Z+1)
	GT&03b	525-555	P	angle resolved ion spectra; high-res; spectral assignments
N <sub>2</sub> O	WB74a	530-575	E	weak cont. features
	SB76a	530-545	T	geometry corrected, Z+1 analogy calc., comp. to expt. (WB74a)
	BB&79	504-600	P	photographic, absolute, pressure dependence
	SSH84a	540	T	$\sigma^*$ -res./bond length relationship - inconsistent with
	MN&86	520-600	P	total ion yield, branching ratios at selected E
	PL&87	550-560	T	shape resonance – bond length refuted
	GC&88	532-600	P,T	absolute photoionisation cross-section, b
	LE&88	540	P,T	DES; spectator versus participator decay
	ME88	500-700	P	Auger-ion coincidence; state-selective frag.; undulator rad.
	SG&89	535-550	T	$\sigma^*$ shape res.; pos. & shape as f(R); approx. cyl. well & ab initio
	H90b	535	P	ionic frag. comp to N <sub>T</sub> , N <sub>C</sub> → π*
	PBV91	520-560	T	MS; comp.to expt; dev. from d(R)
	SK&91	540-600	P,T	absolute; comp to N <sub>C</sub> , N <sub>T</sub> ; ab initio; O 1s like N <sub>C</sub> ; E( $\sigma^*$ ) const. in partials
	K92	530-550	R	survey of numerical XANES
	KA&92b	520-570	P	symmetry resolved using ion angular distribution.
	ZZ&92	530-540	T	DSCF; core hole localisation; gen. rules for MO shifts in 2nd row
	BSS93a	526-576	P	PEPICO-, PIY-, PIPICO-yield, b; comp. of b for N <sub>2</sub> , NO, N <sub>2</sub> O, O <sub>2</sub>
	PV&93	530-550	T	quasi-atomic calc; short-range order (bond length) correlation
	L94	530,540	T	X-ray emission at π*, $\sigma^*$ ; comp. to resonant AI
	AK&95a	530-570	P,T	ab-initio DSCF-CI; symmetry resolved ion yields; Renner-Teller; Ryd.-val. mixing; $\sigma^*$ identified; large bending in π*
	F95	535	T	de-excitation spectrum of π*
	K96b	530-543	P,R	symmetry resolved (energetic ion axial recoil); comp. to CO <sub>2</sub> , CH <sub>4</sub> where excited state geom. does affect angle-resolved signal
	NM96	540-600	P,R	partial cross-sect.; comp. to calc
	PL&87	530-560	T	shape-resonance bond length refutation
	PV&99	530-540	P	π* 165(15) lifetime width
	C07	525-540	T	density functional calc. mean error of only 0.26 eV
	DH&09	546	P	(O <sup>+</sup> , N <sub>2</sub> <sup>+</sup> ) KRD (e,ion, ion) site-selective fragmentation
N <sub>2</sub> O <sub>2</sub>	PT&95	525-570	P,T	(NO) <sub>2</sub> ; multilayer NEXAFS; DFT calc; low-lying $\sigma^*(N-N)$ consistent with long bond (2.24 Å); 1.5 eV fwhm resol.
O <sub>2</sub>	NM&71	530-550	P	photographic
	BS&74	525-575	P	photographic
	VZ&74	525-560	P	distorted intensities
	WB74c	522-565	E	Z+1 analogy, res. at thresh.
	L75b	525-560	P	res. at thresh.
	VA&75	525-560	P	comp. to CO <sub>2</sub> , C <sub>2</sub> H <sub>5</sub> OH
	B76	525-540	P	pre-edge, absolute
	BB&79	504-600	P	photographic, absolute, pressure dependence
	KMK79	530-550	T	ab initio calc., comp. to expt. (WB74c)
	GA&80	520-600	T	ab initio calc., absolute, cont. shape
	HB80a	522-562	E	res. at thresh., comp. to theory
	AVZ82a	525-535	P	comp. among N <sub>2</sub> , NO & O <sub>2</sub> , cont. to discrete shape res. shift
	BB84	526-534	P	abs. by mono. crystal (KAP) distorts O1s spectra (L75b, BB&79)
	RL&85	520-580	P	comp. of multilayer PSID & ISEELS
	SSH84a	540	T	$\sigma^*$ -res./bond length relationship

(O <sub>2</sub> cont'd)	YKS85b	500-1000	P	EXAFS, non-standard phase shifts indicated
	THY86	546	P	luminescence from O <sub>2</sub> <sup>2+</sup> (K*)
	YKS86	500-950	P	EXAFS, corrected for second order radiation
	YKS87	500-550	P	EXAFS; comp. of CO,CO <sub>2</sub> ,COS,Me <sub>2</sub> CO,CH <sub>3</sub> OH,EtOEt;furan,C <sub>8</sub> H <sub>8</sub> O <sub>2</sub>
	CT88	531	E,T	Auger-loss coinc., DES, strong t-vibn interference, comp to calc.
	YHT88	500-700	P	luminescence ion, abs, comp., selective decay
	SG&89	535-550	T	$\sigma^*$ shape res.; pos. & shape as f(R); approx. cyl. well & ab initio
	SS89a	520-560	P	electron yield; O <sup>+</sup> ,O <sup>2+</sup> yields; ion b's ( $\pi^* = -1$ ; 3p Ryd = 1.2)
	SS89d	520-560	P	partial IY; ion KERDs; diss. pathways; $\pi^*$ partly non-dissoc.
	CT90	531	E	DES; (e,2e); comp. to Auger and calc; participator decay strong
	H90b	500-700	P,R	comp. of abs. luminescence and TIY; fluorescence decay
	LK&90	510-600	P	total ion ang. distr.; b-params
	LL&90a	531,560	P	AI and Auger spectra at $\pi^*$ , $\sigma^*$ , cont.
	LL&90b	490-590	P	total ion yield; DES at $\pi^*$ , $\sigma^*$ and continuum (AI and Auger)
	S90b	525-570	R,P	ionic frag; KERD; ang. dist.
	SS90	531	P	KERD in (O <sup>+</sup> ,O <sup>2+</sup> ); PIPICO
	SU&90c	520-560	P	total ion yield; mol. orientation param. (-0.8 at $\pi^*$ ; 1 at both $\sigma^*$ )
	JJ&91	530-800	T	MS calc; NEXAFS and EXAFS; CO and O <sub>2</sub>
	MC&91	525-560	P	50 meV; Ryd. structure resolved on "exchange split" $\sigma^*$
	SB91b	500-950	P,T	MS-Xa calc of EXAFS and edge; comp to YKS87
	SS&91	520-560	P	total ion yield and molecular orient. parameters (peaks B, C are s)
	TC91	531	E,T	DES; lifetime-vibrational interference; hole state lifetime deduced
	DM&92	530-545	P	high resolution (120 meV)
	HL&92	531	P	(e- <sub>Auger</sub> ,ion) coinc.; multi-det; intermediate state ident.
	K92	530-550	R	survey of numerical XANES
	KA&92b	531	P	ion ang. dist. at $\pi^*$ ; claims external axial recoil approx is not valid in polyatomics
	KSY92	525-565	P,T	comp. of TEY, TIY (po. dep.); high res. 84 meV; ab initio; DSCF of Ryd.; only weak Ryd-val mixing
	MH&92	520-3000	E	luminescence from O <sup>+</sup> , O <sup>2+</sup> attributed to decay of O <sub>2</sub> <sup>K+</sup>
	RE&92	526-570	P	high res (<100meV); detailed Ryd. struct. in 538-543 eV
	RF&92	528-570	P	comp. to MC&91; improved Ryd. resolution; instr. description
	S92	525-900	EPTR	MS-Xa, EXAFS, comp. to surf. ads. O <sub>2</sub> on Pt, Ag
	YS92	525-565	P	sym. resolved by ion yield; BOTH features are $\sigma^*$ ; high res (84 meV)
	HF&93	520-560	E,T	absolute; comp. of <sup>1</sup> D- <sup>3</sup> S; DSCF-CI calc; magnetic splitting in <sup>3</sup> D
	NR&93	530-545	P	autoionization (DES) used as selective detector of $\sigma^*$ ; exchange split only 0.6 eV (both $\sigma^*$ in B)
	RAZ93	540-1000	P,T	comp. of MS-Feff with expt.; reproduces $\sigma^*$ & EXAFS if >13 legs
	SC&93	520-560	P	Auger, autoionization at $\pi^*$ (530.9); 540 ( $\sigma^*$ ), 542 ( $\sigma^*$ ), 552 (1s <sup>-1</sup> ); atomic O <sup>K</sup> decay detected (ultrafast decay)
	NR&94	529-532	P,T	DES at $\pi^*$ ; lifetime-vib'n interference strong in partials; comp. to CO, N <sub>2</sub>
	YND94	538-570	T	absolute; ab initio Z+1; multi-excitation; comp to (BB&79); strong (1s <sup>-1</sup> ,p <sup>-1</sup> ,p <sup>4</sup> ) 2e- state at 539 eV in $\sigma^*$ region
	YSK94	535-550	P,T	ultrahigh res.; ion-b and state symmetries; DSCF pot. curves; Ryd-val mix and exchange split $\sigma^*(O-O)$
	AK&95a	535-550	P,T	ab-initio DSCF-CI; symmetry resolved ion yields; Renner-Teller; Ryd.-val. mixing; $\sigma^*$ identified; large bending in $\pi^*$
	BM&95	530-540	P	HERMON at SRC; 1e5 resolving power
	CC&95	530-540	P	SGM at SRBC performance test; high resolution
	MBN95	550	T	calc of core hole localisation; N <sub>2</sub> O (78%), CO <sub>2</sub> (60), C <sub>2</sub> H <sub>4</sub> (86%)
	QO&95	538-544	P	Elettra; high resolution
	RL&95	540-546	P	(ZEKE-X-ray) coinc; peak 0.45 eV below ZEKE peak; no PCI in coinc.

(O <sub>2</sub> cont'd)	AL&96	529-545	T	STEX; <sup>2</sup> S channel only one with exchange split of σ*; <sup>4</sup> S channel dominated by Rydberg; supports Kuiper & Dunlap assignments
	GC&96	532-547	P	resonant X-ray em. (RIXS); no sym. breaking; supports 539 eV peak (B) as comprising BOTH σ* states
	L96b	529-531	P,R	participator Auger through π* (from NR&94); vibrational - lifetime interference
	NM96	529-533	P,R	review, lifetime-vibrational interereference; line-shape simulation (NR&94)
	SST96	530-560	T	constant chemical potential LDA; π*, σ* res. rel. position; comp. of p-s sep. in CO, C <sub>2</sub> H <sub>2</sub> , C <sub>2</sub> H <sub>4</sub> , N <sub>2</sub> , O <sub>2</sub>
	STS96	528-560	T	analytical resonance shapes for diatomics; bond length determination
	NG&97	531	P,R	resonant X-ray emission (RIXS)
	GM98	531	T	Auger resonant Raman; time dependent picture; classical; detuning; comp to N <sub>2</sub> , CO (GTM98)
	KK&98a	528-548	P	relative; high res.; symmetry det'n; unresolved vib'ns affect π*
	SA&98c	529-532	P	resonant Auger,ultrafast; 140 meV
	PV&99	530-540	P	π* 149(10) lifetime width
	BB&00	539	P,T	atomic Auger = ultrafast decay at σ*; pol. dep. Auger; Doppler shift associated with localized core hole; measurement-dependent localization ('disentanglement of entangled states')
	AC&01	525-550	P	relative; XAS and XPS; metastable a <sup>1</sup> Δ spectrum; π*, not shape resonance
	SF&01	530-533	P	high res; vibrations; DES
	SO&01	535.4	P	sub-natural linewidths by resonant Auger
	K02	530-560	P,TR	symmetry resolved, high resolution; review
	PK&02	535-547	P,T	CIS; (1π <sub>g</sub> ) and (1π <sub>u</sub> ) participator decay plots; σ*, <sup>4</sup> Σ, <sup>2</sup> Σ complex; CIPSI
	AR&05	542-546	P	X-ray emission threshold coincidence (XETECO); no-PCI threshold spectra; 0.15 eV u-g splittin; quartet-doublet split 1.09 eV 40 meV fwhm
	KYN09	536-544	P,T	Rydberg-valence, vibronic coupling explains underlying broad σ* signal
	VK&09	536-544	P,T	Rydberg-valence, vibronic coupling explains underlying broad σ* signal
	LU&11	539	P,T	resonant Auger decay, localization & decoherence
	AP&12	573	P	PES-Auger coincidence, core-hole decay dynamics
	MM12	530-544	P,R	ultra-fast decay (HBr-Br3d; DCI, HCl-Cl2p; H <sub>2</sub> S - S2p, O <sub>2</sub> -O1s)
	GT&03b	536-546	P	high resolution Ryd-σ*; BL4B UVSOR-II commissioning
	FH&20	526-550	T	coupled cluster calc; comp. to many solid species
	LK&20a	530-545	P	super-accurate energy scale, 3s (v=0) at 539.377(35) eV
	HV&20	529-545	P	TEY, 189 meV, VerSoX end-station test
	BH&21	518-556	P	in situ, Ag-catalysed ethylene epoxidation; Ag affects gas spectrum
	RS&92b	520-560	P	PIY, TIY, TEY of cluster versus molecular O <sub>2</sub>
O <sub>2</sub> S	AVZ82c	525-555	P	comp. to S2p (VZ71b) & S1s (MB&72) spectra of SO <sub>2</sub>
	TKM82	525-540	T	X-alpha (MSM), comp. to expt (K77)
	B85	525-545	E	high res. (0.09eV FWHM)
	SB&87	525-545	E	high res., comp. to MCQD calc & other edges
	BS&88	520-580	E,R	IEELS, E <sub>0</sub> =3700eV, 0°, compare NO <sub>2</sub> SO <sub>2</sub>
	PK&93	500-900	P	EXAFS; comp to SO <sub>2</sub> (multi & monolayer) on Cu; 1st intramolecular bond length from SEXAFS
	FT&99	527-547	P	TIY, TPES; TPEPICO; TPE2PICO; relative cross sections
	JC02	525-555	P,T	relative, Gaussian94 calc (Z+1)
	LS&04	528-542	P	TIY, PIPICO, core-hole loacalization symmetry breaking
	GT&03b	528-546	P	angle resolved ion yield, spectral assignments
	S09	528-541	P	(O <sup>+</sup> ,O <sup>+</sup> ) PIPICO KER profiles, symmetry breaking, vibrational effects
O <sub>3</sub>	PC&81b	520-600	T	ab initio calc., absolute osc.str.s, discrete shape res.
	ZZ&92	530-540	T	DSCF; core hole localisation; gen. rules for MO shifts in 2nd row
	GOI97	525-555	P,T	relative; discharge O <sub>2</sub> ; spectral stripped; 2π* @ 529.1,535.4 eV; GSCF3

(O <sub>3</sub> cont;d)	OK02	530	T	ab initio CI calc, geometry dependence; TDM not aligned along O-O bonds
	MM&07	528-548	P	relative, TIY, PEPEPICO; PIY; dissociative mechanisms at $\pi^*$
	S09	536	P	(O <sup>+</sup> ,O <sup>+</sup> ) PIPICO KER profiles, symmetry breaking, vibrational effects

### Palladium 2p (31.7, 33.3 keV)

C <sub>6</sub> H <sub>10</sub> Pd	DFL92	3.16-3.17	T	Pd(C <sub>3</sub> H <sub>5</sub> ) <sub>2</sub> ; absolute; ab initio-SCF-CI; comp. of 3d spectra of 5 TM compounds; supports MO model of edge structure
-----------------------------------	-------	-----------	---	--

### Phosphorous 2p (140 eV)

B <sub>5</sub> C <sub>12</sub> H <sub>18</sub> P	HLD91	130-220	E	Ph <sub>2</sub> PB <sub>5</sub> H <sub>8</sub>
B <sub>5</sub> C <sub>19</sub> FeH <sub>17</sub> O <sub>2</sub> P	HLD91	130-220	E	Cp(CO) <sub>2</sub> FeB <sub>5</sub> H <sub>2</sub> P(Ph) <sub>2</sub>
Br <sub>3</sub> P	II&87	130-270	P	PBr <sub>3</sub> ; absolute, high res. (0.03-0.07 eV)
CCl <sub>2</sub> F <sub>3</sub> P	HBC96	130-170	P	CF <sub>3</sub> PCl <sub>2</sub> ; absolute; ab initio; TIY,PIY,PIPICO; comp. to PF <sub>3</sub> ,PCl <sub>3</sub>
	NJ&98	120-170	P,T	absolute; GSCF3 calc.; LS-state; comp of PX <sub>3</sub> , YPF <sub>3</sub> . X=Cl,F, Y=O,S)
	NH&03	130-200	P	absolute; TIY, PIY, quantitative fragmentation; comp to (e, e+ion)
<b>C<sub>3</sub>H<sub>9</sub>P</b>	SB85c	130-210	E	P(CH <sub>3</sub> ) <sub>3</sub> ; strong cont. res.
	LC&90	125-210	P,T	high res.; MS-Xa; Ryd.; pot. barr. shape res.; PX <sub>3</sub> (X=H,F,CH <sub>3</sub> )
	HH&98	128-150	E	absolute; comp. of (t-Bu) <sub>2</sub> PCl, PCl <sub>3</sub> , PMe <sub>3</sub>
<b>C<sub>8</sub>ClH<sub>18</sub>P</b>	HH&98	128-150	E	(t-Bu) <sub>2</sub> Cl; absolute; comp. of (t-Bu) <sub>2</sub> PCl, PCl <sub>3</sub> , PMe
Cl <sub>3</sub> OP	GM&76	123-136	P	Rydberg structure, no analysis
	TKM82	133-144	T	X-alpha (MSM), comp. to expt (GM&76)
	SB85c	130-200	E	strong cont. res.
	LC&92a	130-180	P,T	relative, high res. (200 meV); comp. of PF <sub>5</sub> , POCL <sub>3</sub> , POF <sub>3</sub> ; cont. res.
<b>Cl<sub>3</sub>P</b>	MK80	132-146	P	res. at thresh.
	TKM81	133-146	P	relative, synchrotron radiation spectrum
	TKM82	133-144	T	X-alpha (MSM), comp. to expt (K77)
	SB85c	130-200	E	cont. res; dipole forbidden trans. (135eV), rapid variation with K
	II&87	130-270	P	absolute, high res. (0.03-0.07 eV)
	H90a	130-150	E	re-assignment of SB85c; dipole forbidden
	N95	130-170	T	DVXa; absolute; comp to II&87; bond length corr. (also PO <sub>x</sub> , SO <sub>x</sub> , ClO <sub>x</sub> )
	HBC96	130-170	P	absolute; ab initio; TIY,PIY,PIPICO; PE2PICO; PF <sub>3</sub> ,PCl <sub>3</sub> ,CF <sub>3</sub> PCl <sub>2</sub> comp.
	AB97	0-350	E	absolute; total and partial ion yield from (e,e+ion); dipole breakdown
	KC&97b	131-149	P,T	absolute; TIY, PF <sub>3</sub> <sup>+</sup> yield; LS-states; GSCF3 ab initio
	HH&98	128-150	E	absolute; comp. of (t-Bu) <sub>2</sub> PCl, PCl <sub>3</sub> , PMe <sub>3</sub>
	NJ&98	120-170	P,T	absolute; GSCF3 calc.; LS-state; comp of PX <sub>3</sub> , YPF <sub>3</sub> . X=Cl,F, Y=O,S)
	NH&03	130-200	P	absolute; TIY, PIY, quantitative fragmentation; comp to (e, e+ion)
<b>Cl<sub>3</sub>PS</b>	TKM82	133-143	T	X-alpha (MSM), comp. to expt (K77)
<b>F<sub>3</sub>P</b>	SB85c	130-205	E	strong cont. res.
	II&87	130-270	P	absolute, high res. (0.03-0.07 eV)
	LC&90	125-210	P,T	high res.; MS-Xa; Ryd.; pot. barr. shape res.; PX <sub>3</sub> (X=H,F,CH <sub>3</sub> )
	VK&92	130-150	P	TEY; res. Auger/AI differ; participant vs. spectator; ultrafast decay
	N95	130-170	T	DVXa; absolute; comp to II&87; bond length corr. (also PO <sub>x</sub> , SO <sub>x</sub> , ClO <sub>x</sub> )
	HBC96	130-170	P,T	absolute; ab initio; TIY, PIY, PIPICO; PF <sub>3</sub> ,PCl <sub>3</sub> ,CF <sub>3</sub> PCl <sub>2</sub> comp.
	KB&96	130-150	P,T	TIY vs PF <sub>3</sub> <sup>+</sup> ; ab initio; (LS) state at 136.4 eV - only 2p <sub>1/2</sub> component
	ACB97	5-300	E	absolute; total absorption; total and partial ion yields; ioniz. eff.
	HN&98	132-142	P	total and partial IY; PEPIPICO; LS-state in PF <sub>2</sub> <sup>+</sup> as well; improved timing
	NJ&98	120-170	P,T	absolute; GSCF3 calc.; LS-state; comp of PX <sub>3</sub> , YPF <sub>3</sub> . X=Cl,F, Y=O,S)
	UM&99	134-166	P,T	relative; TIY; symmetry resolved – isotropic; 50 meV; DVXα; quasi isotropic ( $\beta < 0.1$ ) even though P-F axial / equatorial differ

(PF <sub>3</sub> cont'd)	KI00	134-140	T	ab initio; spin-orbital Breit-Pauli; molecular field; comp. of SO <sub>2</sub> , COS, PF <sub>3</sub>
	HN02	130-170	P,R	PIY, selective fragmentation; conditions for quantitative yields
	NH&03	130-200	P	absolute; TIY, PIY, quantitative fragmentation; comp to (e, e+ion)
F <sub>3</sub> OP	SB85d	130-210	E	strong cont. res.
	LC&92a	130-180	P,T	relative, high res. (200 meV); comp. of PF <sub>5</sub> , POCL <sub>3</sub> , POF <sub>3</sub> ; cont. res.
	JKC99	134-160	P,T	relative, GSCF3; comp. to NSF <sub>3</sub>
F <sub>3</sub> PS	HN&98	130-205	P	total and partial IY; PEPIPICO; site- and state-selective fragmentation
	HN02	130-170	P,R	PIY, selective fragmentation
F <sub>5</sub> P	SB85d	130-210	E	strong cont. res.
	TL91	135-145	P	relative; gas-sol. comp.; Ryd. structure suppressed in sol.
	LC&92a	130-180	P,T	relative, high res. (200 meV); comp. of PF <sub>5</sub> , POCL <sub>3</sub> , POF <sub>3</sub> ; cont. res.
H <sub>3</sub> P	HB72	120-220	P	absolute, Rydberg analysis IP (137.3, 138.2)
	C73	100-120	P,R	review
	R75	130-140	T	alternate assignment of HB72
	S75a,b	130-140	T	Z+1 analogy calc., alternate assignment of HB72
	F76	130-140	P	absolute, gas-solid comp.
	FS&79	130-140	P,T	absolute, photographic, gas-solid comp.
	SYD82	130-165	T	ab initio, absolute, comp. to expt (HB72)
	SB85c	130-210	E	broad cont. maximum (delayed thresh.?)
	II&87	130-270	P	absolute, high res. (0.03-0.07 eV)
	LC&90	125-210	P,T	high res.; MS-Xa; Ryd.; pot. barr. shape res.; PX <sub>3</sub> (X=H,F,CH <sub>3</sub> )
	ZCB90	120-220	E	absolute; ion yields; comp. to other PA (FS&79, HB72; II&87), atomic theory; supports atomic cont. normalisation at E > IP+25eV
	LB&95	130-170	T	MS-Xa; comp. of XH <sub>n</sub> (X=Si,P,S,Cl)
	U98	131-132	P,R	resonant Auger; ultrafast dissociation

#### Phosphorus 1s (2155 eV)

Br <sub>3</sub> P	CJ99	2.14-2.15	P	chemical shifts of P1s→1e <sup>*</sup> ; correlation to XPS, Auger
CCl <sub>2</sub> H <sub>3</sub> P	CJ99	2.14-2.15	P	chemical shifts of P1s→1e <sup>*</sup> ; correlation to XPS, Auger
CCl <sub>2</sub> H <sub>3</sub> OP	CJ99	2.14-2.15	P	chemical shifts of P1s→1e <sup>*</sup> ; correlation to XPS, Auger
CCl <sub>2</sub> H <sub>3</sub> OP	CJ99	2.14-2.15	P	chemical shifts of P1s→1e <sup>*</sup> ; correlation to XPS, Auger
CCl <sub>2</sub> H <sub>3</sub> PS	CJ99	2.14-2.15	P	chemical shifts of P1s→1e <sup>*</sup> ; correlation to XPS, Auger
C <sub>2</sub> ClH <sub>6</sub> PO <sub>2</sub> S	CJ99	2.14-2.15	P	chemical shifts of P1s→1e <sup>*</sup> ; correlation to XPS, Auger
C <sub>3</sub> H <sub>9</sub> P	CJ99	2.14-2.15	P	chemical shifts of P1s→1e <sup>*</sup> ; correlation to XPS, Auger
C <sub>3</sub> H <sub>9</sub> O <sub>4</sub> P	CJ99	2.14-2.15	P	chemical shifts of P1s→1e <sup>*</sup> ; correlation to XPS, Auger
C <sub>3</sub> H <sub>9</sub> O <sub>3</sub> P	CJ99	2.14-2.15	P	chemical shifts of P1s→1e <sup>*</sup> ; correlation to XPS, Auger
C <sub>3</sub> H <sub>9</sub> O <sub>3</sub> PS	CJ99	2.14-2.15	P	chemical shifts of P1s→1e <sup>*</sup> ; correlation to XPS, Auger
C <sub>6</sub> H <sub>15</sub> P	CJ99	2.14-2.15	P	chemical shifts of P1s→1e <sup>*</sup> ; correlation to XPS, Auger
C <sub>18</sub> H <sub>15</sub> PO <sub>3</sub>	KC&92	2.14-2.19	P,T	(C <sub>6</sub> H <sub>5</sub> O) <sub>3</sub> P; relative, MS-Xa of PO <sub>3</sub> <sup>3-</sup> clusters
C <sub>18</sub> H <sub>15</sub> PO <sub>4</sub>	KC&92	2.14-2.19	P,T	(C <sub>6</sub> H <sub>5</sub> O) <sub>3</sub> PO; relative, MS-Xa of PO <sub>4</sub> <sup>4-</sup> clusters
Cl <sub>3</sub> OP	CJ99	2.14-2.15	P	chemical shifts of P1s→1e <sup>*</sup> ; correlation to XPS, Auger
Cl <sub>3</sub> P	GDT97	2.14-2.20	P,T	relative; TIY, MS-Xa; pot. barr.; AsCl <sub>3</sub> , PCl <sub>3</sub> , GeCl <sub>4</sub> , SnCl <sub>4</sub> comp.
	CJ99	2.14-2.15	P	chemical shifts of P1s→1e <sup>*</sup> ; correlation to XPS, Auger
Cl <sub>3</sub> PS	CJ99	2.14-2.15	P	chemical shifts of P1s→1e <sup>*</sup> ; correlation to XPS, Auger
F <sub>3</sub> P	CJ99	2.14-2.15	P	chemical shifts of P1s→1e <sup>*</sup> ; correlation to XPS, Auger
	NT&99b	2.12-2.20	P	TIY, PIY; PEPIPICO; pol. dep.; selective frag.; cascade processes
	JC01	2.14-2.18	P	relative; comparison of NX <sub>3</sub> , PX <sub>3</sub> 1s edges; pot. barr. effects
F <sub>3</sub> PS	CJ99	2.14-2.15	P	chemical shifts of P1s→1e <sup>*</sup> ; correlation to XPS, Auger
	NT&99a	2.12-2.20	P	TIY, PIY; PEPIPICO; pol. dep.; selective frag.; cascade processes
	NT&99b	2.14-2.17	P,T	symmetry resolved PIY; GSCF3
	HN02	2.14-2.17	P,R	symmetry resolved PIY

F <sub>3</sub> OP	CJ99	2.13-2.18	P	chemical shifts of P1s→1e <sup>*</sup> ; correlation to XPS, Auger
	NT&99B	2.12-2.20	P	TIY, PIY; PEPICO; pol. dep.; selective frag.; cascade processes
F <sub>5</sub> P	CJ99	2.14-2.15	P	chemical shifts of P1s→1e <sup>*</sup> ; correlation to XPS, Auger
H <sub>3</sub> P	CJ99	2.14-2.15	P	chemical shifts of P1s→1e <sup>*</sup> ; correlation to XPS, Auger
	JC01	2.14-2.18	P	relative; comparison of NX <sub>3</sub> , PX <sub>3</sub> 1s edges; pot. barr. effects
H <sub>4</sub> P	KNP91	2.14-2.19	T	PH <sub>4</sub> , SCF-CI in (Z+1); comp. of CH <sub>4</sub> , SiH <sub>4</sub> , PH <sub>4</sub> , NH <sub>4</sub> K-shell spectra
NiP <sub>2</sub>	DCT98	2.15	T	partial localization of core hole
O <sub>6</sub> P <sub>4</sub>	KC&92	2.14-2.16	P,T	relative, EXAFS; MS-Xa of PO <sub>3</sub> <sup>3-</sup> ; bond length corr.
	EK&97d	2.13-21.8	P,T	relative; ioniz. yield; comp. of PO <sub>n</sub> X cage compounds; DFT
O <sub>6</sub> P <sub>4</sub> S	EK&97d	2.13-21.8	P,T	relative; ioniz. yield; comp. of PO <sub>n</sub> X cage compounds; DFT
O <sub>6</sub> P <sub>4</sub> Se	EK&97d	2.13-21.8	P,T	relative; ioniz. yield; comp. of PO <sub>n</sub> X cage compounds; DFT
O <sub>7</sub> P <sub>4</sub>	EK&97d	2.13-21.8	P,T	relative; ioniz. yield; comp. of PO <sub>n</sub> X cage compounds; DFT
O <sub>10</sub> P <sub>4</sub>	KC&92	2.14-2.16	P,T	relative, EXAFS; MS-Xa of PO <sub>4</sub> <sup>4-</sup> ; no match of shape res. & d(R)

#### Potassium 1s (3.61 keV)

BrK	EK&95b	3.60-3.63	P	comp. of alkali halide spectra; cluster contribution identified
FK	TW&99	3.60-3.62	P	comp. to clusters, solid
(FK) <sub>n</sub>	TW&99	3.59-3.66	P	cluster spectra s f(<n>) n= 2 –18; comp. to KF, solid

#### Rhenium 4f (42 eV)

C <sub>12</sub> H <sub>15</sub> N <sub>2</sub> O <sub>2</sub> Re	30-280	HS92	E	Cπ*Re(CO) <sub>2</sub> N <sub>2</sub>
--	--------	------	---	---------------------------------------

#### Selenium 3d (60 eV)

C <sub>4</sub> H <sub>4</sub> Se	HTB89	50-160	E	(selenophene), comp. to solid
C <sub>5</sub> H <sub>6</sub> Se	HTB89	50-160	E	(3-methylselenophene), comp. to solid
SeF <sub>6</sub>	SB90	60-160	E	comp of TeF <sub>6</sub> , SeF <sub>6</sub> , SF <sub>6</sub> ; Z-dependence of pot. barr.s
Se <sub>2</sub>	CM77b	50-160	P	photographic, double excitation, comp. to solid Se

#### Selenium 3p, 3s (180, 220 eV)

SeF <sub>6</sub>	AT&86b	160-210	P	absolute, comp. to SF <sub>6</sub> , SF <sub>5</sub> Cl, weak Se 4d cont. res.
	SB90	160-270	E	comp of TeF <sub>6</sub> , SeF <sub>6</sub> , SF <sub>6</sub> ; Z-dependence of pot. barr.s
C <sub>4</sub> H <sub>4</sub> Se	HTB89	160-210	E	(selenophene), comp. to solid
C <sub>5</sub> H <sub>6</sub> Se	HTB89	160-210	E	(3-methylselenophene), comp. to solid

#### Selenium 1s (12660 eV)

SeO <sub>2</sub>	H31	12.3-13.0	P	1 <sup>st</sup> chemical state XAS ; photographic; compare Se <sub>8</sub> , SeO <sub>2</sub>
Se <sub>2</sub>	NY&02	12.3-13.9	P	TIY, PEPICO; cluster-size selective EXAFS through PIY; R <sub>Se-Se</sub> = 2.17
Se <sub>5</sub>	NY&02	12.3-13.9	P	TIY, PEPICO; cluster-size selective EXAFS through PIY
Se <sub>6</sub>	NY&02	12.3-13.9	P	TIY, PEPICO; cluster-size selective EXAFS through PIY; R <sub>Se-Se</sub> = 2.35
Se <sub>7</sub>	NY&02	12.3-13.9	P	TIY, PEPICO; cluster-size selective EXAFS through PIY
Se <sub>8</sub>	H31	12.3-13.0	P	1 <sup>st</sup> chemical state XAS ; photographic; compare Se <sub>8</sub> , SeO <sub>2</sub>

Silicon 2p, 2s (110, 160 eV)

Br <sub>4</sub> Si	PV&79 PDK97 PDK98	100-140 90-120 105-112	T P P	X-alpha (MSM) calc. of cont. shape high res.; vibrational structure -> excited geom, SiX <sub>4</sub> , X=H,D,F,Cl,Br relative; TIY; high res. (15 meV); comp. of SiX <sub>4</sub> , X=H,D,F,Cl,Br,Me; Z+1 tests; Franck-Condon analysis; G of 40-85 meV
CCl <sub>3</sub> H <sub>3</sub> Si	BL&98	50-450	P,T	relative, TIY, PIY
	FZ&70	102-112	P	MeSiCl <sub>3</sub> ; pot. barr. effects
	BNZ72	102-112	T	semi-empirical calc., comp. to expt. (FZ&70)
CF <sub>3</sub> H <sub>3</sub> Si	BBT90 BT&92	100-200 100-140	P,T P	MeSiF <sub>3</sub> ; relative, 0.15 eV fwhm; Xa; res. incr. with more F relative; TEY, TIY, PA compared; quadrupole-MS PIMS; CH <sub>3</sub> more labile than F; CH <sub>3</sub> <sup>+</sup> enhanced in discrete res.; F 1s mass spec
	NMK97	100-180	P,R	site-specific fragmentation; comp. to SiMe <sub>4</sub> ; surface desorption
C <sub>2</sub> Cl <sub>2</sub> H <sub>6</sub> Si	NF&02	1001-20	P	site-specific fragmentation; comp. of X <sub>3</sub> Si-y-SiMe <sub>3</sub> , X=F,Cl, y = (C <sub>x</sub> H <sub>y</sub> )
	FZ&70	102-112	P	Me <sub>2</sub> SiCl <sub>2</sub> ; pot. barr. effects
	BNZ72	102-112	T	semi-empirical calc., comp. to expt. (FZ&70)
	CL&97	102-104	P	60 meV; comp. to solid; valence/Rydberg char.
	CL&05	103-117	P	SiMe <sub>2</sub> Cl <sub>2</sub> , luminescence yield, Si <sup>*</sup> , Si <sup>+</sup> , CH*, H*, , excited diatomic
C <sub>2</sub> F <sub>2</sub> H <sub>6</sub> Si	BBT90 BT&92	100-200 100-140	P,T P	Me <sub>2</sub> SiF <sub>2</sub> ; relative, 0.15 eV fwhm; Xa; res. incr. with more F relative; TEY, TIY, PA compared; quadrupole-MS PIMS; CH <sub>3</sub> more labile than F; CH <sub>3</sub> <sup>+</sup> enhanced in discrete res.; F 1s mass spec
	FZ&70	102-112	P	Me <sub>3</sub> SiCl; pot. barr. effects
C <sub>3</sub> ClH <sub>9</sub> Si	BNZ72	102-112	T	semi-empirical calc., comp. to expt. (FZ&70)
	NO&93	100-112	P	Me <sub>3</sub> Si-SiCl <sub>3</sub> ; site-specific ionic. fragm.; PEPICO, PIPICO resonant Auger; comp. of SiMe <sub>4</sub> , SiCl <sub>4</sub> ; Si <sub>2</sub> Me <sub>6</sub> and Cl <sub>3</sub> Si-SiMe <sub>3</sub>
C <sub>3</sub> FH <sub>9</sub> Si	NF&02	100-120	P	site-specific fragmentation; comp. of X <sub>3</sub> Si-y-SiMe <sub>3</sub> , X=F,Cl, y = (C <sub>x</sub> H <sub>y</sub> )
	NE&14	100-120	P	Auger and resonant-PES, electronic basis for site-specific fragmentation
C <sub>3</sub> F <sub>3</sub> H <sub>9</sub> Si <sub>2</sub>	BBT90	100-200	P,T	Me <sub>3</sub> SiF; relative, 0.15 eV fwhm; Xa; res. incr. with more F
	BT&92	100-140	P	relative; TEY, TIY, PA compared; quadrupole-MS PIMS; CH <sub>3</sub> more labile than F; CH <sub>3</sub> <sup>+</sup> enhanced in discrete res.; F 1s mass spec
C <sub>3</sub> H <sub>6</sub> Si	NF&02	1001-20	P	site-specific fragmentation; comp. of X <sub>3</sub> Si-y-SiMe <sub>3</sub> , X=F,Cl, y = (C <sub>x</sub> H <sub>y</sub> )
C <sub>4</sub> F <sub>3</sub> H <sub>9</sub> O <sub>3</sub> SSi	TWM95	93-100	T	c-(SiMe) <sub>3</sub> ; cyclo-polysilanes; ab initio EICVOM calc.
C <sub>4</sub> F <sub>3</sub> H <sub>11</sub> Si <sub>2</sub>	UH94a	100-200	E	Me <sub>3</sub> SiOSO <sub>2</sub> CF <sub>3</sub> ; comp of SI-O-X species re inductive, resonance effects
C <sub>4</sub> F <sub>3</sub> H <sub>11</sub> Si <sub>2</sub>	NMK97	100-180	P,R	F <sub>3</sub> Si(CH <sub>2</sub> )SiMe <sub>3</sub> ; site-specific frag.; comp. to SiMe <sub>4</sub> ; surface desorption
C <sub>4</sub> F <sub>3</sub> H <sub>14</sub> Si <sub>2</sub>	NF&02	1001-20	P	site-specific fragmentation; comp. of X <sub>3</sub> Si-y-SiMe <sub>3</sub> , X=F,Cl, y = (C <sub>x</sub> H <sub>y</sub> )
C <sub>4</sub> F <sub>3</sub> H <sub>14</sub> Si <sub>2</sub>	NO&95	100-120	P	CF <sub>3</sub> SiCH <sub>2</sub> SiMe <sub>3</sub> , ionic fragmentation; site specific (SiF <sub>3</sub> vs. SiMe <sub>3</sub> ) partial yields identify chemical shift undetected in absorption
C <sub>4</sub> H <sub>8</sub> Si	TWM95	93-100	T	c-(SiMe) <sub>4</sub> ; cyclo-polysilanes; ab initio EICVOM calc.
C <sub>4</sub> H <sub>12</sub> OSi	SK&93b	90-190	P,T	Me <sub>3</sub> Si(OMe); gas phase analogs of solid SiC/SiO <sub>2</sub> ; 2p vs. 1s; good at 2p poor at 1s; MS-Xa calc; Si(OMe) <sub>x</sub> (Me) <sub>4-x</sub> x=0-4 series
	UH94a	100-200	E	comp of SI-O-X species re inductive, resonance effects
	WMT94b	95-140	E,T	EICVOM SCF (gammess) calc.; Ryd.-val mix; Me <sub>x</sub> Si(OMe) <sub>4-x</sub> , x=0-4
C <sub>4</sub> H <sub>12</sub> O <sub>2</sub> Si	UT&97	90-110	P	absolute; Si-Si & Si-O-R
	SK&93b	90-190	P,T	Me <sub>2</sub> Si(OMe) <sub>2</sub> ; gas phase analogs of solid SiC/SiO <sub>2</sub> ; 2p vs. 1s; good at 2p poor at 1s; MS-Xa calc; Si(OMe) <sub>x</sub> (Me) <sub>4-x</sub> x=0-4 series
C <sub>4</sub> H <sub>12</sub> O <sub>3</sub> Si	WMT94b	95-140	E,T	EICVOM SCF (gammess) calc.; Ryd.-val mix; Me <sub>x</sub> Si(OMe) <sub>4-x</sub> , x=0-4
	SK&93b	90-190	P,T	MeSi(OMe) <sub>3</sub> ; gas phase analogs of solid SiC/SiO <sub>2</sub> ; 2p vs. 1s; good at 2p poor at 1s; MS-Xa calc; Si(OMe) <sub>x</sub> (Me) <sub>4-x</sub> x=0-4 series
	WMT94b	95-140	E,T	EICVOM SCF (gammess) calc.; Ryd.-val mix; Me <sub>x</sub> Si(OMe) <sub>4-x</sub> , x=0-4

$C_4H_{12}O_4Si$	SK&93b	90-190	P,T	$Si(OMe)_4$ ; gas phase analogs of solid $SiC/SiO_2$ ; 2p vs. 1s; good at 2p poor at 1s; MS-Xa calc; $Si(OMe)_x(Me)_{4-x}$ x=0-4 series
$C_4H_{12}Si$	WMT94b	95-140	E,T	EICVOM SCF (gumes) calc.; Ryd.-val mix; $Me_xSi(OMe)_{4-x}$ , x=0-4
	FZ&70	102-112	P	$Me_4Si$ ; pot. barr. effects
	BNZ72	102-112	T	semi-empirical calc., comp. to expt. (FZ&70)
	SD&84	50-280	E	cont. res., comp. to $SiH_4$ , $SiF_4$
	M85	100-110	P	shape res. at thresh., coupling to valence states, ionic
	SD&85	50-280	E	cont. res., fragmentation is state selective
	SMN85	100-150	P	shape res. at thresh.; partial cross-sections
	MS&86	100-112	P	PES & ionic fragmentation (PIPICO) around edge, 2 res.
	BT&87	100-200	P,T	0.3 eV FWHM, comp to other expt, X-alpha calc
	NB87	100-120	P,R	decay effects, Auger, ion yields (review)
	N88	100-110	P,R	electron & ion yield spectra, discrete (DES) & cont. states
	BBT90	100-200	P,T	$Me_4Si$ ; relative, 0.15 eV fwhm; Xa; res. incr. with more F
	BT&92	100-140	P	relative; TEY, TIY, PA compared; quadrupole-MS PIMS; $CH_3$ more labile than F; $CH_3^+$ enhanced in discrete res.; F 1s mass spec
$C_5Cl_3H_9Si_2$	W92	100-150	E	comp. of $SiMe_4$ , $Si_2Me_6$ , $Si_6Me_{12}$ ; $\sigma^*(Si-Si)$
	NO&93	100-112	P	site-specific ionic. fragm.; PEPICO, PIPICO resonant Auger; comp. of $SiMe_4$ , $SiCl_4$ ; $Si_2Me_6$ and $Cl_3Si-SiMe_3$
	SK&93b	90-190	P,T	gas phase analogs of solid $SiC/SiO_2$ ; 2p vs. 1s; good at 2p poor at 1s; MS-Xa calc; comparison of $Si(OMe)_x(Me_{4-x})$ x=0-4 series
	SL&93	100-117	P	total ion yield; PEPICO
	UX&94	90-170	E	comp. of edges of Si-Si compounds
	WMT94b	95-140	E,T	EICVOM SCF (gumes) calc.; Ryd.-val mix; $Me_xSi(OMe)_{4-x}$ , x=0-4
	NMK97	110-120	P,R	site-specific fragmentation; comp. to $SiMe_4$ ; surface desorption
	PDK98	105-112	P	relative; TIY; high res. (15 meV); comp. of $SiX_4$ , X=H,D,F,Cl,Br,Me; Z+1 tests; Franck-Condon analysis; G of 40-85 meV
	NF&02	100-120	P	site-specific fragmentation; comp. of $X_3Si-y-SiMe_3$ , X=F,Cl, y = ( $C_xH_y$ )
	NO99	95-120	P	$Cl_3SiC:::CsMe_3$ ; TIY, PIY; site specific fragmentaiton
	NF&02	1001-20	P	site-specific fragmentation; comp. of $X_3Si-y-SiMe_3$ , X=F,Cl, y = ( $C_xH_y$ )
$C_5F_3H_9Si_2$	NF&02	1001-20	P	site-specific fragmentation; comp. of $X_3Si-y-SiMe_3$ , X=F,Cl, y = ( $C_xH_y$ )
$C_5F_3H_{11}Si_2$	NF&02	1001-20	P	site-specific fragmentation; comp. of $X_3Si-y-SiMe_3$ , X=F,Cl, y = ( $C_xH_y$ )
$C_5F_3H_{13}Si$	NMK97	100-180	P,R	$F_3Si(CH_2)_2SiMe_3$ ; site-specific frag.; comp. to $SiMe_4$ ; surface desorption
$C_6H_{10}Si$	NF&97	100-120	P	site-specific fragmentation; no e- migration between two ends
	NF&02	1001-20	P	site-specific fragmentation; comp. of $X_3Si-y-SiMe_3$ , X=F,Cl, y = ( $C_xH_y$ )
	NP&07	104-115	P,T	site-specific fragmentation; ab initio
	NT&08	1990	P	AEPIPICO, site selective fragmentation, Si 2p & Si 1s compared
	TWM95	93-100	E,T	c-( $SiMe_5$ ); cyclo-polysilanes; ab initio EICVOM calc.; expt. comp. to ETS
	TC&02	85-220	E	$Me_3SiOEt$ ; absolute; comp. to vinyl silanes
	UH94b	90-200	E	$Me_3Si(NMe_2)$ ; comp. of Si-N cmpds; models for $SiN_xO_y$ films
	NF&02	1001-20	P	site-specific fragmentation; comp. of $X_3Si-y-SiMe_3$ , X=F,Cl, y = ( $C_xH_y$ )
	C <sub>6</sub> H <sub>6</sub> OSi	UT&97	P	$Ph_3SiOH$ ; absolute; Si-Si & Si-O-R
	C <sub>6</sub> H <sub>12</sub> Si	TWM95	93-100	c-( $SiMe_6$ ); cyclo-polysilanes; ab initio EICVOM calc.; expt. comp. to ETS
	C <sub>6</sub> H <sub>16</sub> OSi	UH94a	100-200	$Et_3SiOH$ ; comp of SI-O-X species re inductive, resonance effects
	C <sub>6</sub> H <sub>18</sub> Si <sub>2</sub>	W92	100-150	$Me_3Si-SiMe_3$ ; comp. of $SiMe_4$ , $Si_2Me_6$ , $Si_6Me_{12}$ ; $\sigma^*(Si-Si)$
$C_6H_{18}OSi_2$	NO&93	100-112	P	site-specific ionic. fragm.; PEPICO, PIPICO resonant Auger; comp. of $SiMe_4$ , $SiCl_4$ ; $Si_2Me_6$ and $Cl_3Si-SiMe_3$
	SL&93	100-117	P	total ion yield; PEPICO; detailed fragmentation map; KERDS
	UX&94	90-170	E	comp. of edges of Si-Si compounds
	XJ&96	90-130	P,T	gas-solid comp.; weak Ryd on strong valence; MS-Xa pred. mixed R,V
	UH94a	100-200	E	$Me_3SiOSiMe_3$ ; comp of SI-O-X species re inductive, resonance effects
	UH94a	100-200	E	c-( $SiMe_2O_3$ ); comp of SI-O-X species re inductive, resonance effects

<b>C<sub>6</sub>H<sub>18</sub>OSi<sub>2</sub></b>	UT&97	90-110	P	Me <sub>3</sub> Si-O-SiMe <sub>3</sub> ; absolute; Si-Si & Si-O-R
<b>C<sub>6</sub>H<sub>18</sub>Si<sub>2</sub></b>	UT&97	90-110	P	Me <sub>3</sub> Si-SiMe <sub>3</sub> ; absolute; Si-Si & Si-O-R
<b>C<sub>7</sub>H<sub>8</sub>N<sub>2</sub>O</b>	UH&95a	100-160	E	phenylurea; absolute; modelling of polyurethane PEELS
<b>C<sub>8</sub>H<sub>12</sub>Si</b>	HS90	90-140	E	HC/C-CH <sub>2</sub> -C/C-SiMe <sub>3</sub> ; absolute; comp. to other ::-bonded species
<b>C<sub>8</sub>H<sub>12</sub>O<sub>3</sub>Si</b>	TC&02	90-200	E	(CH <sub>2</sub> =CH)Si(OAc) <sub>3</sub> ; absolute; vinyl silanes
<b>C<sub>8</sub>H<sub>18</sub>O<sub>3</sub>Si</b>	TC&02	90-200	E	(CH <sub>2</sub> =CH)Si(OEt) <sub>3</sub> ; absolute
<b>C<sub>8</sub>H<sub>24</sub>N<sub>4</sub>Si</b>	UH94b	90-200	E	Si(NMe <sub>2</sub> ) <sub>4</sub> ; comp. of Si-N cmpds; models for SiN <sub>x</sub> O <sub>y</sub> films
<b>C<sub>8</sub>H<sub>24</sub>O<sub>4</sub>Si<sub>4</sub></b>	UH94a	100-200	E	c-(SiMe <sub>2</sub> O) <sub>4</sub> ; comp of SI-O-X species re inductive, resonance effects
<b>C<sub>9</sub>H<sub>27</sub>NSi<sub>3</sub></b>	UH94b	90-200	E	N(SiMe <sub>3</sub> ) <sub>3</sub> ; comp. of Si-N cmpds; models for SiN <sub>x</sub> O <sub>y</sub> films
<b>C<sub>9</sub>H<sub>28</sub>Si<sub>4</sub></b>	UX&94	90-170	P	HSi(SiMe <sub>3</sub> ) <sub>3</sub> ; Xa; search for σ*(Si-Si)
<b>C<sub>10</sub>H<sub>20</sub>N<sub>2</sub>Si</b>	UH&98	95-170	E,T	c-Si(RNCH=CHNR), R=tBu, silylene; absolute; delocal. in Si-N-C=C
<b>C<sub>10</sub>H<sub>22</sub>N<sub>2</sub>Si</b>	UH&98	95-170	E,T	c-Si(RNCH <sub>2</sub> CH <sub>2</sub> NR), R=tBu, unsat. silylene; absolute;
<b>C<sub>10</sub>H<sub>22</sub>N<sub>2</sub>Si</b>	UH&98	95-170	E,T	c-H <sub>2</sub> Si(RNCH=CHNR), R=tBu, silylene; absolute; no delocal.
<b>C<sub>10</sub>H<sub>24</sub>N<sub>2</sub>Si</b>	UH&98	95-170	E,T	c-H <sub>2</sub> Si(RNCH <sub>2</sub> CH <sub>2</sub> NR), R=tBu, unsat. silylene; absolute
<b>C<sub>11</sub>H<sub>21</sub>NOSi<sub>2</sub></b>	NF&96	100-130	P,T	Me(SiMe <sub>3</sub> N=)COSiMe <sub>3</sub> ; PEPICO; ion yields; PIPICO; no Si site select.; gs. calc of MeCF <sub>3</sub> , SiH <sub>3</sub> CF <sub>3</sub> , MeSiF <sub>3</sub> , SiH <sub>3</sub> SiF <sub>3</sub> ; LUMO of SiH <sub>3</sub> SiF <sub>3</sub> is p
<b>C<sub>12</sub>H<sub>36</sub>Si<sub>5</sub></b>	W92	90-140	E	Si[Si(CH <sub>3</sub> ) <sub>3</sub> ] <sub>4</sub>
	UX&94	90-170	E	comp. of edges of Si-Si compounds
	XJ&95	90-130	P,T	MS-Xa calc of Si 2p and Si 1s
<b>C<sub>12</sub>H<sub>36</sub>Si<sub>6</sub></b>	W92	100-150	E	c-Si <sub>6</sub> Me <sub>12</sub> ; comp. of SiMe <sub>4</sub> , Si <sub>2</sub> Me <sub>6</sub> , Si <sub>6</sub> Me <sub>12</sub> ; σ*(Si-Si)
	UX&94	90-170	E	comp. of edges of Si-Si compounds; σ*(Si-Si)
<b>C<sub>18</sub>H<sub>16</sub>OSi</b>	UT&97	100-145	E,T	triphenylsilanol, comp. of Si-O-X species
<b>C<sub>30</sub>H<sub>30</sub>Si<sub>2</sub></b>	UT&97	90-110	P	Bz <sub>3</sub> Si-SiBz <sub>3</sub> ; absolute; Si-Si & Si-O-R
<b>C<sub>30</sub>H<sub>30</sub>Si<sub>2</sub>O</b>	UT&97	90-110	P	Bz <sub>3</sub> Si-O-SiBz <sub>3</sub> ; absolute; Si-Si & Si-O-R
<b>ClH<sub>3</sub>Si</b>	WM&89	100-110	T	comp. of ETS, ISEELS; orb. order; {SiH <sub>x</sub> Cl <sub>4-x</sub> (x=0-4),SiF <sub>4</sub> } SE 6.1eV
	WM&91	100-110	T	comp. of ETS, ISEELS; orb. order; {SiH <sub>x</sub> Cl <sub>4-x</sub> (x=0-4)}, SE 6.1 eV
	T94	100-120	T	comp. of ISEELS TV and <sup>29</sup> Si nmr shielding; {SiH <sub>x</sub> Cl <sub>4-x</sub> (x=0-4)}
	WMT94a	100-140	E,T	ab initio; ISEELS vs. ETS; questions 'constancy of stabilization energy'- (TV-EA); comp. of SiH <sub>x</sub> Cl <sub>4-x</sub> , x= 0-3
<b>Cl<sub>2</sub>H<sub>2</sub>Si</b>	WM&89	100-110	T	comp. of ETS, ISEELS; orb. order; {SiH <sub>x</sub> Cl <sub>4-x</sub> (x=0-4),SiF <sub>4</sub> } SE 6.1eV
	WM&91	100-110	T	comp. of ETS, ISEELS; orb. order; {SiH <sub>x</sub> Cl <sub>4-x</sub> (x=0-4)}, SE 6.1 eV
	T94	100-120	T	comp. of ISEELS TV and <sup>29</sup> Si nmr shielding; {SiH <sub>x</sub> Cl <sub>4-x</sub> (x=0-4)}
	WMT94a	100-140	E,T	ab initio; ISEELS vs. ETS; questions 'constancy of stabilization energy'- (TV-EA); comp. of SiH <sub>x</sub> Cl <sub>4-x</sub> , x= 0-3
<b>Cl<sub>3</sub>HSi</b>	WM&89	100-110	T	comp. of ETS, ISEELS; orb. order; {SiH <sub>x</sub> Cl <sub>4-x</sub> (x=0-4),SiF <sub>4</sub> } SE 6.1eV
	WM&91	100-110	T	comp. of ETS, ISEELS; orb. order; {SiH <sub>x</sub> Cl <sub>4-x</sub> (x=0-4)}, SE 6.1 eV
	T94	100-120	T	comp. of ISEELS TV and <sup>29</sup> Si nmr shielding; {SiH <sub>x</sub> Cl <sub>4-x</sub> (x=0-4)}
	WMT94a	100-140	E,T	ab initio; ISEELS vs. ETS; questions 'constancy of stabilization energy'- (TV-EA); comp. of SiH <sub>x</sub> Cl <sub>4-x</sub> , x= 0-3
<b>Cl<sub>4</sub>Si</b>	FZ&70	102-112	P	pot. barr. effects
	ZV71	100-140	P,R	pot. barr. effects
	BNZ72	102-112	T	semi-empirical calc., comp. to expt. (FZ&70)
	D72	100-140	P,R	pot. barr. effects
	GM&76	103-115	P	Rydberg structure, no analysis
	PV&79	100-140	T	X-alpha (MSM) calc. of cont. shape, comp. to expt.
	TD84	100-300	T	X-alpha calc. (MSM), comp. to expt.
	CS&86	115-142	P,T	absolute, bs, MS-Xalpha, e & two t <sub>2</sub> res. identified
	BT&87	100-200	P,T	0.3 eV FWHM, comp to other expt, X-alpha calc
	AS&88	100-110	P	DES, spectator dominates
	CG&88	100-130	P,T	DES, bs, spectator dominates

(SiCl <sub>4</sub> cont'd)	CM&88b	100-113	P	DES, weak non-spectator (participator) obs; 2p<--7t <sub>2</sub> strongest absolute, X-alpha calc.; cont. & discrete; Rydbergs
	TL&89	90-140	T	comp. of ETS, ISEELS; orb. order; {SiH <sub>x</sub> Cl <sub>4-x</sub> (x=0-4,SiF <sub>4</sub> ) SE 6.1 eV
	WM&89	100-110	T	TEY, fluoresc. (SiCl <sub>4</sub> <sup>+</sup> , Si) yields; comp. to abs (YL&89); enhanced Fl at val. & Rydbergs
	RW&90a	102-112	P	wavelength-res. lum.; comp. of FY and PA
	RW&90b	100-140	P	DV-Xa; comp. to exp: SiX <sub>4</sub> , X=H,Cl,F; Virt. val. MOs dominate
	IF&91	100-170	T	comp. of TEY sol and gas PA (BT&87); distinguish val & Ryd.
	RF91	102-112	P	comp. of ETS, ISEELS; orb. order; {SiH <sub>x</sub> Cl <sub>4-x</sub> (x=0-4), SE 6.1 eV
	WM&91	100-110	T	fluorescence from core hole decay; comp. of SiF <sub>4</sub> , SiCl <sub>4</sub>
	D92a	100-140	P,R	comp of SiCl <sub>4</sub> , Si <sub>2</sub> Cl <sub>6</sub>
	W92	100-150	E	Me <sub>3</sub> Si-SiCl <sub>3</sub> ; site-specific ionic. fragm.; PEPICO, PIPICO resonant Auger;
	NO&93	100-112	P	comp. of SiMe <sub>4</sub> , SiCl <sub>4</sub> ; Si <sub>2</sub> Me <sub>6</sub> and Cl <sub>3</sub> Si-SiMe <sub>3</sub> , C <sub>6</sub> H <sub>18</sub> Si <sub>2</sub>
	T94	100-120	T	comp. of ISEELS TV and <sup>29</sup> Si nmr shielding; {SiH <sub>x</sub> Cl <sub>4-x</sub> (x=0-4)
	WMT94a	100-140	E,T	ab initio; ISEELS vs. ETS; questions 'constancy of stabilization energy'- (TV-EA); comp. of SiH <sub>x</sub> Cl <sub>4-x</sub> , x= 0-3
	CK&95	102-115	P	ion yields; compared TEY and CL <sup>+</sup> PSID scaled; 60 meV fwhm; mostly valence except p6d Ryd. at 109 eV; non-standard S-O splitting
	DP&95	104-112	P	TIY; high resolution; vibrations and hot bands identified
	PDK97	90-120	P	high res.; vibrational structure -> excited geom, SiX <sub>4</sub> , X=H,D,F,Cl,Br
	MG&98	102-125	P	resonant Auger; strong participator; comp. of SiF <sub>4</sub> , SiCl24
	PDK97	90-120	P	high res.; vibrational structure -> excited geom, SiX <sub>4</sub> , X=H,D,F,Cl,Br
	PDK98	105-112	P	relative; TIY; high res. (15 meV); comp. of SiX <sub>4</sub> , X=H,D,F,Cl,Br,Me; Z+1 tests; Franck-Condon analysis; G of 40-85 meV
	LC&11	200-225	P	PIY, TEY, state-specific frag; comp. to solid
	SK&13	1.84-1.89	P, T	TIY, STOBE-deMon calc, sym. forbidden 1s →a <sub>1</sub> obs. & calc (vibronic)
Cl <sub>6</sub> Si <sub>2</sub>	W92	100-150	E	comp of SiCl <sub>4</sub> , Si <sub>2</sub> Cl <sub>6</sub>
D <sub>4</sub> Si	SB&92	101-108	P	high res. (50 meV); vib'ns in Rydberg; analysed rel. to PES; isotope effect
	SL&94	101-109	P	high resolution; vibrationally-resolved Rydbergs; comp. of SiH <sub>4</sub> , SiD <sub>4</sub> ,
	PDK97	90-120	P	high res.; vibrational structure -> excited geom, SiX <sub>4</sub> , X=H,D,F,Cl,Br
Si <sub>2</sub> H <sub>6</sub>	PD&97	102-108	P	relative; TIY; high res. (15 meV); G=50(5) meV for all nl Rydberg; molecular distortion; Ryd.-val. mix; Franck-Condon analysis for geom.
	PDK98	105-112	P	relative; TIY; high res. (15 meV); comp. of SiX <sub>4</sub> , X=H,D,F,Cl,Br,Me; Z+1 tests; Franck-Condon analysis; G of 40-85 meV
F <sub>2</sub> Si	ZV72	100-150	P,R	pot. barr. Effects
F <sub>4</sub> Si	VZ71a	100-120	P	pot. barr. effects
	ZV71	100-140	P,R	pot. barr. effects
	D72	100-140	P,R	pot. barr. effects
	HB72	100-120	P	absolute, Rydberg analysis IP (110.8, 111.4)
	ZV72	100-170	P,R	pot. barr. effects
	R75	100-120	T	alternate assignment of HB72
	SM&78	100-120	T	X-alpha (MSM), comp. to expt (VZ71a)
	PV&79	100-140	T	X-alpha (MSM) calc. of cont. shape, comp. to expt. (VZ71a)
	FP&80	100-170	P	absolute, gas-solid comp., Z+1 analogy calc.
	PVK80	100-140	T	X-alpha (MSM) calc., comp. to expt., cont. shape res.
	AP&82	100-140	T	absolute, comp. to (VZ71a), cont. shape res.
	DV82	100-140	P	absolute, comp. to theory (AP&82), SiF <sub>6</sub> <sup>2-</sup> (sol)
	PVZ82	100-140	T	multiple scattering, cont. res., comp. to expt. (VZ71a,FP&80)
	PV&82	100-140	P,T	relative, cont. res., comp. to theory (PV&79)
	N84	110-125	P	resonant Auger, cont. res.
	TD84	100-300	T	X-alpha calc. (MSM), comp. to expt.
	AT&86a	100-110	P	resonant Auger at σ*(a <sub>1</sub> ), 4s & 3d, comp. to normal Auger

(SiF <sub>4</sub> cont'd)	BA&86	116-150	P,T	absolute, MS-Xalpha, t <sub>2</sub> res., bs
	R86	100-170	P	comp. of F <sup>+</sup> , e-, PSID of cond. MLs with gas abs.; F <sup>+</sup> yield lower
	FP&88	100-160	P	partial IY & Auger X-sect; comp. to abs.(FP&80), strong shake-up
	LS&89	100-125	P	absolute, comp. of abs., total, partial IYs; double PI X-sect; PCI
	SMN89	100-125	P	thresh. e-; partial e- yields; resonant Auger (DES)
	WM&89	100-110	T	ETS, ISEELS comp.; orb. order; {SiH <sub>x</sub> Cl <sub>4-x</sub> (x=0-4, SiF <sub>4</sub> ) SE 6.1 eV
	RW&90a	100-140	P	comp. of fluorescence yield and PA; selective decay into neutrals
	RW&90c	100-140	P	wavelength-res. lum.; comp. of FY and PA
	BT&92	100-140	P	relative; TEY, TIY, PA compared; quadrupole-MS PIMS; CH <sub>3</sub> more labile
				than F; CH <sub>3</sub> <sup>+</sup> enhanced in discrete res.; F 1s mass spec
	IB&91	100-160	P	absolute; ion yields; PIPICO; quantitative ion collection; KERD
	IF&91	100-170	T	DV-Xa; comp. to exp: SiX <sub>4</sub> , X=H,Cl,F; Virt. val. MOs dominate
	S91b	130	P	Auger-ion coincidence
	BT&92	100-140	P	relative; TEY, TIY, PA compared; quadrupole-MS PIMS; CH <sub>3</sub> more labile
				than F; CH <sub>3</sub> <sup>+</sup> enhanced in discrete res.; F 1s mass spec
	D92a	100-140	P,R	fluorescence from core hole decay; comp. of SiF <sub>4</sub> , SiCl <sub>4</sub>
	GC&92	0-350	E	absolute; ion frag.; challenges atomic cont. normal. - need IP+100 eV;
				differs from earlier spectra (LS&89, IB&91)
	SK&92b	130	P	Auger-ion coincidence; apparatus described
	PD&96	105-113	P	high res. (85 meV); vibn'l struct; mixed Ryd-val; Franck-Condon analysis
	SH&96a	130,145	P	(Auger, ion) coinc; fragment ions resolve states
	OC&97b	5-200	E,R	absolute, VTKR sum rule; derived molecular properties
	PDK97	90-120	P	high res.; vibrational structure -> excited geom, SiX <sub>4</sub> , X=H,D,F,Cl,Br
	MG&98	102-125	P	resonant Auger; strong participator; comp. of SiF <sub>4</sub> , SiCl <sub>4</sub> ; continuum Auger
				signal ascribed to nuclear motion (ultrafast decay precursor)
	PDK98	105-112	P	relative; TIY; high res. (15 meV); comp. of SiX <sub>4</sub> , X=H,D,F,Cl,Br,Me; Z+1
				tests; Franck-Condon analysis; G of 40-85 meV
	FL01	100-190	E	GOS.K-max = 5
	SLS01	105-120	P	TIY, PIY, branching ratios differ from LS&89, IB&91
	SLS02	70-110	P	PEPICO, PIPICO, fragmentation mechanisms
H <sub>4</sub> Si	HBK71	100-200	P	absolute, Rydberg analysis IP (107.2, 107.8)
	HB72	100-200	P	absolute, Rydberg analysis IP (107.2, 107.8)
	C73	100-120	P,R	review
	R75	100-120	T	alternate assignment of HB72
	S75a,b	100-120	T	Z+1 analogy calc., alternate assignment of HB72
	S76a	100-120	T	Z+1 analogy, EICVOM
	BF&79	100-170	P	absolute, gas-solid comp.
	FS&79	100-140	P,T	absolute, photographic, gas-solid comp.
	PVK80	100-140	T	X-alpha (MSM) calc., comp. to expt. (FS&79)
	PV&80	100-140	T	X-alpha (MSM) calc, comp. to expt. (FS&79)
	PVZ82	100-140	T	multiple scattering, cont. res., comp. to expt. (FS&79)
	SYD82	105-135	T	ab initio, absolute, comp. to expt (HB72)
	TD84	100-300	T	X-alpha calc. (MSM), comp. to expt.
	SMN86	100-115	P	resonant Auger (DES), dissociation prior to AI
	YA&86	100-115	P	total ion yield; 80 meV fwhm; DES at σ*(Si-H)
	N87	103-123	P	resonant Auger, diss. prior to AI, comp. to Si 1s (BNM86), PIPICO
	N88	100-110	P,R	electron & ion spectra of decay of discrete (DES) & cont. states
	NM&88	103-123	P	ionic decay, partial ion & electron X-sect, PIPICO
	SU90a	100-200	P	partial & total ion yields; PIPICO yields; selective frag.
	CIB90	90-180	E	absolute; comp. to Si(g), Si(sol) [Astrophys. J. 40 (79) 865]; TOF MS at
	WM&89	100-110	T	103 (σ*) & 120 eV; proposes 30% fluorescence yield at σ*
				ETS, ISEELS comp.; orb. order; {SiH <sub>x</sub> Cl <sub>4-x</sub> (x=0-4,SiF <sub>4</sub> ) SE 6.1 eV}

(SiH <sub>4</sub> cont'd)	IF&91	100-170	T	DV-Xa; comp. to exp: SiX <sub>4</sub> , X=H,Cl,F; Virt. val. MOs dominate
	WM&91	100-110	T	comp. of ETS, ISEELS; orb. order; {SiH <sub>x</sub> Cl <sub>4-x</sub> (x=0-4), SE 6.1 eV
	SB&92	101-108	P	high res. (50 meV); vibrational structure in Rydberg; analysed rel. to PES; isotope effect
	YP&93	101-135	T	absolute; MC-HF, comp. to expt. [HB72]
	SL&94	101-109	P	high res.; vibrationally-resolved Rydbergs; comp. of SiH <sub>4</sub> , SiD <sub>4</sub> , Si <sub>2</sub> H <sub>6</sub>
	T94	100-120	T	comp. of ISEELS TV and <sup>29</sup> Si nmr shielding; {SiH <sub>x</sub> Cl <sub>4-x</sub> (x=0-4)}
	CB&95	80-350	E	absolute; use of S(0) and S(-2) sum rules for accurate osc. str.
	LB&95	100-180	T	MS-Xa; comp. of XH <sub>n</sub> (X=Si,P,S,Cl)
	ISN97	90-150	P	mass spectra & abs.; filtered white light to enhance SiH <sub>4</sub> -> Si CVD
	OC&97b	5-200	E,R	absolute, VTKR sum rule; derived molecular properties
	PDK97	90-120	P	high res.; vibrational structure -> excited geom, SiX <sub>4</sub> , X=H,D,F,Cl,Br
	PD&97	102-108	P	relative; TIY; high res. (15 meV); G=50(5) meV for all nl Rydberg; molecular distortion; Ryd.-val. mix; Franck-Condon analysis for geom.
	PDK98	105-112	P	relative; TIY; high res. (15 meV); comp. of SiX <sub>4</sub> , X=H,D,F,Cl,Br,Me; Z+1 tests; Franck-Condon analysis; G of 40-85 meV
H <sub>6</sub> Si <sub>2</sub>	SB&92	101-108	P	SiH <sub>3</sub> -SiH <sub>3</sub> ; high res. (50 meV); vibrational structure in Rydberg; analysed rel. to PES; isotope effect
	SL&94	101-109	P	high resolution; vibrationally-resolved Rydbergs; comp. of SiH <sub>4</sub> , SiD <sub>4</sub> , Si <sub>2</sub> H <sub>6</sub> ; low-lying σ*(Si-Si)
H <sub>8</sub> Si <sub>3</sub>	SB&92	101-108	P	SiH <sub>3</sub> -SiH <sub>2</sub> -SiH <sub>3</sub> ; high res. (50 meV); vibrational structure in Rydberg; analysed rel. to PES; isotope effect
(O <sub>2</sub> Si) <sub>n</sub>	ABL13	106-115	P	size selected np; aerodynamic lenses & diff. pump; refractive indx

### Silicon 1s (1850 eV)

Br <sub>4</sub> Si	BM&89a	1.80-2.04	P	double excitation (1s,2p) multiplets
	BMN90	1.80-2.15	P,T	relative, chem. comp.; KL, KV 2e- excit; Ryd-val mix; CI calc
CCl <sub>3</sub> H <sub>3</sub> Si	HC&87a	1.84-1.90	P	shape res.
	FBN90	1.83-1.90	P	discrete & cont. shape res.; double excitation
C <sub>2</sub> Cl <sub>2</sub> H <sub>2</sub> Si	HC&87a	1.84-1.90	P	shape res.
	FBN90	1.80-2.35	P	discrete & cont. shape res.; KL double excitation
C <sub>3</sub> ClH <sub>3</sub> Si	HC&87a	1.84-1.90	P	shape res.
	FBN90	1.83-1.90	P	discrete & cont. shape res.; double excitation
C <sub>3</sub> Cl <sub>3</sub> H <sub>9</sub> Si <sub>2</sub>	SE&13	1.83-1.87	P	TIY, site dependent, KLL resonant Auger
C <sub>4</sub> H <sub>10</sub> OSi	UT&97	1.83-1.87	P	trimethylsilanol; absolute; Si-Si & Si-O-R
C <sub>4</sub> H <sub>12</sub> O <sub>4</sub> Si	BMN90	1.80-2.15	P,T	(OMe) <sub>4</sub> Si; rel.; chem. comp.; KL, KV 2e- excit; Ryd-val mix; CI calc
C <sub>4</sub> H <sub>20</sub> O <sub>4</sub> Si	BMN90	1.80-2.15	P,T	(OEt) <sub>4</sub> Si; rel.; chem. comp.; KL, KV 2e- excit; Ryd-val mix; CI calc
C <sub>4</sub> H <sub>12</sub> Si	BN86	1.83-1.88	P	Si(Me) <sub>4</sub> ; relative, comp. to SiX <sub>4</sub> , X=F,Cl,H,CH <sub>3</sub>
	BNM86	1.84-1.88	P,T	comp. to SiX <sub>4</sub> , X=F,Cl,H,CH <sub>3</sub> , Si2p (SD&85,MS&86)
	HC&87a	1.84-1.90	P	shape res.
	BM&89a	1.96-2.04	P	double excitation (1s,2p) multiplets
	BMN90	1.80-2.15	P,T	relative, chem. comp.; KL, KV 2e- excit; Ryd-val mix; CI calc
	DS&92	1.82-2.60	P,T	XANES and EXAFS interpreted by MS-Xa; MS paths analysed
	FT&93	1.95-2.02	P,T	KL 2e- exc.(data from BM&89a; comp. of solid Si, P, S, Cl species
	HT&93	1.82-1.86	P	comp. of SiMe <sub>4</sub> , Si(GeMe <sub>3</sub> ) <sub>4</sub> , Si(SiMe <sub>3</sub> ) <sub>4</sub> , Ge(SiMe <sub>3</sub> ) <sub>4</sub> ; Si-Ge ALS
	SK&93b	1.83-1.89	P,T	gas phase analogs of solid SiC/SiO <sub>2</sub> ; 2p vs. 1s; good at 2p poor at 1s; MS-Xa calc; Si(OMe) <sub>x</sub> (Me) <sub>4-x</sub> x=0-4 series
	UX&94	1.82-1.90	P	comp. of edges of Si-Si compounds; search for σ*(Si-Si)
	XJ&96b	1.83-2.60	P	xanes, xafs; comp. of SiMe <sub>4</sub> , Si(SiMe <sub>3</sub> ) <sub>4</sub> , Si(GeMe <sub>3</sub> ) <sub>4</sub> , Ge(SiMe <sub>3</sub> ) <sub>4</sub>
	SK&11	1.83-1.86	P	resonant Auger

C <sub>4</sub> H <sub>12</sub> SiO	SK&93b	1.83-1.89	P,T	Me <sub>3</sub> Si(OMe); gas phase analogs of solid SiC/SiO <sub>2</sub> ; 2p vs. 1s; good at 2p poor at 1s; MS-Xa calc; Si(OMe) <sub>x</sub> (Me) <sub>4-x</sub> x=0-4 series
C <sub>4</sub> H <sub>12</sub> SiO <sub>2</sub>	UT&97	1.83-1.87	P	absolute; Si-Si & Si-O-R
C <sub>4</sub> H <sub>12</sub> SiO <sub>2</sub>	SK&93b	1.83-1.89	P,T	Me <sub>2</sub> Si(OMe) <sub>2</sub> ; gas phase analogs of solid SiC/SiO <sub>2</sub> ; 2p vs. 1s; good at 2p poor at 1s; MS-Xa calc; Si(OMe) <sub>x</sub> (Me) <sub>4-x</sub> x=0-4 series
C <sub>4</sub> H <sub>12</sub> SiO <sub>3</sub>	SK&93b	1.83-1.89	P,T	MeSi(OMe); gas phase analogs of solid SiC/SiO <sub>2</sub> ; 2p vs. 1s; good at 2p poor at 1s; MS-Xa calc; Si(OMe) <sub>x</sub> (Me) <sub>4-x</sub> x=0-4 series
C <sub>4</sub> H <sub>12</sub> SiO <sub>4</sub>	SK&93b	1.83-1.89	P,T	Si(OMe) <sub>4</sub> ; gas phase analogs of solid SiC/SiO <sub>2</sub> ; 2p vs. 1s; good at 2p poor at 1s; MS-Xa calc; Si(OMe) <sub>x</sub> (Me) <sub>4-x</sub> x=0-4 series
C <sub>5</sub> H <sub>15</sub> NSi	UH&94b	1.82-2.20	P	Me <sub>3</sub> Si(NMe <sub>2</sub> ); comp. of Si-N cmpds; models for SiN <sub>x</sub> O <sub>y</sub> films
C <sub>5</sub> F <sub>3</sub> H <sub>13</sub> Si <sub>2</sub>	SN&09	1.84-1.87	P, T	F <sub>3</sub> Si(CH <sub>2</sub> ) <sub>2</sub> Si(CH <sub>3</sub> ) <sub>3</sub> , site selective fragmentation, TIY, STOBE-DEMON
	NT&08	1990	P	AEPPIPO, site selective fragmentation, Si 2p & Si 1s compared
C <sub>6</sub> H <sub>8</sub> Si	UT&97	1.83-1.87	T	phenylsilane; ab initio; EHMO; comp to Ph <sub>3</sub> Si-X
C <sub>6</sub> H <sub>18</sub> N <sub>2</sub> Si	UH&94b	1.82-2.20	P	Me <sub>2</sub> Si(NMe <sub>2</sub> ) <sub>2</sub> ; comp. of Si-N cmpds; models for SiN <sub>x</sub> O <sub>y</sub> films
C <sub>6</sub> H <sub>18</sub> N <sub>3</sub> Si	UH&94b	1.82-2.20	P	HSi(NMe <sub>2</sub> ) <sub>3</sub> ; comp. of Si-N cmpds; models for SiN <sub>x</sub> O <sub>y</sub> films
C <sub>6</sub> H <sub>18</sub> OSi <sub>2</sub>	UT&97	1.83-1.87	P	Me <sub>3</sub> Si-OSiMe <sub>3</sub> ; absolute; Si-Si & Si-O-R
C <sub>6</sub> H <sub>18</sub> O <sub>3</sub> Si <sub>3</sub>	UH94a	1.82-2.20	P	c-(SiMe <sub>2</sub> O) <sub>3</sub> ; comp of SI-O-X species re inductive, resonance effects
C <sub>6</sub> H <sub>18</sub> O <sub>3</sub> Si <sub>3</sub>	UX&94	1.82-1.90	P	Me <sub>3</sub> Si-SiMe <sub>3</sub> ; comp. of edges of Si-Si compounds; search for σ*(Si-Si)
C <sub>6</sub> H <sub>18</sub> Si <sub>2</sub>	XJ&96a	1.82-1.84	P,T	gas-solid comp.; weak Ryd. on strong valence; MS-Xa pred. mixed R,V
	XJ&96b	1.83-2.60	P	xanes, xafs; comp. of SiMe <sub>4</sub> , Si(SiMe <sub>3</sub> ) <sub>4</sub> , Si(GeMe <sub>3</sub> ) <sub>4</sub> , Ge(SiMe <sub>3</sub> ) <sub>4</sub>
	UT&97	1.83-1.87	P	triphenylsilanol; absolute; Si-Si & Si-O-R
C <sub>7</sub> H <sub>21</sub> N <sub>3</sub> Si	UH94b	1.82-2.20	P	MeSi(NMe <sub>2</sub> ) <sub>2</sub> ; comp. of Si-N cmpds; models for SiN <sub>x</sub> O <sub>y</sub> films
C <sub>8</sub> H <sub>20</sub> O <sub>4</sub> Si	UH94a	1.82-2.20	P	Si(OEt) <sub>4</sub> ; comp of SI-O-X species re inductive, resonance effects
C <sub>8</sub> H <sub>20</sub> Si	BMN90	1.80-2.15	P,T	(Et) <sub>4</sub> Si; rel.; chem. comp.; KL, KV 2e- excit; Ryd-val mix; CI calc
C <sub>8</sub> H <sub>24</sub> N <sub>4</sub> Si	UH94b	1.80-2.20	P	Si(NMe <sub>2</sub> ) <sub>4</sub> ; comp. of Si-N cmpds; models for SiN <sub>x</sub> O <sub>y</sub> films
C <sub>8</sub> H <sub>24</sub> O <sub>4</sub> Si <sub>4</sub>	UH94a	1.80-2.20	P	c-(SiMe <sub>2</sub> O) <sub>4</sub> ; comp of SI-O-X species re inductive, resonance effects
C <sub>9</sub> H <sub>14</sub> Si	UT&97	1.83-1.87	P	trimethylphenylsilane; a initio; EHMO
C <sub>9</sub> H <sub>27</sub> NSi <sub>3</sub>	UH94b	1.80-2.20	P	N(SiMe <sub>3</sub> ) <sub>3</sub> ; comp. of Si-N cmpds; models for SiN <sub>x</sub> O <sub>y</sub> films
C <sub>10</sub> H <sub>20</sub> N <sub>2</sub> Si	UH&98	1.83-1.86	P,T	c-Si(RNCH=CHNR), R=tBu, silylene; absolute; delocal. in Si-N-C=C
C <sub>10</sub> H <sub>22</sub> N <sub>2</sub> Si	UH&98	1.83-1.86	P,T	c-Si(RNCH <sub>2</sub> CH <sub>2</sub> NR), R=tBu, unsat. silylene; absolute;
C <sub>10</sub> H <sub>22</sub> N <sub>2</sub> Si	UH&98	1.83-1.86	P,T	c-H <sub>2</sub> Si(RNCH=CHNR), R=tBu, silylene; absolute; no delocal.
C <sub>10</sub> H <sub>24</sub> N <sub>2</sub> Si	UH&98	1.83-1.86	P,T	c-H <sub>2</sub> Si(RNCH <sub>2</sub> CH <sub>2</sub> NR), R=tBu, unsat. silylene; absolute;
C <sub>12</sub> GeH <sub>36</sub> Si <sub>4</sub>	HT&93	1.82-1.86	P	comp. of SiMe <sub>4</sub> , Si(GeMe <sub>3</sub> ) <sub>4</sub> , Si(SiMe <sub>3</sub> ) <sub>4</sub> , Ge(SiMe <sub>3</sub> ) <sub>4</sub> ; Si-Ge ALS
	XJ&96b	1.83-2.60	P	xanes, xafs; comp. of SiMe <sub>4</sub> , Si(SiMe <sub>3</sub> ) <sub>4</sub> , Si(GeMe <sub>3</sub> ) <sub>4</sub> , Ge(SiMe <sub>3</sub> ) <sub>4</sub>
C <sub>12</sub> Ge <sub>4</sub> H <sub>36</sub> Si	HT&93	1.82-1.86	P	comp. of SiMe <sub>4</sub> , Si(GeMe <sub>3</sub> ) <sub>4</sub> , Si(SiMe <sub>3</sub> ) <sub>4</sub> , Ge(SiMe <sub>3</sub> ) <sub>4</sub> ; Si-Ge ALS
	XJ&96b	1.83-2.60	P	xanes, xafs; comp. of SiMe <sub>4</sub> , Si(SiMe <sub>3</sub> ) <sub>4</sub> , Si(GeMe <sub>3</sub> ) <sub>4</sub> , Ge(SiMe <sub>3</sub> ) <sub>4</sub>
C <sub>12</sub> H <sub>36</sub> Si <sub>5</sub>	HT&93	1.82-1.86	P	comp. of SiMe <sub>4</sub> , Si(GeMe <sub>3</sub> ) <sub>4</sub> , Si(SiMe <sub>3</sub> ) <sub>4</sub> , Ge(SiMe <sub>3</sub> ) <sub>4</sub> ; Si-Ge ALS
	UX&94	1.82-1.90	P	comp. of edges of Si-Si compounds; search for σ*(Si-Si)
	XJ&95	1.82-1.90	P,T	MS-Xa calc of Si 2p and Si 1s
	XJ&96b	1.83-2.60	P	xanes, xafs; comp. of SiMe <sub>4</sub> , Si(SiMe <sub>3</sub> ) <sub>4</sub> , Si(GeMe <sub>3</sub> ) <sub>4</sub> , Ge(SiMe <sub>3</sub> ) <sub>4</sub>
C <sub>12</sub> H <sub>36</sub> Si <sub>6</sub>	UX&94	1.82-1.90	P	c-(SiMe <sub>2</sub> ) <sub>6</sub> ; comp. of edges of Si-Si compounds; search for σ*(Si-Si)
C <sub>18</sub> H <sub>16</sub> OSi	UT&97	1.83-1.87	P	triphenylsilanol; absolute; Si-Si & Si-O-R
C <sub>30</sub> H <sub>30</sub> Si <sub>2</sub>	UT&97	1.83-1.87	P	Bz <sub>3</sub> Si-SiBz <sub>3</sub> ; absolute; Si-Si & Si-O-R
Cl <sub>4</sub> Si	M66	1.83-2.13	P	extended fine structure (EXAFS)
	BN86	1.83-1.88	P	relative, comp. to SiX <sub>4</sub> , X=F,Cl,H,CH <sub>3</sub>
	BNM86	1.84-1.88	P,T	comp. to SiX <sub>4</sub> , X=F,Cl,H,CH <sub>3</sub> , Si2p (SD&85,MS&86)
	BF&87	1.84-1.90	P,T	shape res.; comp. to Cl1s; ab initio-CI calc.
	HC&87a	1.84-1.90	P	shape res.
	BM&89a	1.96-2.04	P	double excitation (1s,2p) multiplets
	TL&89	1.83-1.88	T	absolute, X-alpha calc.; cont. & discrete; Rydbergs
	BMN90	1.80-2.15	P,T	relative, chem. comp.; KL, KV 2e- excit; Ryd-val mix; CI calc
	FBN90	1.83-1.90	P	discrete & cont. shape res.; double excitation

(SiCl <sub>4</sub> cont'd)	DS&92	1.82-2.60	P,T	XANES and EXAFS interpreted by MS-Xa; MS paths analysed
	FT&93	1.95-2.02	P,T	KL 2e- exc.(data from BM&89a); comp. of solid Si, P, S, Cl species
	SK&13b	1.84-1.86	P	resonant Auger, cascade Auger
D <sub>4</sub> Si	BMN90	1.80-2.15	P,T	relative, chem. comp.; KL, KV 2e- excit; Ryd-val mix; CI calc
FH <sub>3</sub> Si	KP92b	1.84-1.85	T	SCF-CI; comp. to SiH <sub>4</sub>
F <sub>2</sub> H <sub>2</sub> Si	KP93	1.84-1.85	T	ab initio; MRD-CI; dipole & quadrupole; comp. to FH <sub>3</sub> Si and SiH <sub>4</sub>
F <sub>4</sub> Si	BN86	1.83-1.88	P	relative, comp. to SiX <sub>4</sub> , X=F,Cl,H,CH <sub>3</sub>
	BNM86	1.84-1.88	P,T	comp. to SiX <sub>4</sub> , X=F,Cl,H,CH <sub>3</sub> , Si2p (SD&85,MS&86)
	BM&89a	1.80-2.30	P	double excitation (1s,2p) multiplets; EXAFS
	BMN90	1.80-2.15	P,T	relative, chem. comp.; KL, KV 2e- excit; Ryd-val mix; CI calc
	OCT91	2.00-2.10	T	double core vacancies (KL); comp. to BM&89a
	DS&92	1.82-2.60	P,T	XANES and EXAFS interpreted by MS-Xa; MS paths analysed
	FT&93	1.95-2.02	P,T	KL 2e- exc.(data from BM&89a); comp. of solid Si, P, S, Cl species
	SK&10	1.83-1.86	P	resonant Auger
	SK&11	1.83-1.86	P	resonant Auger
	SK&13b	1.84-1.86	P	resonant Auger, Cascade Auger
H <sub>4</sub> Si	BN86	1.83-1.88	P	relative, comp. to SiX <sub>4</sub> , X=F,Cl,H,CH <sub>3</sub>
	BNM86	1.84-1.88	P,T	comp. to SiX <sub>4</sub> , X=F,Cl,H,CH <sub>3</sub> , Si2p (SD&85,MS&86)
	BM&89a	1.96-2.04	P	double excitation (1s,2p) multiplets
	US&89b	1.84-1.86	P	partial & total ion yields; strong multiple ionis.; no sel. frag.
	BMN90	1.80-2.15	P,T	relative, chem. comp.; KL, KV 2e- excit; Ryd-val mix; CI calc
	SU90b	1.84-1.86	P	partial & total IYs; strong. frag.; 12 eV KER; vacancy cascades
(SiH <sub>4</sub> cont'd)	OCT91	2.0-2.1	T	double core vacancies (KL); comp. to BM&89a
	DS&92	1.82-2.60	P,T	XANES and EXAFS interpreted by MS-Xa; MS paths analysed
	KNP92	1.84-1.85	T	SCF-CI; (Z+1); comp. of simpl. ab initio methods; comp. to ext [BMN90]
	KP92b	1.84-1.85	T	SCF-CI; comp. to expt [BMN90] and SiFH <sub>3</sub> calc.
	FT&93	1.95-2.02	P,T	KL 2e- exc.(data from BM&89a); comp. of solid Si, P, S, Cl species
	KP94a	1.84-1.85	T	SCF-CI; Jahn-Teller effect
OSi	BE&91	1.83-1.88	P	SiO; comp. to sol; strong π* (like CO); gas.NE.sol!!; Z+1 (PO)

### Sodium 2p, 2s (50 eV)

Cl <sub>4</sub> Na	YS&02	190-230	T	relative; MS-Xα plus DFT; geometry dependence
Na <sub>2</sub>	DCZ83	30-160	T	one-electron, cont. X-section, absolute, no shape res., EXAFS or Cooper minimum

### Sodium 1s (1072 eV)

BrNa	EK&94b	1050-1100	P	comp. of alkali halides vapors; clusters; Na <sup>-</sup> states speculated
	TE&01	1.070-1080	P	relative, comparison of gas, solid of NaX
ClNa	RSW76	1050-1100	P	photographic, gas-solid comp., cont. res.
	TE&01	1.070-1080	P	relative, comparison of gas, solid of NaX
Cl <sub>4</sub> Na <sub>4</sub> (ClNa) <sub>n</sub>	YS&02	1050-1100	T	relative; MS-Xα plus DFT; geometry dependence
	RC&01	1070-1100	P,T	EXAFS as f(<n>); TEY, PIY, MS calc; 2.2 – 2.8 Å
FNa	TE&00	1070-1100	P	relative; comp. to Kr-matrix clusters & solid; strong 3s, 3p Ryd disappears
	TE&01	1.070-1080	P	relative, comparison of gas, solid of NaX
INa	TE&01	1.070-1080	P	relative, comparison of gas, solid of NaX

Sulfur 2p, 2s (175, 235 eV)

<b>BHS</b>	EH99	160-240	E,T	absolute; transient from H <sub>2</sub> S+B+SiO <sub>2</sub> ; comp of HBO, HBS, H <sub>3</sub> B <sub>3</sub> O <sub>3</sub>
	H00	160-250	E,R	transient ISEELS; comp of HBO,HBS, H <sub>2</sub> S
	HE&01	160-240	E	absolute; transient ISEELS
<b>CF<sub>8</sub>S</b>	KA&10	168-210	PT,	absolute, comp. to SF <sub>6</sub> , DFT calculation
<b>CH<sub>4</sub>O<sub>3</sub>S</b>	HH14	160-200	E	(methane sulfonic acid), references for PFSA (Nafion)
<b>CH<sub>4</sub>S</b>	DTH90	150-290	E	CH <sub>3</sub> SH, absolute; comp. to S1s, other RSH
<b>COS</b>	WB74e	155-200	E	weak cont. feature
	KGM77	162-174	P	Rydberg analysis IP (170.49)
	TL&84	162-174	P	Auger, PES X-sections, bs, absolute
	CG&88	160-200	P,T	DES, bs, spectator dominates
	NH&88	160-195	R	comp. of ETS, CO <sub>2</sub> , COS, CS <sub>2</sub> re location of σ*; decay of core states
	MH&89	140-280	E,T	absolute, ab initio, comp. of CO <sub>2</sub> , COS & CS <sub>2</sub> - all edges
	AEB97b	160-180	P	TIY,PIY; charge state mapping
	EK&97a	163-183	P	TIY, PEPICO; b ; high res.(35 meV); PEPICO; bs
	EK&97b	162-172	P	TIY, PEPICO; fragmentation mechanisms; S <sup>3+</sup> from (S2p, π*)
	EK&97c	163-183	P	TIY, PIY; PE3PICO; fragmentation mechanisms
	BNP98	160-172	T	MR-CI, compared to experiment (Thomas, Morin, unpub)
	MB&98	162-174	P	resonant Auger; vibrational resolved; Renner-Teller; lifetime-vib'n interfer.
	FE&99	161-173	P	TIY; ionic frag; branching ratios; state selective fragmentation
	MG&99	160-195	P,T	TIY, STEX, resonant emission; atomic like ultra-fast decay of σ*
	FCB00	50-360	E	absolute; sum rule analysis
	KI00	172-178	T	ab initio; spin-orbital Breit-Pauli; molecular field; comp. of SO <sub>2</sub> , COS, PF <sub>3</sub>
	MA&03	170-205	P	luminescence (300-650 nm) yield, spectroscopy
	FE&04	163-168	P,T	long lived atomic S <sup>L*</sup> at 165.6 eV; XRF detected; no resonant Auger (p-p)
	GA&05a	174-198	P, T	PAD, comp of S2p, C1s, O1s at selected energies, MS-Xα
	GA&05b	174-198	P, T	AR-PEPICO, comp of S2p, C1s, O1s at selected energies, MS-Xα
	FE&06	182	P	untra-fast decay, PIY, S* produced
	IIS12	166-172	P	resonant Auger, NEXAFS maps, participator Auger after π* excitation
<b>CS<sub>2</sub></b>	VZ71b	160-210	P	absence of barr. effects
	D72	160-200	P,R	absence of pot. barr. effects
	ZV72	160-200	P,R	absence of pot. barr. effects
	WB74e	156-202	E	absence of pot. barr. effects
	KGM77	162-172	P	Rydberg structure analysis
	MK80	162-172	P	vibnl struct.
	H87	150-190	P	total & partial ion yields, comp. to C1s, quadrupole
	CG&88	160-200	P,T	DES, bs, spectator dominates
	NH&88	160-195	R	comp. of ETS, CO <sub>2</sub> , COS, CS <sub>2</sub> re location of σ*; decay of core states
	MH&89	140-280	E,T	absolute, ab initio, comp. of CO <sub>2</sub> , COS & CS <sub>2</sub> - all edges
	HE90	178	P	DES; Auger-ion coinc.; ion KE
	AEB97b	160-180	P	TIY,PIY; charge state mapping
	AB98	164, 177	P	(Auger, ion) coinc.; comp. to spin-selective double charge transfer calc; fragmentation mech.; S <sub>2</sub> <sup>+</sup> detected at π*
	KE&98	161-173	P	TIY, angle-resolved PEPICO; 30 meV fwhm; vibronic symmetry breaking; core hole localized in Rydbergs
	FE&99	161-173	P	TIY, state-selective fragmentation
	L99	165	P	full angle/energy/mass (64 ch) multi-detector; 0 dead-time multi-hit; PIY
	ET&07	160-180	E,T	absolute, OOS, non-dipole, triplet states
	TR&07	160-180	E,T	absolute, OOS, GOS to 30 a.u. <sup>-1</sup> , MP-CI calc
<b>C<sub>2</sub>F<sub>3</sub>H<sub>3</sub>O<sub>3</sub>S</b>	HH14	160-200	E	(Methyl trifluoromethanesulfonate), absolute, comp to Nafion
<b>C<sub>2</sub>H<sub>3</sub>NS</b>	HTM89	150-285	E	(CH <sub>3</sub> SCN), comp to CH <sub>3</sub> NCS, vibrational ELS

	CE&09	160-180	P	TIY, PEPICO, fragmentation dynamics
C <sub>2</sub> H <sub>3</sub> NS	HTM89	150-285	E	(CH <sub>3</sub> NCS), comp to CH <sub>3</sub> SCN, vibrational ELS
C <sub>2</sub> H <sub>6</sub> OS	TB&88	160-280	E	(CH <sub>3</sub> ) <sub>2</sub> S=O, DMSO, comp. to S1s
<b>C<sub>2</sub>H<sub>6</sub>O<sub>3</sub>S</b>	HH14	160-200	E	(CH <sub>3</sub> )SO <sub>3</sub> CH <sub>3</sub> , absolute, comp. to PFSA (Nafion) spectra
C <sub>2</sub> H <sub>6</sub> S	BS&12	160-190	P, T	(CH <sub>3</sub> ) <sub>2</sub> S dimethyl sulfide, TIY, PIY; IS-CASSCF calc.
C <sub>2</sub> H <sub>6</sub> S <sub>2</sub>	BS&12	160-190	P, T	(CH <sub>3</sub> ) <sub>2</sub> S dimethyl di-sulfide, TIY, PIY; IS-CASSCF calc.
<b>C<sub>4</sub>H<sub>4</sub>S</b>	H86b	160-195	E,R	thiophene, comp. to thiolane
	HHS86	160-255	E,P	S2p, S2s, S1s; comp. to sol. ml; MS-Xa calc; $\sigma^*(C-S)$
	HE90	200-250	P	Auger-ion coinc. (but e-'s signal wrong); S2p/C1s comp.; sel. frag.
	HT&90	160-285	E	absolute, comp. to 3-alky-thiophenes
	HE91	(white)	P	(hv;e <sub>Auger,ion</sub> ) coinc.; mass spectra at C1s, S2p with Auger
	TG&18	162-172	P,T	benzo-b-thiophene, TIY; DFT calc, comp.C <sub>4</sub> H <sub>4</sub> S, C <sub>8</sub> H <sub>6</sub> S, C <sub>8</sub> H <sub>6</sub> S (S-rings)
<b>C<sub>4</sub>H<sub>8</sub>S</b>	H86b	160-195	E,R	comp. to thiophene
	HHS86	160-255	E,P	(thiolane), S2p, S2s, S1s; $\sigma^*(C-S)$
	HE91	(white)	P	(hv;e <sub>Auger,ion</sub> ) coinc.; mass spectra at C1s, S2p with Auger
C <sub>5</sub> H <sub>6</sub> S	HT&90	150-285	E	absolute, 3-alkyl-thiophenes; no mod. of $\pi^*$ (cf. polymer cond.)
C <sub>5</sub> H <sub>12</sub> NO <sub>2</sub> S	SD&20	160-175	P,T	protonated methionine, selective ionic dissociation @ $\sigma^*(C-S)$
<b>C<sub>6</sub>H<sub>4</sub>N<sub>2</sub>S</b>	HD&91	160-280	E	c-BzN <sub>2</sub> S fused ring; comp. of S-N heterocycles, aromaticity
<b>C<sub>6</sub>H<sub>4</sub>N<sub>2</sub>S<sub>2</sub></b>	HD&91	160-280	E	c-BzN <sub>2</sub> S <sub>2</sub> fused ring; comp. of S-N heterocycles, aromaticity
<b>C<sub>6</sub>H<sub>4</sub>N<sub>2</sub>S<sub>3</sub></b>	HD&91	160-280	E	c-BzN <sub>2</sub> S <sub>3</sub> fused ring; comp. of S-N heterocycles, aromaticity
<b>C<sub>6</sub>H<sub>9</sub>S</b>	HT&90	150-285	E	absolute, 3-alkyl-thiophenes; no mod. of $\pi^*$ (cf. polymer cond.)
C <sub>8</sub> H <sub>6</sub> S	TG&18	162-172	P,T	benzo-b-thiophene, TIY; DFT calc, comp.C <sub>4</sub> H <sub>4</sub> S, C <sub>8</sub> H <sub>6</sub> S, C <sub>8</sub> H <sub>6</sub> S (S-rings)
<b>C<sub>8</sub>H<sub>13</sub>S</b>	HT&90	150-285	E	absolute, 3-alkyl-thiophenes; no mod. of $\pi^*$ (cf. polymer cond.)
<b>C<sub>10</sub>H<sub>17</sub>S</b>	HT&90	150-285	E	absolute, 3-alkyl-thiophenes; no mod. of $\pi^*$ (cf. polymer cond.)
C <sub>12</sub> H <sub>8</sub> S	TG&18	162-172	P,T	dibenzothiophene, TIY; DFT calc, compare C <sub>4</sub> H <sub>4</sub> S, C <sub>8</sub> H <sub>6</sub> S, C <sub>8</sub> H <sub>6</sub> S (Srings)
<b>C<sub>12</sub>H<sub>21</sub>S</b>	HT&90	150-285	E	absolute, 3-alkyl-thiophenes; no mod. of $\pi^*$ (cf. polymer cond.)
C <sub>14</sub> H <sub>24</sub> S	HT&90	150-285	E	absolute, 3-alkyl-thiophenes; no mod. of $\pi^*$ (cf. polymer cond.)
ClF <sub>5</sub> S	AT&86b	165-215	P	absolute, comp. to SF <sub>6</sub> & SeF <sub>6</sub> (Se3p)
Cl <sub>3</sub> PS	TKM82	162-173	P	X-alpha (MSM) calc., comp. to expt (K77)
	NS&98	150-240	P	absolute; PIY, TIY, PEPICO
D <sub>2</sub> S	HS&94	160-240	P	30 meV fwhm; comp. of H <sub>2</sub> S/D <sub>2</sub> S; vibn'l struct.; val-Ryd. identified
F <sub>2</sub> OS	T91	160-172	T	SCF, EICVOM; orbital char, comp. to expt & Diss. Att.
	BHK92	160-172	T	ab initio DSCF, large basis set calc.
F <sub>2</sub> O <sub>2</sub> S	T91	160-172	T	SCF, EICVOM; orbital char, comp. to expt & Diss. Att.
F <sub>3</sub> NS	JKC99	164-194	P,T	relative; GSCF3; ion current; two LS-coupled states; comp. to OPF <sub>3</sub>
F <sub>3</sub> OS	NS&98	150-240	P	absolute; PIY, TIY, PEPICO
<b>F<sub>4</sub>S</b>	BZ&67	140-188	P	relative, large background comp. to SF <sub>6</sub> S 2p
	BH87	160-250	E	S2p, S2s, S1s & F1s comp.
	KBH90	160-180	T	ab initio, comp. to BH87; revised $\sigma^*(S-F)$ assignments
	T91	160-172	T	SCF, EICVOM; orbital char, comp. to expt & Diss. Att.
	BHK92	160-172	E,T	ab initio DSCF, large basis set calc.
F <sub>4</sub> OS	T91	160-172	T	SCF, EICVOM; orbital char, comp. to expt & Diss. Att.
<b>F<sub>6</sub>S</b>	BZ&67	170-240	P	pot. barr. effects
	ZF67	170-300	P	photographic, pot. barr. effects, S 2s structure
	N70	130-300	T	pot. barr. effects, MO interpretation
	NM&71	150-240	P	photographic, pot. barr. effects, weak Rydberg structure
	BH&72	150-250	P	gas-solid comp., cont. res.
	D72	150-250	P,R	pot. barr. effects
	GGL72	160-250	T	ab initio calc., pot. barr. effects
	VZ72	170-230	P	absolute
	ZV72	170-260	P,R	pot. barr. effects
	SP&74	175-190	T	X-alpha (MSM) calc., cont. shape res.

(SF <sub>6</sub> cont'd)				
	VK&74	175-210	T	cont. shape res., extended fine structure (EXAFS)
	B76b	160-460	E	cont. shape res., extended fine structure (EXAFS)
	M76b	175-190	T	X-alpha (MSM) calc., cont. shape res.
	VK76	170-220	T	Green's function calc., pot. barr. effects, res. theory
	GKM77a	170-220	P	0.12eV FWHM, weak Rydberg structure
	H77b	170-190	T	HF improved VO; comp. to expt.
	HB78c	180-280	E	pot. barr. effects, Rydbergs, dipole forbidden transitions, S 2s
	HBW78	40-240	E	absolute, ionic fragmentation of cont. res.
	W80	220-290	E	extended fine structure (EXAFS), dissociative double ionisation
	BD&82	180-190	E,R	calibration ( $t_{2g}=184.54$ eV)
	GN&83	180-200	P,T	comparison of core & valence cont. shapes
	SB84	184.54(5)	E	calibration standard( $2p_{1/2} \rightarrow t_{2g}$ )
	VA&85	130-175	P,R	comp. to BF <sub>3</sub> , N <sub>2</sub> , NO <sub>3</sub> ; KPF <sub>6</sub> (s); shape resonances
	AT&86b	165-215	P	absolute, comp. to SF <sub>5</sub> Cl & SeF <sub>6</sub> (Se3p)
	H86a	170-186	E	74 eV final energy, new quadrupole state claimed
	TC86	180-210	T	local density calc, comp to expt (BH&82, HB78)
	FL&88	170-250	P	partial PI, shape resonant & multi-electron at e <sub>g</sub> , no effect of t <sub>2g</sub> res. on b, combined 1-e <sup>-</sup> /multi-e <sup>-</sup> model
	AT&89	160-270	P,T	relative, comp. to valence partial X-sect, SeF <sub>6</sub> , "F <sub>6</sub> "; X-alpha calc.
	KBH90	160-180	T	ab initio, comp. to SF <sub>4</sub> (BH87)
	NMA90	160-260	T	MSXa calc; order of res. identified; comp. to expt. (ZV71)
	SB90	160-240	E	comp of TeF <sub>6</sub> , SeF <sub>6</sub> , SF <sub>6</sub> ; Z-dependence of pot. barr's
	NMA91	160-210	T	absolute; DVXa calc; comp. to expt. (ZV71); H <sub>2</sub> S
	T91	160-172	T	SCF, EICVOM; orbital char, comp. to expt & Diss. Att.
	TL91	170-180	P	relative; gas-sol. comp. in Rydberg region; crystal quality of sol. important (MS); 177.2,178.4 eV peaks (gas) 6 broad line ( $t_{1u}$ ?) in sol.
	BHK92	160-240	E,T	DSCF, comp. to expt (all edges)
	SU&92b	166-204	P	PIPICO yield spectra; Auger-ion coinc; t <sub>2g</sub> /e <sub>g</sub> PIPICO differ; new shake-up
	HS&93	170-215	P,T	high res (45 meV); comp. of exp; theory & Ryd. analysis; lineshapes; vibn'l structure of Ryd. analysed; IPs (180.27, 181.48)
	YML93	160-210	E	generalised osc. str.; large increase in rel. intensity of t <sub>1u</sub> ( $K^2_{max} \sim 6au$ )
	HH&95	68-214	E	2 kV impact; 1°; parallel detector-phosphor-CCD described
	FT&95	165-210	E,T	dipole and non-dipole; 2 new quadrupole states; DSCF calc (non-relativistic)
	TF&95	165-210	E	GOS for all states, differences from YML93 explained
	FCM96	170-185	T	GOS, extrapolation to $K^2=0$ , comp. to YML93
	FM&98	160-200	E	4 keV impact; (Auger,ion) coinc.; no bound SF <sub>6</sub> <sup>++</sup> states
	HE&98	150-280	E	absolute; S 2p and S 2s GOS
	ETH99	160-260	E	absolute; GOS; B-state strongest for $K^2 > 50 au^{-2}$ ; S 2s GOS
	PV&99	170-180	P	Ryd lifetime width 3d 43(7), 5s, 4d 35(1) meV
	EF&00	160-270	E	GOS; strong e $\rightarrow$ e quadrupole; confirms TF&95
	H00	165-210	E,R	extreme non-dipole, B-state largest
	OM02	23-210	P	TIY, β-parameter
	SM&02	170-205	P	negative ion PIY; state interpretation; Rydberg region
	SR&02	165-205	P	DES vs PES; ERAMICO, vibration-dissociation correlation
	KA&03	170-205	P	TIY, AEPICO, EREICO, (SF <sub>2</sub> <sup>2+</sup> ) observed, spectator resonant below IP, decay of t <sub>2g</sub> and e <sub>g</sub> resonances DIFFERS due to additional 2e- states
	MA&03	170-205	P	luminescence (300-650 nm) yield, spectroscopy
	OM03	80-220	P	TIY, KERD for all ions; β-parameter
	K04	168-212	P,T	spin-orbit ; singlet-triplet as function of R(S-F)
	SR&04	170-189	P	(e-(E), ion) coinc (EREICO); state dependent dissociation; comp. to val <sup>-1</sup>

(SF <sub>6</sub> cont'd)	PS&05	170-210	P	relative, TIY, PIY, all +ves and S <sup>-</sup> , F <sup>-</sup> ; anion signals specific to shape resonances
	KA&10	168-210	P,T	absolute, comp. to SF <sub>5</sub> CF <sub>3</sub> , DFT calculation
	KC&16	170-2105	P,T	XAS, XES compared; 4e <sub>g</sub> resonance is multi-electron
	SK&22a	684-705	P	high accuracy E-caib (1s→α <sub>1g</sub> 688.448 eV), 0.5 eV lower than prior position and line shape in cluster vs. molecule
(SF <sub>6</sub> ) <sub>n</sub>	PB&08	180-186	T	SCF, EICVOM; orbital char, comp. to expt & Diss. Att.
F <sub>10</sub> S <sub>2</sub>	T91	160-172	T	absence of pot. barr. effects
H <sub>2</sub> S	VZ71b	155-205	P	absence of pot. barr. effects
	ZV71	160-200	P,R	absence of pot. barr. effects
	D72	160-200	P,R	absence of pot. barr. effects
	HB72	160-175	P	photoelectric yield, absolute, Rydberg analysis IP (171.1, 172.2)
	ZV72	160-210	P,R	comp. to SO <sub>2</sub> , CS <sub>2</sub> & SF <sub>6</sub> , absence of pot. barr. effects
	R75	160-175	T	alternate assignment of HB72
	S75a,b	160-175	T	Z+1 analogy calc., alternate assignment of HB72
	S76a	160-175	T	Z+1 analogy, EICVOM
	SYD82	160-175	T	ab initio, absolute, comp. to expt (HB72)
	CCM88	170-260	T	ab initio, absolute, Stieljes imag; discrete TV & OS, comp [HB72]
	NMA91	160-210	T	DV-Xa; comp. to expt. (ZV71)
	AA&92c	165-167	P	resonant autoionisation (DES); comp. of Cl <sub>2</sub> , HCl, H <sub>2</sub> S
	HS&94	160-240	P	30 meV fwhm; comp. of H <sub>2</sub> S/D <sub>2</sub> S; vibn'l struct.; val-Ryd. identified
	LB&95	160-220	T	MS-Xa; comp. of XH <sub>n</sub> (X=Si,P,S,Cl)
	SA&95a	173-180	P	ultrafast decay of LM 2e excited state detected by HS <sup>L*</sup> lines
	NN&97	164-167	P,T	ultrafast decay; time domain; 'core hole clock' (5.3 +/- 1.5 fs)
	NS&97	164-167	P	ultra-fast decay; Auger; molecular split states of HS (3s <sub>1/2</sub> -1p <sub>3/2</sub> = 90 meV)
	SA97	165	P	Auger resonant Raman; ultrafast decay to HΣ*-H); no Raman narrowing in ion fragment lines; core hole decay as femtosecond clock
	EH99	160-240	E,T	absolute; transient from H <sub>2</sub> S+B+SiO <sub>2</sub> ; comp of HBO, HBS, H <sub>3</sub> B <sub>3</sub> O <sub>3</sub>
	FCB99	50-270	E	absolute; sum rule normalized
	H00	160-250	E,R	transient ISEELS; comp of HBO,HBS, H <sub>2</sub> S
	KH&01a	170-200	P,T	spin-orbit resolved; partial cross-sections; MSXα
	HE&01	160-240	E	absolute; transient ISEELS
	HL&04	220-245	P	S 2s; TIY, threshold e-; ( threshold e-, Auger e- coincidence)
	GS&05	164-180	P	relative; TIY, PIY; ultrafast signal, +ve, -ve signals
	VM&06	162-173	P	TIY, TFY, pFY, excited H detected from Lyman & Balmer lines, ultrafast
	VM&07	162-173	P	TIY, TFY, pFY, excited H detected from Lyman & Balmer lines, ultrafast
	MM12	68-72	P,R	ultra-fast decay (HBr-Br3d; DCl, HCl-Cl2p; H <sub>2</sub> S - S2p, O <sub>2</sub> -O1s)
O <sub>2</sub> S	VZ71b	160-210	P,R	pot. barr. effects
	ZV71	160-210	P,R	pot. barr. effects
	D72	160-210	P,R	pot. barr. effects
	ZV72	160-215	P,R	pot. barr. effects
	KG&76	162-178	P	Rydberg analysis IP (174.8, 176.0)
	SMM79	164-167	T	ab initio calc., comp. to expt. (KG&76)
	KMN80a	160-210	P,T	ab initio calc., comp. to expt., pot. barr. effects
	SB&87	160-260	E	(55meV fwhm; comp to MCQD calc, PA (KG&76), S1s (BE85)
	TH&87	160-220	P	relative, no shape res. in b plot
	BS&88	163-178	E,R	ISEELS, Eo=3700eV, 0°, compare NO <sub>2</sub> SO <sub>2</sub>
	DH&89	165-185	P	negative (O <sup>-</sup> ) & positive (O <sup>+</sup> , O <sub>2</sub> <sup>+</sup> ) yields from S2p (→SO <sup>2+</sup> + O <sup>-</sup> )?
	CZ&91	150-260	E	absolute; comp. to atomic & other; ion TOF MS (e; e+ion)
	T91	160-172	T	SCF, EICVOM; orbital char, comp. to expt & Diss. Att.
	GP&98	164-176	P	realitive; 30 meV; state sym. from – FC analysis; ΔE <sub>SO</sub> = 1.20; O <sub>h</sub> =0.095eV
	FT&99	163-180	P	TIY, TPES; TPEPICO; TPE2PICO; relative cross sections; PCI; Anisotropic ion ang. distribution; fragmentation; KERD; site-specific

(SO <sub>2</sub> cont'd)	KI00	172-178	T	ab initio; spin-orbital Breit-Pauli; molecular field; comp. of SO <sub>2</sub> , COS, PF <sub>3</sub>
	KH&01b	163-167	P	angle-resolved Ion yield spectra, high res., singlet-triplet states identified
	K04	163-167	P,T	angle-resolved photoion yield, S-O; molecular field exchange splittings
	FCH05	155-245	P	PIPICO, PEPIPICO, fragmentation
S <sub>n</sub>	TGR99	154-194	P,T	n = 2-8 – sulfur aggregates; selected ion yields; PEPIPICO; fragmentation mechanisms
	TG&99	160-175	P	relative, TIY, PEPIPICO; large changes in discrete with cluster ion
(Na <sub>2</sub> SO <sub>4</sub> .10H <sub>2</sub> O) <sub>n</sub>	ABL13	170-200	P	size selected nanoparticles; aerodynamic lenses * diff. pump
(NH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub>	MG&16	166-180	P	ammonium sulfate clusters

### Sulfur 1s (2470 eV)

CCuHOS <sub>2</sub>	TV93	2.47-2.48	T	CuS <sub>2</sub> COH; ab initio-SCF-EICVOM; pre-edge res. ( $\pi^*$ , $\sigma^*_{O-O}, \sigma^*_{S-S}$ )
CF <sub>8</sub> S	LD72	2.47-2.51	P	CF <sub>3</sub> SF <sub>5</sub> ; pot. barr. Effects
	IS&05	2.46-2.49	P	PEPICO, PIPICO, site-selective fragmentation
CH <sub>2</sub> S <sub>2</sub>	TV93	2.47-2.48	T	thio-formic acid; ab initio-SCF-EICVOM; pre-edge res. ( $\pi^*, \sigma^*_{O-O}, \sigma^*_{S-S}$ )
CH <sub>4</sub> S	BE85	2.46-2.49	P	CH <sub>3</sub> SH, equivalent core model, comp. to ETS
	DTH90	2.46-2.51	P	absolute; comp. to other RSH and RSR ( $\sigma^*(S-C)$ )
	DTM91	2.46-2.49	P	comp. to ETS; $\sigma^*(S-C)$ bond length correl.
	SDT92	2.46-2.49	T	SCF-CI (geometry) calc. of pot. energy curves; comp. to [DTH90]
	TV93	2.47-2.48	T	ab in.-SCF-EICVOM; pre-edge res. ( $\pi^*, \sigma^*_{O-O}, \sigma^*_{S-S}$ ), comp to DTH90
	SHU11	2.43 – 2.49	P,T	comp. thiol & thioethers; CH <sub>3</sub> SH, C <sub>2</sub> H <sub>5</sub> SH, CH <sub>3</sub> SCH <sub>3</sub> , C <sub>4</sub> H <sub>8</sub> S, C <sub>6</sub> H <sub>5</sub> SH, C <sub>5</sub> H <sub>11</sub> NOS; GSCF3-IVO HF calculations
COS	PL84	2.46-2.49	P	comp. to emission, S2p (WB74) & calc, S1s/S2p shift=0.2-0.7eV
	NH&88	2.47-2.51	R	comp. of ETS, all edges for CO <sub>2</sub> , COS & CS <sub>2</sub> ; $\sigma^*$ loc.; hole decay
	MH&89	2.45-2.55	P,T	absolute, ab initio, comp. of CO <sub>2</sub> , COS & CS <sub>2</sub> - all edges
	BA&96	2.45-2.50	P	average charge; pre-edge ioniz. by -10 eV
	AT&96b	2.46-2.51	P	relative, angle-resolved PIY; $\beta$ s; Renner-Teller $\pi^*$ ; 10 $\sigma^*$ at 2474 eV
	AEB97a	2.45-2.51	P	partial ion yields; branching ratios; triple coinc. analysis
	EA&97	2.45-2.51	P	total and partial ion yields; average charge; triple coincidence det.
	MA&98	2.46-2.48	P,T	relative; abs. Emission comp; polarized XES; ab initio calc
	NTH99	2.45-2.50	P	TIY, PIY; PE3PICO; selective bond breaking
	HN02	2460	P,R	TPEPIPIPICO; high charge states
CS <sub>2</sub>	PL84	2.46-2.49	P	comp. to emission, S2p (WB74) & calc, S1s/S2p shift=0.2-0.7eV
	BE85	2.45-2.55	P	relative
	NB87	2.47-2.51	P,R	comp. to Cl 2p, S 2p EELS (WB74); constant term values
	NH&88	2.47-2.51	R	comp. of ETS, all edges for CO <sub>2</sub> , COS & CS <sub>2</sub> ; $\sigma^*$ loc.; hole decay
	MH&89	2.45-2.55	P,T	absolute, ab initio, comp. of CO <sub>2</sub> , COS & CS <sub>2</sub> - all edges
	FD&95	2.45-3.20	P,T	xafs; detailed MS analysis; very strong forward focussing
	BA&96	2.45-2.50	P	average charge; pre-edge ioniz. by -10 eV
	SL&96	2.50	P,R	PE3PICO; anisotropic angular dist. of ions; polarization effects
	AEB97	2.45-2.51	P	partial ion yields; branching ratios; triple coinc. analysis
	EA&97	2.45-2.51	P	total and partial ion yields; average charge; triple coincidence det.
	CB&01	2.42-2.52	P	Auger-ion coinc; site selective frag; comp. to SO <sub>2</sub>
	HN02	2.460	P,R	PEPIPIPICO; high charge states from Auger cascade
	GD&15	2.460	P,T	fragmentation; PE ang. Dist., localized core hole, Schroedinger cat
C <sub>2</sub> H <sub>3</sub> NS	DTM91	2.46-2.49	P	CH <sub>3</sub> SCN; comp. to ETS; $\sigma^*(S-C)$ bond length correl.
C <sub>2</sub> H <sub>3</sub> NS	DTM91	2.46-2.49	P	CH <sub>3</sub> SNC; comp. to ETS; $\sigma^*(S-C)$ bond length correl.
C <sub>2</sub> H <sub>6</sub> OS	TB&88	2.46-2.51	P	(CH <sub>3</sub> ) <sub>2</sub> S=O, DMSO, comp. to S2p,O1s,C1s
C <sub>2</sub> H <sub>6</sub> S	HBT89	2.46-2.51	P	(CH <sub>3</sub> ) <sub>2</sub> S, comp. to (CH <sub>3</sub> ) <sub>2</sub> S <sub>2</sub> , $\sigma^*(S-S)$
	DTH90	2.46-2.51	P	absolute; comp. to other RSH and RSR; $\sigma^*(S-C)$
	DB&98	2.46-2.49	P	relative; ioniz. yield; low-lying $\sigma^*(Si-Si)$ level; correl. with ETS

C <sub>2</sub> H <sub>6</sub> S	DTM91	2.46-2.49	P	C <sub>2</sub> H <sub>5</sub> SH; comp. to ETS; $\sigma^*(S-C)$ bond length correl.
	SHU11	2.43 – 2.49	P,T	comp. thiol & thioethers; CH <sub>3</sub> SH, C <sub>2</sub> H <sub>5</sub> SH, CH <sub>3</sub> SCH <sub>3</sub> , C <sub>4</sub> H <sub>8</sub> S, C <sub>6</sub> H <sub>5</sub> SH, C <sub>5</sub> H <sub>11</sub> NOS; GSCF3-IVO HF calculations
C <sub>2</sub> H <sub>6</sub> S <sub>2</sub>	HBT89	2.46-2.51	P	(CH <sub>3</sub> ) <sub>2</sub> S <sub>2</sub> , comp. to (CH <sub>3</sub> ) <sub>2</sub> S, $\sigma^*(S-S)$
	DTH90	2.46-2.51	P	absolute; comp. to other RSH and RSR; $\sigma^*(S-C)$
	CH&97	2.46-2.49	P	R(S-S) <sub>n</sub> -R; dependence of $\sigma^*(S-S)$ , $\sigma^*(S-C)$ on R, n
	DB&98	2.46-2.49	P	relative; ioniz. yield; low-lying $\sigma^*(Si-Si)$ level; correl. with ETS
C <sub>2</sub> H <sub>6</sub> S <sub>3</sub>	DB&98	2.46-2.49	P	Me-S <sub>3</sub> -Me; ioniz. yield; low-lying $\sigma^*(Si-Si)$ level; correl. with ETS
	SHU11	2.43 – 2.49	P,T	comp. thiol & thioethers; CH <sub>3</sub> SH, C <sub>2</sub> H <sub>5</sub> SH, CH <sub>3</sub> SCH <sub>3</sub> , C <sub>4</sub> H <sub>8</sub> S, C <sub>6</sub> H <sub>5</sub> SH, C <sub>5</sub> H <sub>11</sub> NOS; GSCF3-IVO HF calculations
<b>C<sub>4</sub>H<sub>4</sub>S</b>	H86b	2.47-2.50	P,R	(thiophene); comp. to thiolane
	HHS86	2.47-2.50	P	S2p, S2s, S1s; comp. to sol., ml; MS-Xa calc; $\sigma^*(C-S)$
	PL86	2.46-2.50	P,T	absolute, fluorescence, STO-3G calc, IP=2477.6eV
	TK&92	2.46-2.49	P	gas comp. to multi- and monolayer; pol. dep.; $\pi^*$ , $\sigma^*_{Si-C}$ components in main res. identified; supports HHS86
<b>C<sub>4</sub>H<sub>8</sub>S</b>	K02	2.46-2.49	P,TR	symmetry resolved, $\pi^*$ below $\sigma^*$ , review
	H86b	2.47-2.50	P,R	(thiolane); comp. to thiophene
	HHS86	2.47-2.50	P	S2p, S2s, S1s; $\sigma^*(C-S)$
C <sub>4</sub> H <sub>10</sub> S	DTH90	2.46-2.51	P	Et-S-Et; absolute; comp. to other RSH and RSR; $\sigma^*(S-C)$
	DTM91	2.46-2.49	P	comp. to ETS; $\sigma^*(S-C)$ bond length correl.
C <sub>5</sub> H <sub>11</sub> NOS	SHU11	2.43-2.49	P,T	comp. thiol & thioethers; CH <sub>3</sub> SH, C <sub>2</sub> H <sub>5</sub> SH, CH <sub>3</sub> SCH <sub>3</sub> , C <sub>4</sub> H <sub>8</sub> S, C <sub>6</sub> H <sub>5</sub> SH, C <sub>5</sub> H <sub>11</sub> NOS; GSCF3-IVO HF calculations
C <sub>6</sub> H <sub>4</sub> N <sub>2</sub> S	HD&91	2.46-2.51	P	BzN <sub>2</sub> S fused ring; absolute; comp. to other edges; matches S2s
C <sub>6</sub> H <sub>4</sub> N <sub>2</sub> S <sub>2</sub>	HD&91	2.46-2.51	P	BzN <sub>2</sub> S <sub>2</sub> fused ring; absolute; comp. to other edges; matches S2s
C <sub>6</sub> H <sub>4</sub> N <sub>2</sub> S <sub>3</sub>	HD&91	2.46-2.51	P	BzN <sub>2</sub> S <sub>3</sub> fused ring; absolute; comp. to other edges; matches S2s
C <sub>6</sub> H <sub>6</sub> S	DTH90	2.46-2.51	P	C <sub>6</sub> H <sub>5</sub> SH, comp. to other RSH and RSR; $\sigma^*(S-C)$
	DTM91	2.46-2.49	P	comp. to ETS; $\sigma^*(S-C)$ bond length correl.
	TY&91	2.46-2.50	P	relative; gas-solid comp.; $\sigma^*(S-C)$ less well-defined; Ryd. disappears; EXAFS stronger; no EXAFS analysis
	SHU11	2.4-2.49	P,T	comp. thiol & thioethers; CH <sub>3</sub> SH, C <sub>2</sub> H <sub>5</sub> SH, CH <sub>3</sub> SCH <sub>3</sub> , C <sub>4</sub> H <sub>8</sub> S, C <sub>6</sub> H <sub>5</sub> SH, C <sub>5</sub> H <sub>11</sub> NOS; GSCF3-IVO HF calculations
C <sub>6</sub> H <sub>14</sub> S <sub>2</sub>	CH&97	2.46-2.49	P	R(S-S) <sub>n</sub> -R, R= iPr; dependence of $\sigma^*(S-S)$ , $\sigma^*(S-C)$ on R, n
C <sub>7</sub> H <sub>8</sub> S	DTH90	2.46-2.51	P	C <sub>6</sub> H <sub>5</sub> SCH <sub>3</sub> , comp. to other RSH and RSR; $\sigma^*(S-C)$
	DTM91	2.46-2.49	P	comp. to ETS; $\sigma^*(S-C)$ bond length correl.
C <sub>8</sub> H <sub>14</sub> S <sub>2</sub>	CH&97	2.46-2.49	P	R(S-S) <sub>n</sub> -R, R=2-but enyl; dependence of $\sigma^*(S-S)$ , $\sigma^*(S-C)$ on R, n
C <sub>8</sub> H <sub>14</sub> S <sub>3</sub>	CH&97	2.46-2.49	P	R(S-S) <sub>n</sub> -R, R=2-but enyl; dependence of $\sigma^*(S-S)$ , $\sigma^*(S-C)$ on R, n
C <sub>8</sub> H <sub>18</sub> S <sub>2</sub>	CH&97	2.46-2.49	P	R(S-S) <sub>n</sub> -R, R=n-butyl; dependence of $\sigma^*(S-S)$ , $\sigma^*(S-C)$ on R, n
C <sub>8</sub> H <sub>18</sub> S <sub>3</sub>	CH&97	2.46-2.49	P	R(S-S) <sub>n</sub> -R, R=n-butyl; dependence of $\sigma^*(S-S)$ , $\sigma^*(S-C)$ on R, n
C <sub>8</sub> H <sub>18</sub> S <sub>4</sub>	CH&97	2.46-2.49	P	R(S-S) <sub>n</sub> -R, R=n-butyl; dependence of $\sigma^*(S-S)$ , $\sigma^*(S-C)$ on R, n
C <sub>8</sub> H <sub>18</sub> S <sub>2</sub>	CH&97	2.46-2.49	P	R(S-S) <sub>n</sub> -R, R=t-butyl; dependence of $\sigma^*(S-S)$ , $\sigma^*(S-C)$ on R, n
C <sub>8</sub> H <sub>18</sub> S <sub>3</sub>	CH&97	2.46-2.49	P	R(S-S) <sub>n</sub> -R, R=t-butyl; dependence of $\sigma^*(S-S)$ , $\sigma^*(S-C)$ on R, n
C <sub>8</sub> H <sub>18</sub> S <sub>4</sub>	CH&97	2.46-2.49	P	R(S-S) <sub>n</sub> -R, R=t-butyl; dependence of $\sigma^*(S-S)$ , $\sigma^*(S-C)$ on R, n
C <sub>12</sub> H <sub>10</sub> S <sub>2</sub>	CH&97	2.46-2.49	P	R(S-S) <sub>n</sub> -R, R=phenyl; dependence of $\sigma^*(S-S)$ , $\sigma^*(S-C)$ on R, n
C <sub>12</sub> H <sub>22</sub> S <sub>2</sub>	CH&97	2.46-2.49	P	R(S-S) <sub>n</sub> -R, R=Me <sub>2</sub> C=CMeCH <sub>2</sub> -; depend. of $\sigma^*(S-S)$ , $\sigma^*(S-C)$ on R, n
C <sub>12</sub> H <sub>22</sub> S <sub>3</sub>	CH&97	2.46-2.49	P	R(S-S) <sub>n</sub> -R, R=Me <sub>2</sub> C=CMeCH <sub>2</sub> -; depend. of $\sigma^*(S-S)$ , $\sigma^*(S-C)$ on R, n
C <sub>12</sub> H <sub>22</sub> S <sub>4</sub>	CH&97	2.46-2.49	P	R(S-S) <sub>n</sub> -R, R=Me <sub>2</sub> C=CMeCH <sub>2</sub> -; depend. of $\sigma^*(S-S)$ , $\sigma^*(S-C)$ on R, n
C <sub>14</sub> H <sub>14</sub> S <sub>2</sub>	CH&97	2.46-2.49	P	R(S-S) <sub>n</sub> -R, R=C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> -; dependence of $\sigma^*(S-S)$ , $\sigma^*(S-C)$ on R, n
ClFO <sub>2</sub> S	HBT89	2.46-2.51	P	ionization yield, comp of SO <sub>2</sub> Cl <sub>2</sub> , SO <sub>2</sub> FCI & SO <sub>2</sub> F <sub>2</sub>
	HT88	2.46-2.56	P	ionization yield, comp to SO <sub>2</sub> Cl <sub>2</sub> , SO <sub>2</sub> FCI

ClF <sub>5</sub> S	RB&92	2.4-3.1	P,T	relative; comp. to SF <sub>6</sub> & SCF-CI calc; EXAFS no S 3d participation
	BR&92	2.4-2.8	P	double core vacancy state (1s,2p); comp. of SF <sub>5</sub> Cl, SF <sub>6</sub>
	NM96	2.4-2.8	P,R	EXAFS; KL double excitation; compared to SF <sub>6</sub>
Cl <sub>2</sub> OS	HBT87	2.46-2.51	P	comp. to other S,Cl,O compounds, $\sigma^*(S-X)$
Cl <sub>2</sub> O <sub>2</sub> S	HBT87	2.46-2.51	P	comp. to other S,Cl,O compounds, $\sigma^*(S-X)$
	HT88	2.46-2.56	P	ionization yield, comp to SO <sub>2</sub> Cl <sub>2</sub> , SO <sub>2</sub> FCI
	HBT89	2.46-2.51	P	ionization yield, comp of SO <sub>2</sub> Cl <sub>2</sub> , SO <sub>2</sub> FCI & SO <sub>2</sub> F <sub>2</sub>
Cl <sub>2</sub> S	CH86	2.46-2.77	P	relative, $\sigma^*(C-S)$ , EXAFS
	HKR86	2.46-2.75	P	EXAFS, xanes
	HBT87	2.46-2.51	P	comp. to other S,Cl,O compounds, $\sigma^*(S-X)$
	HT88	2.46-2.56	P	ionization yield, comp to SO <sub>2</sub> Cl <sub>2</sub> , SO <sub>2</sub> FCI
Cl <sub>2</sub> S <sub>2</sub>	HBT87	2.46-2.51	P	comp. to other S,Cl,O compounds, $\sigma^*(S-X)$
D <sub>2</sub> S	HA&98c	2.46-2.49	P	relative; PIT, TIY; photofragmentation asymmetry
	DA&98c	2.46-2.49	P	TIY, PIY, neutral D observed; $\beta$ for fragmentation
F <sub>2</sub> OS	LD72	2.47-2.50	P	SF <sub>2</sub> O; pot. barr. effects
	T91	2.46-2.48	T	SCF, EICVOM; orbital char, comp. to expt & Diss. Att.
	BHK92	2.46-2.48	P,T	DSCF, comp of all edges; spectrum from BH87 (err. report as SF <sub>4</sub> )
F <sub>2</sub> O <sub>2</sub> S	LD72	2.47-2.50	P	SF <sub>2</sub> O <sub>2</sub> ; pot. barr. effects
	BK74	2.48-2.50	P	pot. barr. effects
	HBT89	2.46-2.51	P	ionization yield, comp of SO <sub>2</sub> Cl <sub>2</sub> , SO <sub>2</sub> FCI & SO <sub>2</sub> F <sub>2</sub>
	HT88	2.46-2.56	P	ionization yield, comp to SO <sub>2</sub> Cl <sub>2</sub> , SO <sub>2</sub> FCI
	HBT89	2.46-2.51	P	ionization yield, comp of SO <sub>2</sub> Cl <sub>2</sub> , SO <sub>2</sub> FCI & SO <sub>2</sub> F <sub>2</sub>
F <sub>3</sub> PS	NTH99	2.45-2.50	P	TIY, PIY; PE3PICO; selective bond breaking
	T91	2.46-2.48	T	SCF, EICVOM; orbital char, comp. to expt & diss. att.
F <sub>4</sub> S	BH87	2.48-2.50	P	SF <sub>4</sub> ; pot. barr. effects
	KBH90	2.48-2.50	T	ab initio, comp. to SF <sub>6</sub> & expt. (BH87), revised $\sigma^*(S-F)$ assignments
	BHK92	2.48-2.54	P,T	revised S1s spectrum (correction to BH87); DSCF, comp. of all edges
	T91	2.46-2.48	T	SCF, EICVOM; orbital char, comp. to expt & Diss. Att.
	BHK92	2.46-2.50	P,T	DSCF, update of BH87; correct S1s spectrum; comp of all edges
F <sub>4</sub> OS	T91	2.46-2.48	T	SCF, EICVOM; orbital char, comp. to expt & Diss. Att.
F <sub>6</sub> S	BM62	2.48-2.50	P	pot. barr. effects, $\sigma^*(S-F)$
	LD66	2.47-2.90	P	pot. barr. effects, absolute, EXAFS
	D72	2.47-2.90	P,R	pot. barr. effects
	F72	2.48-2.55	T	pot. barr. effects, review
	GGL72	2.48-2.52	T	ab initio calc., pot. barr. effects
	BK73	2.49-2.51	P	Rydberg structure claimed
	BK74	2.48-2.50	P	pot. barr. effects
	B76b	2.48-2.78	E	extended fine structure (EXAFS)
	BH86	2.48-2.52	P	comp. to SF <sub>4</sub> , $\sigma^*(S-F)$
	FL&86	2.47-2.58	P	Auger & AI yields, cont. res. not all shape
	THH87	2.47-2.52	P,T	XANES, EXAFS, multiple scattering analysis
	QL89	2.46-2.52	E,P	enhanced X-ray emission of SF <sub>6</sub> vs. H <sub>2</sub> S & SO <sub>2</sub> at discrete a <sub>1g</sub> peak
	TB&89	2.47-3.20	P,T	XANES, EXAFS, MS-calc; correction for inelastic scatt. of PE
	KBH90	2.48-2.50	T	ab initio, comp. to SF <sub>4</sub> (BH87)
	NMA90	2.47-2.58	T	MSXa calc; order of res. identified; comp. to expt. (ZV71)
	NMA91	2.47-2.49	T	absolute; DVXa calc; comp. to expt. (L75, BE85)
	T91	2.46-2.48	T	SCF, EICVOM; orbital char, comp. to expt & Diss. Att.
	BR&92	2.4-2.8	P	double core vacancy state (1s,2p); comp. of SF <sub>5</sub> Cl, SF <sub>6</sub>
	RB&92	2.45-2.80	P,T	1-e- & 2-e- excitation; ab initio calc; comp. of SF <sub>6</sub> & SF <sub>5</sub> Cl; symmetry breaking; 3d Ryd & 3d val. orb. differ.; EXAFS ( $k_{\max}=13\text{\AA}^{-1}$ )
	TH&92a	2.8-3.8	T,P	MS calc of EXAFS ampl. reduction factor; comp. of Br <sub>2</sub> , GeCl <sub>4</sub> , SF <sub>6</sub>
	BR&95	2.48-2.55	P	laser generated (3ps) continuum; laser photodissociation

(SF <sub>6</sub> cont'd)	RW&95	2.45-2.58	P	500 fs pump-probe; bleaching of t <sub>1u</sub> resonance in first 10 ps; fast diss.
	NM96	2.4-2.8	P,R	EXAFS; KL double excitation; compared to SF <sub>5</sub> Cl
	RG&96a	2.67-2.69	P,T	KL 2- exc.; CAS-MCSCF calc; (Z+2) interp.; comp. of H <sub>2</sub> S, SO <sub>2</sub> , SF <sub>6</sub>
	RG&96b	2.4-2.8	P,T	absolute; KL 2- exc.; CAS-MCSCF calc; (Z+2) interpretation
	RW&96	2.45-2.58	P, R	ps-res. spectra; bleach by terawatt lasers; <b>summary of sub-ns XAS</b>
	NL99	2.50-2.63	T	$\sigma$ resonances in ionization continuum; l = 9 at 2550 eV
F <sub>10</sub> S <sub>2</sub>	T91	2.46-2.48	T	SCF, EICVOM; orbital char, comp. to expt & Diss. Att.
H <sub>2</sub> S	LD66	2.47-2.50	P	absolute
	M71	2.47-2.52	P	photographic
	MS71	2.47-2.52	P	MO interpretation
	MS&73	2.47-2.52	T	semiempirical calc.
	L75a	2.46-2.49	P	Rydberg structure
	SYD82	2.46-2.50	T	ab initio, absolute, comp. to expt (L75a)
	BE85	2.46-2.52	P	equivalent core analogy, comp. to ETS res.
	CH86	2.46-2.50	P	relative, double excitation
	D86b	2.47-2.49	P	comp. of emission & absorption [L75a]; multivacancy effects
	ML&91	2.47-2.48	P	absorp. and polarised fluorescence; determ. of MO symmetry
	NMA91	2.47-2.48	T	DV-Xa; comp. to expt. (ZV71)
	BR&92	2.4-2.8	P,T	MC-SCF calc; improved singlet-triplet; double core vacancy states
	ML&94	2.473	P	ion yields at 3b <sub>2</sub> resonance
	AHB96	1-15	P	triple coinc. (Auger,ion,ion) PEPICO; triple ioniz.
	AT&96a	2.46-1.51	P	relative; TIY; angle resolved; 3b <sub>2</sub> /6a <sub>2</sub> $\Delta E \sim 0.15$ eV; weak anisotropy
	NM96	2.66-2.72	P,R	KL double excitation; Rydbergs; 1.5% contribution
	RG&96a	2.67-2.69	P,T	KL 2- exc.; CAS-MCSCF calc; (Z+2) interp.; comp. of H <sub>2</sub> S, SO <sub>2</sub> , SF <sub>6</sub>
	RG&96b	2.4-2.8	P,T	absolute; KL 2- exc.; CAS-MCSCF calc; (Z+2) interpretation
	DA&98c	2.46-2.49	P	TIY, PIY, neutral D observed; $\beta$ for fragmentation
	HA&98c	2.46-2.49	P	relative; PIT, TIY; photofragmentation asymmetry
H <sub>2</sub> S <sub>2</sub>	TV93	2.47-2.48	T	ab initio-SCF-EICVOM; pre-edge res. ( $\pi^*$ , $\sigma^*_{O-O}, \sigma^*_{S-S}$ )
O <sub>2</sub> S	BM62	2.48-2.50	P	atomic charge analysis
	MB&72	2.47-2.49	P	pre-thresh. structure
	MS&73	2.47-2.49	T	semiempirical calc.
	KMN80a	2.47-2.49	T	ab initio calc., comp. to expt., pot. barr. effects
	ME&84	2.46-2.49	P	comp. free & 12% SO <sub>2</sub> in p-hydroquinone clathrate, sharper peaks, Z+1 analysis, comp. to ETS
	BE85	2.46-2.52	P	equivalent core analogy, comp. to ETS res.
	BS&88	163-178	P,T,R	BE85; Eo=3700eV, 0°, compare NO <sub>2</sub> SO <sub>2</sub> MQDT calculation
	NB87	2.46-2.52	P,R	review, equivalent core analogy
	HT88	2.46-2.56	P	ionization yield, confirmed identical to absorption
	T91	2.46-2.48	T	SCF, EICVOM; orbital char, comp. to expt & diss. Attachment
	SR&95	2.45-2.50	P	107 ppm in He; in-situ E-chem. cell; surf. studies (S/Cu re tarnishing); 0.8 eV fwhm; $\pi^*$ narrower than BE85; 0.54 eV est. resol.; G = 0.59 eV
	RG&96a	2.67-2.69	P,T	KL 2- exc.; CAS-MCSCF calc; (Z+2) interp.; comp. of H <sub>2</sub> S, SO <sub>2</sub> , SF <sub>6</sub>
	RG&96b	2.4-2.8	P,T	absolute; KL 2- exc.; CAS-MCSCF calc; (Z+2) interpretation
	AT&98	2.47-2.49	P,T	relative, TIY; KERD; angle resolved; state sym; GSCF3
	CB&01	2.42-2.52	P	Auger-ion coinc; site selective frag; comp. to CS <sub>2</sub>
	K02	2.46-2.49	P,T,R	symmetry resolved, Renner-Teller; GSCF3; review
S <sub>2</sub>	DO&96	2.46-2.50	P	relative; comp. of gas, sol. polymer - S <sub>8</sub> vs. S <sub>n</sub> <sup>-</sup> chain; comp. to O <sub>2</sub> ( <sup>3</sup> S <sub>g</sub> <sup>-</sup> g.s.); bond-length correlation

### Tellurium 4d (40 eV)

Te <sub>2</sub>	STZ73	37-130	P	photographic
TeF <sub>4</sub>	BST80	40-55	P,T	relative, Z+1 analogy used to predict valence spectrum of IF <sub>4</sub>
TeF <sub>6</sub>	SB90	40-90	E	comp of TeF <sub>6</sub> , SeF <sub>6</sub> , SF <sub>6</sub> ; Z-dependence of pot. barr.s
	PV&86	40-90	T	shape res.
	PV90	40-90	T	quasi-atomic treatment

### Tellurium 4s, 4p (120, 172 eV)

TeF <sub>6</sub>	SB90	100-190	E	comp of TeF <sub>6</sub> , SeF <sub>6</sub> , SF <sub>6</sub> ; Z-dependence of pot. barr.s
------------------	------	---------	---	---

### Tellurium 3d (600 eV)

TeF <sub>6</sub>	SB90	580-680	E	comp of TeF <sub>6</sub> , SeF <sub>6</sub> , SF <sub>6</sub> ; Z-dependence of pot. barr.s
------------------	------	---------	---	---

### Tellurium 3p (830 eV)

TeF <sub>6</sub>	SB90	810-870	E	comp of TeF <sub>6</sub> , SeF <sub>6</sub> , SF <sub>6</sub> ; Z-dependence of pot. barr.s
------------------	------	---------	---	---

### Thorium 5d (110 eV)

ThF <sub>4</sub>	CP&80	70-150	P	photographic, broad res., comp. to Th (solid)
	CM&91	70-150	P,R	laser-plasma; comp. to Th(sol) and Th(vap)

### Tin 4d (25 eV)

C <sub>4</sub> H <sub>12</sub> Sn	SN&86	21-41	P	Sn(CH <sub>3</sub> ) <sub>4</sub> ; threshold e-;
	NSK88	28-41	P	thresh. e-, ionic frag. yields, comp. of M(Me) <sub>4</sub> M=Ge,Sn,Pb
	NS&90	28-41	P	ZEKE, PI yield, BR, comp. of M(Me) <sub>x</sub> frag. (Bi, Ga, Zn, Ge, Sn, Pb)

### Tin 4p,4s (85,135)

C <sub>4</sub> H <sub>12</sub> Sn	US&90b	60-260	P	partial ion yields, PIPICO
-----------------------------------	--------	--------	---	----------------------------

### Tin 3d (510 eV)

C <sub>4</sub> H <sub>12</sub> Sn	US&89a	400-600	P	tot. & part. IY; enhanced Si-C breakage; mult. ionis.; cascade
	US&90a	400-600	P	total & partial IY; enhanced Si-C breakage; mult. ionis.; cascade

### Tin 2p (3900, 4180 eV)

Cl <sub>4</sub> Sn	GDT97	3.90-4.30	P,T	relative; TIY, MS-Xa; pot. barr.; AsCl <sub>3</sub> , PCl <sub>3</sub> , GeCl <sub>4</sub> , SnCl <sub>4</sub> comp.; σ*(X-Cl) bond length correlation
--------------------	-------	-----------	-----	--

### Titanium 2p (460 eV)

Br <sub>4</sub> Ti	DF&94	450-470	T	ab initio CI; relaxed hole; comp. of TiX <sub>4</sub> , X=F,Cl,Br
C <sub>5</sub> Cl <sub>3</sub> H <sub>5</sub> Ti	W92	450-490	E,T	CpTiCl <sub>3</sub> ; comnp. to TiCl <sub>4</sub> ; EHMO
	WH93	450-490	E,T	abs.; comp. of Cp <sub>x</sub> TiCl <sub>4-x</sub> , x=0-2; diff '10Dq' at each edge
C <sub>10</sub> Cl <sub>2</sub> H <sub>10</sub> Ti	WH93	450-490	E	Cp <sub>2</sub> TiCl <sub>2</sub> ; abs.; comp. of Cp <sub>x</sub> TiCl <sub>4-x</sub> , x=0-2; diff '10Dq' at each edge

<b>Cl<sub>4</sub>Ti</b>	W92 WH93 DF&94	450-490 450-490 450-470	E,T E,T T	TiCl <sub>4</sub> ; absolute; EHMO; comp. to at.mult.-ligand field calc. abs.; comp. of Cp <sub>x</sub> TiCl <sub>4-x</sub> , x=0-2; diff '10Dq' at each edge ab initio CI; relaxed hole; comp. of TiX <sub>4</sub> , X=F,Cl,Br; comp. to WH93; $t_2 < e$ ; strong CI mixing
F <sub>4</sub> Ti	HT&00 DF&94	450-470 450-470	P T	resonant X-ray emission; comp to WH93; high P – absorption saturated ? ab initio CI; relaxed hole; comp. of TiX <sub>4</sub> , X=F,Cl,Br
Ti <sub>2</sub> <sup>+</sup>	MG&16	448-472	P	Ti <sub>n</sub> <sup>+</sup> , n=1-5,7,10; atoomic ion to solid comparison, selected ion NEXAFS
Ti <sub>3</sub> <sup>+</sup>	MG&16	448-472	P	Ti <sub>n</sub> <sup>+</sup> , n=1-5,7,10; atoomic ion to solid comparison, selected ion NEXAFS
Ti <sub>4</sub> <sup>+</sup>	MG&16	448-472	P	Ti <sub>n</sub> <sup>+</sup> , n=1-5,7,10; atoomic ion to solid comparison, selected ion NEXAFS
Ti <sub>5</sub> <sup>+</sup>	MG&16	448-472	P	Ti <sub>n</sub> <sup>+</sup> , n=1-5,7,10; atoomic ion to solid comparison, selected ion NEXAFS
Ti <sub>7</sub> <sup>+</sup>	MG&16	448-472	P	Ti <sub>n</sub> <sup>+</sup> , n=1-5,7,10; atoomic ion to solid comparison, selected ion NEXAFS
Ti <sub>10</sub> <sup>+</sup>	MG&16	448-472	P	Ti <sub>n</sub> <sup>+</sup> , n=1-5,7,10; atoomic ion to solid comparison, selected ion NEXAFS

### Titanium 1s (4966 eV)

Br <sub>4</sub> Ti	DF&94	4.96-4.98	T	ab initio CI; relaxed hole; comp. of TiX <sub>4</sub> , X=F,Cl,Br; strong 3d res.
Cl <sub>4</sub> Ti	KH90	4.96-5.00	P	relative
	DF&94	4.96-4.98	T	ab initio CI; relaxed hole; TiX <sub>4</sub> , X=F,Cl,Br; strong 3d res.; comp. to KH90
F <sub>4</sub> Ti	DF&94	4.96-4.98	T	ab initio CI; relaxed hole; comp. of TiX <sub>4</sub> , X=F,Cl,Br; strong 3d res.

### Uranium 5d (120 eV)

UF <sub>4</sub>	CM&80	70-145	P	photographic, comp. to U solid, shape res. -cont.? (see PC83)
-----------------	-------	--------	---	---

### Uranium 4d (3560 eV)

UCl <sub>4</sub>	GE&89	3.53-3.62	P,T	absolute, comp. to UO <sub>2</sub> (calc.); MS-calc. of res.
------------------	-------	-----------	-----	--

### Uranium 4p (4304 eV)

UCl <sub>4</sub>	GE&89	4.28-4.37	P,T	absolute, comp. to UO <sub>2</sub> (calc.); MS-calc. of res.
------------------	-------	-----------	-----	--

### Vanadium 2p,2s (520,630 eV)

C <sub>6</sub> O <sub>6</sub> V	TD&92a	500-660	P,E	V(CO) <sub>6</sub> , absolute
Cl <sub>3</sub> OV	DF&94	510-530	T	ab initio CI; relaxed orb.; MO <sub>x</sub> X <sub>y</sub> (Ti,V,Cr,Mn); more coval. as Cl $\div$ F
F <sub>3</sub> OV	DF&94	510-530	T	ab initio CI; relaxed orb.; MO <sub>x</sub> X <sub>y</sub> (Ti,V,Cr,Mn); more coval. as Cl $\div$ F

### Vanadium 1s (5465 eV)

Cl <sub>3</sub> OV	DF&94	5.46-5.48	T	ab initio CI; relaxed orb.; MO <sub>x</sub> X <sub>y</sub> (Ti,V,Cr,Mn); more coval. as Cl $\div$ F
F <sub>3</sub> OV	DF&94	5.46-5.48	T	ab initio CI; relaxed orb.; MO <sub>x</sub> X <sub>y</sub> (Ti,V,Cr,Mn); more coval. as Cl $\div$ F

### Xenon 4d, 4p (65, 145 eV)

XeC <sub>60</sub>	PN93	60-140	P	absolute; comp. of atom and Xe in C <sub>60</sub> cage; EXAFS
XeF <sub>2</sub>	CH&73	50-160	P	absolute, gas-solid comp., ligand field core level splitting
	S74	66-73	P,R	review, ligand field core level splitting
	T88	60-130	T	X-a; val. partials at Xe 4d; effect of R(Xe-F) on cont. res.
XeF <sub>4</sub>	CH&73	50-160	P	absolute, gas-solid comp., ligand field core level splitting
XeF <sub>6</sub>	NHS74	50-170	P	absolute, evidence for octahedral symmetry

Zinc 3d (14 eV)

C<sub>2</sub>H<sub>6</sub>Zn            NS&90    13-18        P        Zn(Me)<sub>2</sub>; threshold e-; ion yield and BR; comp. of MMe<sub>x</sub>  
(M=Bi,Ge,Pb,Sn,Zn)

---

## REFERENCES

---

**ref. codes      year of publication (ONLY last 2 digits!!! (earliest is 31 = 1931 !!) preceeded by:  
initials of all authors (if <3) or initials of first two then &  
if code is not unique, small a,b,c, .. distinguishes different references**

---

- A80** V.N. Akimov, Dissertation. Leningrad, 1980. ( $\text{H}_2\text{O}$  - O1s,  $\text{NH}_3$  - N1s,  $\text{CH}_4$  - C1s)
- A96** M.Ya. Amusia, "Theory of Photoionization" in VUV and Soft X-ray Photoionization, U. Becker, D.A. Shirley, eds. (Plenum, NY, 1996) 1. (Ar1s, Mn3p, Xe4d)
- A95** H. Aksela, J. Electron Spectrosc. 72 (1995) 235. (Kr3d,Xe4d)
- AA84** H. Agren and R. Arneberg, Physica Scripta 30 (1984) 55. (CO-C1s,O1s)
- AA&80** G.B. Armer, T. Aberg, J.C. Levin, B. Craseman, M.H. Chen, G.E. Ice and G.S. Brown, Phys. Rev. Lett. 54 (1980) 1142. (Xe2p)
- AA&82** R. Arneberg, H. Agren, J. Muller and R. Manne, Chem. Phys. Lett. 91 (1982) 362. (N<sub>2</sub>-N1s)
- AA&84** R. Arneberg, H. Agren, J. Muller and R. Manne, Chem. Phys. 83 (1984) 53. (N<sub>2</sub>-N1s)
- AA&85** G.B. Armen, J. Aberg, J.C. Levin, B. Craseman, M.H. Chen, G.E. Ice and G.S. Brown, Phys. Rev. Lett 54 (1985) 1142.
- AA&86a** H. Aksela, S. Aksela, G.M. Bancroft, K.H. Tan and H. Pulkkinen, Phys. Rev A 33 (1986) 3867. (Xe4d)
- AA&86b** H. Aksela, S. Aksela, G.M. Bancroft, H. Pulkkinen and K.H. Tan Phys. Rev A 33 (1986) 3876. (Kr3d)
- AA&87** S. Aksela, H. Aksela, M. Levasalmis, K.H. Tan and G.M. Bancroft, Phys. Rev A 36 (1987) 3449. (Kr3d)
- AA&88** H. Aksela, S. Aksela, H. Pulkkinen, G.M. Bancroft and K.H. Tan, Phys. Rev A 37 (1988) 1798. (Ar2p)
- AA&89a** H. Aksela, S. Aksela, J. Tulkki, T. Aberg, G.M. Bancroft and K.H. Tan, Phys. Rev A 39 (1989) 3401. (Ne1s)
- AA&89b** H. Aksela, S. Aksela, H. Pulkkinen and A. Yagashita, Phys. Rev A 40 (1989) 6275. (Kr3d)
- AA&90a** H. Aksela, S. Aksela, H. Pulkkinen and O.P. Sairanen Phys. Rev A 41 (1990) 425. (Ar2p,Kr3d,Ne1s,Xe4d)
- AA&90b** H. Aksela, S. Aksela, O.P. Sairanen, M. Hotokka, G.M. Bancroft, K.H. Tan and J. Tulkki, Phys. Rev A 41 (1990) 6000. (HCl-Cl2p)
- AA&92a** H. Aksela, S. Aksela, M. Hotokka, A. Yagashita and E. Shigemasa, J. Phys. B 25 (1992) 3357 (HCl-Cl2p)
- AA&92b** H. Aksela, S. Aksela, A. Montybentta, J. Tulkki, E. Shigemasa, A. Yagashita and Y. Furusawa, Phys. Scripta T 41 (1992) 113 (Ar2p, Kr3d)
- AA&92c** H. Aksela, S. Aksela, O.P. Sairanen, A. Kivimaki, G.M. Bancroft and K.H. Tan, Phys. Scripta T 41 (1992) 122 (Cl<sub>2</sub>,HCl-Cl2p; H<sub>2</sub>S-S2p)

- AA&94** H. Aksela, A. Ausmees, O.P. Siaranen, S.J. Osborne, A. Naves de Brito, A. Kivimaki, J. Jauhainen, S. Svensson and S. Aksela, Phys. Rev. Lett. 73 (1994) 2031. (Xe4d)
- AA&01** P. Andersen, T. Andersen, F. Folkmann, V.K. Ivanov, H. Kjeldsen and J.B. West, J. Phys. B 34 (2001) 2009. (Xe4d)
- AB97** J.W. Au and C.E. Brion, Chem. Phys. 218 (1997) 87. (PCl<sub>3</sub> - P2p, Cl2p)
- AB98** U. Alkemper and F. Von Busch, J. Electron Spectrosc. 93 (1998) 115. (CS<sub>2</sub> - S2p)
- ABC75** M. Y. Amusia, N.B. Berezina and L.V. Chernysheva, Phys. Lett. A 51 (1975) 101. (Xe4d)
- ABL13** Antonsson E, Bresch H, Lewinski RFree nanoparticles studied by soft X-rays. Chem Phys Lett 559 (2013) 1–11, (Na<sub>2</sub>SO<sub>4</sub>.10H<sub>2</sub>O)<sub>n</sub> – S2p, O1s; (SiO<sub>2</sub>)<sub>n</sub> – Si2p)
- ABZ96** M.Y. Amusia, A.S. Baltenkov and G.I. Zhuravleva, J. Phys. B 29 (1996) L151. (Ar1s, K1s)
- AB&95** L. Avaldi, P. Belotti, P. Bolognesi, R. Camilloni and G. Stefani, Phys. Rev. Lett. 75 (1995) 1915. (Xe4d)
- AB&96** L. Avaldi, P. Bolognesi, R. Camilloni, E. Fainelli, R.A. Muttari and G. Stefani, Phys. Rev. A 54 (1996) 2930. (Xe4d)
- ACB97** J.W. Au, G. Cooper and C.E. Brion, Chem. Phys. 215 (1997) 397. (PF<sub>3</sub> - P2p)
- ACS90** L. Avaldi, R. Camilloni and G. Stefani, Phys. Rev. A 41 (1990) 134. (C<sub>2</sub>H<sub>2</sub>-C1s)
- AC&76** M.Y. Amusia, N.A. Cherepkov, D. Zivanovic and V. Radojevic, Phys. Rev. A 13 (1976) 1466. (Li1s)
- AC&90** M.Ya Amusia, L.V. Chernyshevo, G.F. Gribakin and K.L. Tsemekhman, J. Phys. B 23 (1990) 393 (Xe4d, Ba4d)
- AC&93** P. d'Angelo, A. di Cicco, A. Filippini and N.V. Pavel, Phys. Rev. A 47 (1993) 2055. (HBr,Br<sub>2</sub> - Br1s)
- AC&94** H. Agren, V. Caravetta, O. Vahtras and L.G.M. Pettersson, Chem. Phys. Lett. 222 (1994) 75. (HCN, CH<sub>3</sub>(CH<sub>2</sub>)<sub>n</sub>CN, n=0,1,2,5,10)
- AC&95** H. Agren, V. Caravetta, O. Vahtras and L.G.M. Pettersson, Phys. Rev B 51 (1995) 17,848. (C<sub>n</sub>F<sub>2n+2</sub>, n=2,4,6,8,10 - C1s, F1s)
- AC&00a** M.Ya. Amusia, N.A. Cherepkov, L.V. Chernysheva and S.T. Manson, J. Phys. B 33 (2000) L37. (Xe4d)
- AC&00b** M.Ya. Amusia, N.A. Cherepkov, L.V. Chernysheva and S.T. Manson, Phys. Rev. A 61 (2000) 020701. (I4d)
- AC&00c** R. D'Arcy, J.T. Costello, E.T. Kennedy, G. McGuiness, J.P. Mosnier and G. O'Sullivan, J. Phys. B 33 (2000) 1383. (Sb4d)
- AC&01** M. Alagia, M. Coreno, M. de Simone, R. Richter and S. Stranges, J. El. Spec. 114-116 (2001) 85. (O1s; O<sub>2</sub> – O1s)
- AC&02** M.Ya. Amusia, L.V. Chernysheva, V.K. Ivanov and S.T. Manson, Phys. Rev. A 65 (2002) 032714. (I4d)

- ADB97** U. Alkemper, J. Doppelfield and F. von Busch, Phys. Rev. A 56 (1997) 2741. (Ar1s)
- ADI83** Y.A. Amusia, V.K. Dolmatov and V.K. Ivanov, Sov. Phys. JETP 58 (1983) 67 (Cr3p)
- ADM90** M.Y. Amusia, V.K. Dolmatov and M.M. Mansurov, J. Phys. B 23 (1990) L491. (Mn3p)
- AD&94** L. Avaldi, G. Dawben, R. Camilloni, G.C. King, M. Roper, M.R.F. Siggel, G. Stefani and M. Zitnik, J. Phys. B 27 (1994) 3953. (Ar2p)
- AD&99** D.P. Almeida, G. Dawber, G.C. King and B. Palasthy, J. Phys. B 32 (1999) 3157. (CO – C1s)
- AD&01** D.P. Almeida, G. Dawber, S.E. Michelin and G.C. King, Chem. Phys. 269 (2001) 159. (N<sub>2</sub> – N1s)
- AEB97a** U. Ankerhold, B. Esser and F. von Busch, J. Phys. B 30 (1997) 1207. (CS<sub>2</sub>, COS - S1s)
- AEB97b** U. Ankerhold, B. Esser and F. von Busch, Chem. Phys. 220 (1997) 393. (Ar2p; CS<sub>2</sub>, COS - S2p)
- AF&92** U. Arp, F. Federnam, E. Kallne, B. Sonntag and S.L. Sorensen, J. Phys. B 25 (1992) 3747 (Mn2p)
- AG&69** V.C. Afrosimov, Yu.S. Gordeev, Y.M. Lavrov and S.G. Schelinin, Sov. Phys. JETP 28 (1969) 821. [Zh. Eksp. Teor. Fiz. 55 (1968) 1569]. (Ar2p, Kr3d, Xe4d)
- AG&23** Olesya S. Ablyasova, Meiyuan Guo, et al., Electronic Structure of the Complete Series of Gas-Phase Manganese Acetylacetones by X-ray Absorption Spectroscopy, J. Phys. Chem. A 127 (2023) 7121. Mn(C<sub>5</sub>H<sub>8</sub>O<sub>2</sub>)<sup>+</sup><sub>m</sub>, m=1,2,3 - C1s, O1s, Mn2p)
- AHB96** U. Alkemper, R. Hornig and F. von Busch, J. Phys. B 29 (1996) 35. (CS<sub>2</sub>-S1s)
- AHG93** E. Apen, A.P. Hitchcock and J.L. Gland, J. Phys. Chem. 97 (1993) 6859. (C<sub>3</sub>H<sub>3</sub>N<sub>2</sub>, C<sub>3</sub>H<sub>3</sub>N<sub>3</sub>, C<sub>5</sub>HN<sub>4</sub> - C1s, N1s)
- AH&91** L. Avaldi, R.I. Hall, G. Dawber, P.M. Rutler and G.C. King, J. Phys. B 24 (1991) 427. (Kr3d, Xe4d)
- AH&99** A. Ausmees, A. Hahlin, S.L. Sorensen, S. Sundin, I. Hjelte, O. Bjorneholm and S. Svensson, J. Phys. B 32 (1999) L197. (Xe4d)
- AH&04** J. Adachi, K. Hosaka, S. Furuya, K. Soejima, M. Takahashi, A. Yagishita, S.K. Semenov, N.A. Cherepkov, J. El. Spec. Rel. Phen. 137-140 (2004) 243. (CO-C1s)
- AH&07** J. Adach, K. Hosaka, T. Teramoto, M. Yamazaki, N. Watanabe, M. Takahashi and A. Yagishita, J. Phys. B. 40 (2007) F285. (C<sub>2</sub>H<sub>2</sub> – C1s)
- AI78** M.Y. Amusia and V.K. Ivanov, Phys. Lett. A 65 (1978) 217. (Xe3d,4d)
- AIC81** M.Y. Amusia, V.K. Ivanov and L.V. Chernysheva, J. Phys. B 14 (1981) L19. (Mn3p)
- AIK81** M.Y. Amusia, V.K. Ivanov and V.A. Kupchenko, J. Phys. B 14 (1981) L667. (Ar1s)
- AI&94** U. Arp, K. Iemura, G. Kutlick, M. Meyer, T. Nagata, M. Sacchi, B. Sonntag, S. Yagi and A. Yagashita, J. Phys. B 27 (1994) 3389. (Cu2p)

- AI&95** U. Arp, K. Iemura, G. Kutlick, T. Nagata, S. Yagi and A. Yagashita, J. Phys. B 28 (1995) 225. (Cr2p)
- AI&99** U. Arp, K. Iemura, G. Kutluk, T. Nagata, S. Yagi and A. Yagashita, J. Phys. B 32 (1999) 1295. (Xe3d, Cs3d, Ba3d)
- AKK88** Z. Altun, M. Kutzner and H.P. Kelly, Phys. Rev A 37 (1988) 4671. (Xe4d)
- AK&94** S. Aksela, A. Kivimaki, A. Naves de Brito, O.-P. Sairanen, S. Svensson and J. Vayrynen, Rev. Sci. Inst. 65 (1994) 831. (Ar2p, Kr3d)
- AK&95a** J.I. Adachi, N. Kosugi, E. Shigemasa and A. Yagashita, J. Chem. Phys. 102 (1995) 7369. (N<sub>2</sub>O-N1s,O1s)
- AK&95b** I. Arcon, A. Kadre, M. Stuhec, D. Glavic-Cindro and W. Drube, Phys. Rev. A 51 (1995) 147. (Xe2p)
- AK&95c** S. Aksela, A. Kivimaki, O.P. Sairanen, A. Naves de Brito, E. Nommiste and S. Svensson, Rev. Sci. Inst. 66 (1995) 1621. (Kr3d, Ar2p, N<sub>2</sub>-N1s)
- AK&96a** J. Adachi, N. Kosugi, E. Shigemasa and A. Yagashita, J. Phys. Chem. 100 (1996) 19783. (CO<sub>2</sub> - C1s)
- AK&96b** J. Adachi, N. Kosugi, et al., , J. Electron Spectrosc. 79 (1996) 491. (N<sub>2</sub>O - N1s)
- AK&97a** J. Adachi, N. Kosugi, E. Shigemasa and A. Yagashita, J. Chem. Phys. 107 (1997) 4919. (CO<sub>2</sub>, COS, CS<sub>2</sub> - C1s)
- AK&97b** H. Aksela, M. Kivilompolo, E. Nommiste and S. Aksela, Phys. Rev. Lett. 79 (1997) 4970. (Kr3d, Xe4d)
- AK&12** J.-I Adachi, M. Kazama, T. Teramoto, N. Miyauchi, T. Mizuno, M. Yamazaki, T. Fujikawaand A.Yagishita, J. Phys. B 45 (2012) 194007. (CO-C1s)
- AJ&97a** J.N. Anderson, U. Johansson, R. Nyholm, S.L. Sorensen and M. Wiklund, MAX report (1997)180. (CH<sub>3</sub>OH – C1s, O1s)
- AJ&97b** J.N. Anderson, U. Johansson, R. Nyholm, S.L. Sorensen and M. Wiklund, MAX report (1997)182. (C<sub>2</sub>H<sub>4</sub> , C<sub>4</sub>H<sub>6</sub>– C1s)
- ALS95** G.B. Armen, J.C. Levin and I.A. Sellin, Phys. Rev. A 53 (1996) 772. (Ar1s)
- AL&87** H. Aksela, R. Lakanen, S. Aksela, O.P. Sairanen, A. Yagashita, M. Meyer, Th. Prescher, E. von Raven, M. Richter and B. Sonntag, Phys Rev A 38 (1988) 3395. (Rb3d)
- AL&93** U. Arp, B.M. Lagutin, G. Materlick, I.D. Petrov, B. Sonntag and V.L. Sukhorukov, J. Phys. B 26 (1993) 438. (Ca1s, Cr1s, Cu1s, Mn1s)
- AL&97** U. Arp, T. LeBrun, S.H. Southworth, M.A. MacDonald and M. Jung, Phys. Rev. A 55 (1997) 4273. (Ar1s)
- AM97** V.G. Asolkar and C. Monde, Ind. J. Phys. A 71 (1997) 47. (CH<sub>x</sub>F<sub>4-x</sub>,x=0-4 - C1s)
- AMK97** D.P. Almeida, S.E. Michelin and T. Kroin, ICPEAC Proceedings (1997)
- AM&90** U. Arp, G. Materlick, M. Richter and B. Sonntag, J. Phys. B 23 (1990) L811. (Ce2p, Er2p, Gd2p, Sm2p, Yb2p)

- AM&02** J. Adachi, S. Motoki, N.A. Cherepkov and A. Yagishita, J. Phys. B 35 (2002) 5023. (CO<sub>2</sub> – C1s)
- AM&05** Y. Azuma, Y. Mishima, Y. Senba, H. Yoshida, A. Hiraya, J. El. Spec. 144-147 (2005) 183. (CH<sub>3</sub>OH(D), C<sub>2</sub>H<sub>5</sub>OH(D), CD<sub>3</sub>CH<sub>2</sub>OH, C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub>OH – O1s)
- AN&95** S. Aksela, E. Nommiste, J. Jouhiainen, E. Kukk, J. Karvonen, H.G. Berry, S.L. Sorensen and H. Aksela, Phys. Rev. Lett. 75 (1995) 2112. (C<sub>60</sub> - C1s)
- AO&95** A. Ausmees, S.J. Osborne, R. Mobery, S. Svensson, S. Aksela, O.P. Siaranen, A. Kivimaki, A. Naves de Brito, E. Nommiste, J. Jauhiainen, and H. Aksela , Phys. Rev. A 51 (1999) 855. (Xe4d)
- AP74** L.V. Azaroff and D.M. Pease, *X-ray Absorption Spectroscopy*, Ch 6 in *X-ray Spectroscopy* (L.V. Azaroff, ed.) (1974, McGraw-Hill, NY) (review)
- AP88** F.X. Araujo and D. Petrini, J. Phys. B 21 (1988) L117. (Na2s)
- AP&82** M.Y. Amusia, A.A. Pavlychev, A.S. Vinogradov, D.E. Onopko and S. A. Titov, Opt. Spectrosc 53 (1982) 91 [Opt.Spectrosk 53 (1982) 157] (SiF<sub>4</sub>-Si2p; CF<sub>4</sub>-C1s)
- AP&12** T. Arion, R. Püttner, C. Lupulescu, R. Ovsyannikov, M. Förstel, G. Öhrwall, A. Lindblad, K. Ueda, S. Svensson, Al.M. Bradshaw, W.Eberhard and, U. Hergenhahn, J. El. Spec. 185 (2012) 234. (O<sub>2</sub>-O1s)
- AP&20** A.R. Abid, E Pelimanni, et al., Electron–ion coincidence spectroscopy of a large organic molecule: photofragmentation of avobenzone after valence and core ionisation, . Phys. B: At. Mol. Opt. Phys. 53 (2020) 244001. (C<sub>19</sub>H<sub>22</sub>O<sub>3</sub> – C1s, O1s).
- AR&89** D. Arvanitis, H. Rabus, L. Wenzel and K. Baberschke, Z. Phys. D 11 (1989) 219. (C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>4</sub>, C<sub>2</sub>H<sub>6</sub> - C1s)
- AR&05** M. Alagia, R. Richter, S. Stranges, M. Agåker, M. Ström, J. Söderström, C. Såthe, R. Feifel, S. Sorensen, A. De Fanis, K. Ueda, R. Fink and J-E. Rubensson, Phys. Rev. B 71 (2005) 012506. (N<sub>2</sub>, N<sub>2</sub>O – N1s; O<sub>2</sub>-O1s)
- ASW75** H. Agren, S. Svensson and U.I. Wahlgren, Chem. Phys. Lett. 35 (1975) 336. (H<sub>2</sub>O)
- AS&88** S. Aksela, O.P. Sairanen, H. Aksela, G.M. Bancroft and K.H. Tan, Phys. Rev. A 37 (1988) 2934. (SiCl<sub>4</sub> - Si2p, Cl2p)
- AS&97** G.B. Armen, H. Southworth, J.C. Levin, U. Arp, T. LeBrun and M.A. MacDonald, Phys. Rev. A 56 (1997) R1079. (Xe2p)
- AT&86a** S. Aksela, K.H. Tan, H. Aksela and G.M. Bancroft, Phys. Rev. A 33 (1986) 258 (SiF<sub>4</sub>-Si2p)
- AT&86b** B.M. Addison, K.H. Tan, G.M. Bancroft and F. Cerrina, Chem. Phys. Lett. 129 (1986) 468. (SF<sub>6</sub>, SF<sub>5</sub>Cl - S2p; SeF<sub>6</sub> - Se3p)
- AT&89** B.M. Addison-Jones, K.H. Tan, B.W. Yates, J.N. Cutler and G.M. Bancroft, J. Electron Spect. 48 (1989) 155. (SF<sub>6</sub> - S2p)
- AT&96a** J. Adachi, Y. Takata, N. Kosugi, A. Hiraya, E. Shigemesa, A. Yagashita and Y. Kitajima, Photon Factory Report (1996) 15. (COS - S1s)
- AT&96a** J. Adachi, Y. Takata, N. Kosugi, A. Hiraya, E. Shigemesa, A. Yagashita and Y. Kitajima, Photon Factory Report (1996) 14. (H<sub>2</sub>S - S1s)

- AT&98** J. Adachi, Y. Takata, N. Kosugi, E. Shigemesa, A. Yagashita and Y. Kitajima, Chem. Phys. Lett. 294 (1999) 559. ( $\text{SO}_2$  - S1s)
- AVC95** H. Agren, O. Vahtras and V. Caravetta, Chem. Phys. 196 (1995) 47. ( $\text{C}_6\text{H}_6$ ,  $\text{C}_{10}\text{H}_8$ ,  $\text{C}_{10}\text{H}_{10}$ ,  $\text{C}_{14}\text{H}_{10}$ ,  $\text{C}_{16}\text{H}_{10}$ ,  $\text{C}_{18}\text{H}_{12}$  - C1s)
- AVZ82a** V.N. Akimov, A.S. Vinogradov and T.M. Zimkina, Opt. Spectrosc. 53 (1982) 63 [Opt. Spectrosk. 53 (1982) 109]. ( $\text{N}_2$ ,  $\text{NO}$ -N1s;  $\text{NO}_2$ -O1s)
- AVZ82b** V.N. Akimov, A.S. Vinogradov and T.M. Zimkina, Opt. Spectrosc. 53 (1982) 280 [Opt. Spectrosk. 53 (1982) 476] ( $\text{H}_2\text{O}$ -O1s,  $\text{NH}_3$ -N1s)
- AVZ82c** V.N. Akimov, A.S. Vinogradov and T.M. Zimkina, Opt. Spectrosc. 53 (1982) 548 [Opt. Spectrosk. 53 (1982) 918]. ( $\text{SO}_2$ -O1s)
- AVZ88** V.N. Akimov, A.S. Vinogradov and A.V. Zhadenov, Opt. Spectrosc. 65 (1988) 210 [Opt. Spectrosk. 65 (1982) 349]. ( $\text{N}_2$ ,  $\text{NH}_3$  - N1s)
- AV&85** V.N. Akimov, A.S. Vinogradov, A.A. Pavlychev and V.N. Sivkov, Opt. Spectrosc. (USSR) 59 (1985) 206. [Opt. Spectrosk. 59 (1985) 342. ( $\text{C}_6\text{H}_6$ ,  $\text{C}_6\text{H}_5\text{CH}_3$ ,  $\text{C}_6\text{H}_5\text{C}_2\text{H}_3$  - C1s;  $\text{C}_5\text{H}_5\text{N}$  - C1s, N1s)]
- AWS87** C. Angonoa, O. Walter and J. Schirmer, J. Chem. Phys. 87 (1987) 6789. (CO-C1s)
- AY&96** H. Agren, L. Yang, V. Caravetta and L.G.M. Pettersson, Chem. Phys. Lett. 259 (1996) 21. ( $\text{O}_2$  -O1s)
- B18** G. Brogren, Nova Acta. Reg. Sci. Uppsaliensis 14 (1918) No. 4. (Nels)
- B54** J. Backovsky, Czech. J. Phys. 4 (1954) 150. (Nels)
- B76a** S. Bodeur, J. Appl. Phys. 47 (1976) 4911. ( $\text{O}_2$ -O1s)
- B76b** R.A. Bonham, in *Momentum Wavefunctions*, AIP Conf. Proc. 86 (1976) 70. ( $\text{SF}_6$  - S2p, F1s, S1s)
- B79** C.F. Bunge, Phys. Rev. A 19 (1979) 936. (Li1s)
- B80** F.C. Brown, 'Inner-shell Threshold Spectra', Ch. 4, *Synchrotron Radiation Research*, Winnick & S. Doniach (eds.) (Plenum, NY, 1980) (Ar1s, Ne1s,  $\text{Cl}_2$ -Cl1s,  $\text{N}_2$ -N1s - review)
- B81** A. Bianconi, EXAFS for Inorganic Systems (DL/SCI/R17) Proc. Daresbury Study Weekend (March, 1981) 13. ( $\text{C}_2\text{H}_2$ ,  $\text{C}_2\text{H}_4$ ,  $\text{CF}_4$ -C1s,  $\text{N}_2\text{O}$ -N1s)
- B82a** C.E. Brion, Physics of Electronic and Atomic Collisions, (Proc. of XII ICPEAC, Tennessee, 1981), S. Datz, ed. (North-Holland, 1982). (CO<sub>2</sub>-C1s, HF, F<sub>2</sub>-F1s, N<sub>2</sub>O-N1s - review)
- B82b** A. Bianconi, in *EXAFS and Near Edge Structure*, A. Bianconi, L. Incoccia and S. Stipcich, eds., (Springer-Verlag, Berlin, 1983) 118. ( $\text{C}_2\text{H}_2$ ,  $\text{C}_2\text{H}_4$  - C1s)
- B85** C.E. Brion, Com. At. Mol. Phys. 16 (1985) 249. (review,  $\text{N}_2$ -N1s,  $\text{SO}_2$ -O1s)
- B97** H.G. Barry, AIP Conf. Proc. 392 (1997) 511. ( $\text{C}_{60}$  - C1s)
- B00a** M.A. Bautista, J. Phys. B 33(2000) 71. (Fe2p)

- B00b** M.A. Bautista, J. Phys. B 33(2000) L419. (Fe2p, Fe1s)
- BAK93** J. Boyle, Z. Altun, and H.P. Kelly, Phys. Rev. A 47 (1993) 4811. (W4f)
- BA&86** G.M. Bancroft, S. Aksela, K.H. Tan, B.W. Yates, L.L. Coatsworth and J.S. Tse, J. Chem. Phys. 84 (1986) 5. (SiF<sub>4</sub>-Si2p)
- BA&94** M.A. Baig, M. Akram, S.A. Bhatti, K. Sommer and J. Hormes, J. Phys. B 27 (1994) 1693. (Cd4d)
- BA&95** H.G. Berry, Y. Azuma, P.L. Cowan, D.S. Gemmell, T. LeBrun, T. LeBrun and M. Y. Amusia, Nucl. Inst. Meth. B 98 (1995) 25. (Ar1s, K1s)
- BA&96** F. von Busch, U. Ankerhold, S. Drees and B. Esser, J. Phys. B 29 (1996) 5343. (Ar2p, Ar1s; Xe2p; CS<sub>2</sub>, COS - S1s)
- BA&01** P. Bolognesi, L. Avaldi, M.C.A. Lopes, G. Dawber, G.C. King, M.A. MacDonald, C. Villani, and F. Tarantelli, Phys. Rev. A 64(2001) 012701. (Kr3d, Xe4d)
- BB84** S. Bodeur and R. Barchevitz, Sol. St. Comm. 49 (1984) 11. (O<sub>2</sub>-O1s)
- BB87** E. Bernieri and E. Burattini, Phys. Rev. A 35 (1987) 3322 (Kr1s)
- BB89** J.I. Bolick and M.S. Banna, Phys. Rev. A 40 (1989) 2756. (Xe4d)
- BB91** R.S. Barbieri and R.A. Bonham, Phys. Rev. A 44 (1991) 7361 (Ne1s)
- BB92** R.S. Barbieri and R.A. Bonham, Phys. Rev. A 45 (1992) 7929 (N<sub>2</sub>-N1s)
- BB01a** K.A. Berrington and C. Balance, J. Phys.B 34 (2001) L383. (Fe3p)
- BB01b** K.A. Berrington and C. Balance, J. Phys.B 34 (2001) 2697. (Fe3p)
- BBB78** F.C. Brown, R.Z. Bachrach and A. Bianconi, Chem. Phys. Lett. 54 (1978) 425. (CH<sub>4</sub>, CH<sub>3</sub>F, CH<sub>2</sub>F<sub>2</sub>, CHF<sub>3</sub>, CF<sub>4</sub> - C1s)
- BBB01** C P Ballance, N R Badnell and K A Berrington, J. Phys. B 34 (2001) 3287. (Fe2p)
- BBP77** W. Butscher, R.J. Buenker and S.D. Peyerimhoff, Chem. Phys. Lett. 52 (1977) 449. (N<sub>2</sub>)
- BBS91** H.M. Boechat-Roberty, C.E. Bielschowsky and G.G.B. de Souza, Phys. Rev A 44 (1991) 1694. (CO<sub>2</sub> - C1s)
- BBT90** J.D. Bozek, G.M. Bancroft and K.H. Tan, Chem. Phys. 145 (1990) 131. (Si(CH<sub>3</sub>)<sub>x</sub>F<sub>4-x</sub>, x=0-4, Si2p,2s)
- BB&79** D.M. Barrus, R.L. Blake, A.J. Burek, K.C. Chambers and A.L. Pregenzer, Phys. Rev. A 20 (1979) 1045. (CO<sub>2</sub>, O<sub>2</sub>, CO, N<sub>2</sub>O - O1s)
- BB&80** A. Barth, R.J. Buenker, S.D. Peyerimhoff and W. Butscher, Chem. Phys. 46 (1980) 149. (C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>4</sub> - C1s)
- BB&85** H.O. Beckman, W. Braun, H.W. Joachim, E. Ruhl and H. Baumgartel, Chem. Phys. Lett. 121 (1985) 499. (C<sub>2</sub>H<sub>4-x</sub>F<sub>x</sub>, x=0,4 - C1s)

- BB&88** C.E. Bouldin, G. Bunker, D.E. McKeown, R.A. Forman and J.J. Ritter, Phys. Rev. B 38 (1988) 10816. (GeCl<sub>4</sub>, GeClH<sub>3</sub>, GeH<sub>4</sub> - Ge1s)
- BB&91** C. Brechignac, M. Broyer, Ph. Cahuzac, M. de Frutos, P. Labastie and J.Ph. Raux, Phys. Rev. Lett. 67 (1991) 1222. (Sb<sub>n</sub>, n=4-16, Sb4d)
- BB&00** O.Bjorneholm, M. Bassler, A. Ausmees, I. Hjelte, R. Feifel, H. Wang, C. Miron, M.N. Piancastelli, S.Svensson, S.L. Sorensen, F. Gel'mukhanov and H. Agren, Phys. Rev. Lett. 84 (2000) 2826. (O<sub>2</sub> – O1s)
- BC81** A. Barth and L.S. Cederbaum, Phys. Rev. A 23 (1981) 1038. (many-body theory of core-excitations)
- BC94** C. Bréchignac and J.P. Connerade, J. Phys. B 27 (1994) 3795. (Sb<sub>5</sub> - Sb4d; Ba3d, Sm3d)
- BC&80** M. Breinig, M.H. Chen, G.E. Ice, F. Parante, B. Crasemann and G.S. Brown, Phys. Rev. A 22 (1980) 520. (Ar1s)
- BC&86** J.M. Bizau, D. Cubaynes, P. Gerard, F.J. Wuilleumier, J.L. Picque, D.L. Ederer, B. Carre and G. Wendum, Phys. Rev. Lett. 57 (1986) 306.(Ba 5d)
- BC&89** J.M. Bizau, D. Cubaynes, P. Gerard and F.J. Wuilleumier, Phys. Rev. A 40 (1989) 3002. (Ba 5d)
- BC&92** G.R. Burton, W.F. Chan, G. Cooper and C.E. Brion, Chem. Phys. 167 (1992) 349. (CH<sub>3</sub>OH - C1s)
- BC&94** G. Burton, W.F. Chan, G. Cooper and C.E. Brion, Chem. Phys. 181 (1994) 147. (CCl<sub>4</sub>-Cl2p, 2s)
- BC&19** Paola Bolognesi, Vincenzo Carravetta et al., Core Shell Investigation of 2-nitroimidazole, Frontiers in Chemistry, 7 (2019) 191. (C<sub>3</sub>H<sub>3</sub>N<sub>3</sub>O<sub>2</sub> – C1s, N1s, O1s)
- BD93** C.E. Blount and D.M. Dickinson, J. Electron Spectrosc. 61 (1993) 367. (CO<sub>2</sub> - C1s)
- BDW79** A.L. Bennani, A. Duguet and H.F. Wellenstein, Chem. Phys. Lett. 60 (1979) 405. (CO<sub>2</sub> - C1s,O1s)
- BD&82** C.E. Brion, S. Daviel, R.N.S. Sodhl and A.P. Hitchcock, Int. Conf. on X-ray and Atomic Inner-Shell Physics, AIP Conf. Proc. 94 (1982) 429. (review of ISEELS - HF, F<sub>2</sub>, NF<sub>3</sub> - F1s; Ne1s; N<sub>2</sub>, NF<sub>3</sub> - N1s; CO-C1s,O1s; SF<sub>6</sub>-S2p, F1s)
- BD&85** M.J. Besnard, G. Dujardin, L. Hellner, S. Leach and D. Winkoun, LURE report (1985) 48. (CH<sub>3</sub>I-I4d)
- BD&92** J. Bruneau, D. Desenne, J.P. LeBreton, M. Louis-Jacque, C. Chenais-Popovics, C.A. Back, P. Renaudin and J.C. Gauthier, J. Phys. B 25 (1992) 5271. (Mg1s)
- BE85** S. Bodeur and J.M. Esteva, Chem. Phys. 100 (1985) 415. (H<sub>2</sub>S, CS<sub>2</sub>, CH<sub>3</sub>SH, SO<sub>2</sub> - S1s)
- BE&89** C. Blancard, J.M. Esteva, R.M. Karnatak, J.P. Connerade, U. Kuetgens and J. Hormes, J. Phys. B 22 (1989) L575. (Tm3d)
- BE&91** E. Bouisset, J.M. Esteva, R.C. Karnatak, J.P. Connerade, A.M. Flank and P. Lagarde, J. Phys. B 24 (1991) 1609. SiO - Si1s)
- BE&18** S. Bari, S.; Egorov, et al., Soft X-ray Spectroscopy as a Probe for Gas-Phase Protein Structure: Electron Impact Ionization from within. Chem.-Eur. J. 24 2018 7631 (C<sub>131</sub>H<sub>229</sub>N<sub>39</sub>O<sub>31</sub> [melittin+qH]<sup>q+</sup>, q=2-4 - )

- BF&79** W. Butscher, H. Friedrich, P. Rabe, W.H.E. Schwarz and B. Sonntag, Chem. Phys. Lett. 64 (1979) 360. (SiH<sub>4</sub> - Si2p)
- BF&87** S. Bodeur, J.L. Ferrer, I. Nenner, P. Millie, M. Benfatto and C.R. Natoli, J. Phys. 48 (1987) C9-1117. (SiCl<sub>4</sub> - Si1s, Cl1s)
- BF&93** S. Brennan, P.H. Fuoss, D.W. Kisker, F.J. Lamelas, P. Imperatori, G.B. Stephenson, J. Tsao, A. Zangwill and T. Kuech, Epitaxial Growth Symposium Proc. (M.R.S.) (1993) 165. (GaAs - Ga 1s, As 1s)
- BF&95a** O. Björneholm, F. Federmann, C. Larsson, U. Hahn, A. Rieck, S. Kakar, T. Möller, A. Beutler and F. Fössing, Rev. Sci. Inst. 66 (1995) 1732. (Ne<sub>n</sub> - Ne1s)
- BF&95b** O. Björneholm, F. Federmann, F. Fössing and T. Möller, Phys. Rev. Lett. 74 (1995) 3017. (Ar, Ar<sub>n</sub> - Ar2p)
- BF&95c** A. von den Borne, F. Federmann, M. Klee and B. Sonntag, J. Phys. B 28 (1995) 2591. (Ba4d)
- BF&96** O. Björneholm, F. Federmann, F. Fössing, T. Möller and P. Stampfli, J. Chem. Phys. 104 (1996) 1846. (Ar<sub>n</sub> - Ar2p)
- BF&99** O. Björneholm, F. Federmann, S. Kakar, and T. Möller, J. Chem. Phys. 111 (1999) 546. ((H<sub>2</sub>O)<sub>n</sub> - O1s)
- BF&02** H.M. Boechat-Roberty, J.D. Freitas, D.P. Almeida and G.G.B. de Souza , J. Phys. B 35 (2002) 1409. (Xe4d)
- BF&07** P. Bolognesi, V. Feyer, A. Lahmam-Bennani, M.E. Staicu Casagrande, L. Avaldi, S.K. Semenov, V.V. Kuznetsov and N.A. Cherepkov, J. El. Spec. 161 (2007) 90. (CO - C1s)
- BF&15** N. Berrah, L. Fang, J. El. Spec. 204 (2015) 284. (CO, CO<sub>2</sub>-C1s; N<sub>2</sub>, N<sub>2</sub>O-N1s; CO<sub>2</sub>-O1s)
- BG&87** J.M. Bizau, P. Girard, F.J. Willeumier and G. Wendum, Phys. Rev. A 36 (1987) 1220 (Ca3p)
- BG&91** S.M. Bharathi, A.M. Grisogono, et al., J. El. Spec. 53 (1991) 271. (C<sub>6</sub>H<sub>6</sub> - C1s)
- BG&12** R.C. Bilodeau, N.D. Gibson, C.W. Walter, A. Aguilar, N. Berrah, J. El. Spec. 185 (2012) 219. ( S2s; Pt 5d; Fe 3p)
- BH81** C.E. Brion and A. Hamnett, *Excited States in Chemical Physics*, part 2. J.W. McGowan, ed. (1981, Wiley) p. 1. (CF<sub>4</sub>-C1s, F1s; N<sub>2</sub>-N1s, CO-C1s)
- BH87** S. Bodeur and A.P. Hitchcock, Chem. Phys. 111 (1987) 467. (SF<sub>4</sub>-S2p, S2s, F1s; SF<sub>4</sub>, SF<sub>6</sub>-S1s, S2p, S2s, F1s)
- BHK92** S. Bodeur, A.P. Hitchcock and N. Kosugi, Chem. Phys. 162 (1992) 293. (SF<sub>4</sub>, SF<sub>2</sub>O - S1s, F1s, S2p, S2s)
- BH&72** D. Blechschmidt, R. Haensel, E.E. Koch, U. Nielsen and T. Sagawa, Chem. Phys. Lett. 14 (1972) 33. (SF<sub>6</sub> - S2p)
- BH&86** U. Becker, R. Holzel, H.G. Kerkhoff, B. Langer, D. Szostak and R. Wehlitz, Phys. Rev. Lett. 56 (1986) 1455. (CO-C1s)
- BH&21** V.I. Bukhtiyarov, M. Hävecker, et al., X-ray Absorption and Photoemission Studies of the Active Oxygen for Ethylene Epoxidation over Silver, Catalysis Letters, 74 (2001) 121. (O<sub>2</sub> - O1s)

- BIB93** R.A. Bonham, M. Inokuti and R.S. Barbieri, J. Phys. B 26 (1993) 3363. (N<sub>2</sub>-N1s)
- BI&85** C.E. Brion, Y. Iida, F. Carnovale and J.P. Thomson, Chem. Phys. 98 (1985) 327. (HBr-Br3d)
- BI&19** Sadia Bari, Ludger Inhester, et al., nner-shell X-ray absorption spectra of the cationic series NH<sub>y</sub><sup>+</sup> (y = 0–3), Phys.Chem.Chem.Phys., 21 (2019) 16505, NH<sub>y</sub><sup>+</sup>(0-3) – N1s
- BK73** R.L. Barinskii and I.M. Kulikova, J. Struct. Chem. 14 (1973) 335. [Zh. Struk. Khim. 14 (1973) 372]. (SF<sub>6</sub> - S1s)
- BK74** R.L. Barinskii and I.M. Kulikova, Bull. Acad. Sci. USSR Phys. Ser. 38 (1974) 16 [Izv. Akad. Nauk. SSSR Ser. Fiz. 38 (1974) 444]. (SF<sub>6</sub>,SOF<sub>2</sub>-S1s; NF<sub>3</sub>-N1s; BCl<sub>3</sub>,BF<sub>3</sub>-B1s)
- BKL73** P.S. Bagus, M. Krauss and R.E. LaVilla, Chem. Phys. Lett. 23 (1973) 13. (CH<sub>4</sub>)
- BKM88** J. Brilly, E.T. Kennedy and J.P. Mosnier, J. Phys. B 21 (1988) 3685. (Al<sup>2+</sup> - Al2p)
- BK&86** U. Becker, H.G. Kerkoff, D.W. Lindle, P.H. Kobrin, T.A. Ferrett, P.A. Heimann, C.M. Truesdale and D.A. Shirley, Phys. Rev. A 34 (1986) 2858. (Eu4d)
- BK&87** U. Becker, H.G. Kerkoff, M. Kupsch, B. Langer, D. Szostak and R. Wehlitz, J. Phys. 48 (1987) C9-497. (Xe3d,4d)
- BK&93** S. Baier, U. Koble, T. Luhmann, M. Martins, M. Richter and P. Zimmermann, J. Phys. B 26 (1993) 4091. (Er4d, Ho4d, Tm4d)
- BL93** G. Bandaroge and R.R. Lucchese, Phys. Rev. A 47 (1993) 1989. (CO - C1s)
- BL97a** S.K. Bolting and R.R. Lucchese, Phys. Rev. A 56 (1997) 3666. (CO - C1s)
- BL97b** N. Berrah and B. Langer, Comm. At. Mol. Phys. 33 (1997) 325. (Xe4d)
- BL&98** B.H. Boo, Z. Liu, S.Y. Lee and I. Koyano, J. Phys. Chem. 102 (1998) 8261. (SiBr<sub>4</sub> – Si2p, Br3d)
- BM62** R.L. Barinskii and B.A. Malyukov, J. Struct. Chem. 3 (1962) 327. [Zh. Struk. Khim. 3 (1962) 343]. (SF<sub>6</sub> - S1s)
- BM95** U. Becker and A. Menzel, Nucl. INst. Meth. B 99 (1995) 68. (CO - C1s; HCl - Cl2p)
- BMN90** S. Bodeur, P. Millie and I. Nenner, Phys. Rev. A 41 (1990) 252. (SiX<sub>4</sub>, X = H, D, F, Cl, Br, CH<sub>3</sub>, C<sub>2</sub>H<sub>5</sub>, OCH<sub>3</sub>, OC<sub>2</sub>H<sub>5</sub> - Si1s)
- BMT88** A. Benitez, J.H. Moore and J.A. Tossell, J. Chem. Phys. 88 (1988) 6691. (C<sub>2</sub>H<sub>3</sub>X, C<sub>6</sub>H<sub>5</sub>X, X=H, F, Br, Cl, I - C1s)
- BM&89a** S. Bodeur, P. Millie, E. Lizon A Lugrin, I. Nenner, A. Filiponi, F. Boscherini and S. Mobilio, Phys. Rev. A 39 (1990) 5075. (SiX<sub>4</sub>, X = H, F, Cl, Br, CH<sub>3</sub>; SiH<sub>2</sub> - Si1s; SiBr<sub>4</sub> - Br2s)
- BM&89b** C.E. Bouldin, D.A. McKeown, R.A. Forman, J.J Ritter and G. Bunker, Physica B 158 (1989) 362. (GeCl<sub>4</sub>, GeClH<sub>3</sub>, GeH<sub>4</sub> - Ge1s)
- BM&90** S. Bodeur, J.L. Marechal, C. Reynaud, D. Bazin and I. Nenner, Z. Phys. D 17 (1990) 291. (HCl,Cl<sub>2</sub> - Cl1s)

- BM&95** M. Bissen, M. Fisher, G. Rogers, D. Eisert, K. Kleman, T. Nelson, B. Mason, F. Middleton and H. Hoescht, Rev. Sci. Inst. 66 (1995) 2072. (Ne1s; CO, O<sub>2</sub> - O1s)
- BN66** R.L. Barinskii and V.I. Nefedov, *X-ray Spectral Determination of the Charge of Atoms in Molecules* (Russian), Nauka Press, Moscow, 1966 (HCl-Cl1s)
- BN86** S. Bodeur and I. Nenner, J. Phys. (Paris) 42 C-8 (1986) 79. (SiX<sub>4</sub>-Si1s, X=Cl,F,H)
- BN97** A.G.H. Barbosa and M.A.C. Nascimento, Chem. Phys. Lett. 279 (1997) 119. (N<sub>2</sub> - N1s)
- BNH92** C.E. Bielschowsky, M.A.C. Nascimento and E. Hollauer, Phys. Rev. A 45 (1992) 7942 (N<sub>2</sub> - N1s)
- BNM86** S. Bodeur, I. Nenner and P. Millie, Phys. Rev. A 34 (1986) 2986. (SiX<sub>4</sub>-Si1s,X = Cl, F, H)
- BNP98** V. Brems, B. M. Nestmann and S. D. Peyerimhoff, Chem. Phys. Lett. 287 (1998) 255. (OCS-S2p)
- BNZ72** V.I. Baranovskii, M.S. Nakhmanson and Yu.M. Zaitsev, J. Struct. Chem. 13 (1972) 793 [Zh. Struk. Khim. 13 (1972) 848]. [SiCl<sub>x</sub>(CH<sub>3</sub>)<sub>4-x</sub> - Si2p]
- BN&84** B. Sonntag, T. Nagata, et al., J. Phys. B 17 (1984) L55. (Xe3d, Cs3d, Ba3d)
- BO&10** Bolognesi P, O'Keeffe P, Ovcharenko Y, Coreno M, Avaldi L, Feyer V et al, Pyrimidine and halogenated pyrimidines near edge x-ray absorption fine structure spectra at C and N K-edges: experiment and theory. J Chem Phys 133 (2010) 034302. (C<sub>4</sub>H<sub>4</sub>N<sub>2</sub>, BrC<sub>4</sub>H<sub>3</sub>N<sub>2</sub>, C<sub>4</sub>ClH<sub>3</sub>N – C1s, N1s)
- BPS97** N.R. Badnell, D. Petrini and S. Stoica, J. Phys. B 30 (1997) L665. (B1s)
- BP&78** A. Bianconi, H. Peterson, F.C. Brown and R.Z. Bachrach, Phys. Rev. A 17 (1978) 1907. (N<sub>2</sub>,N<sub>2</sub>O - N1s)
- BP&86** U. Becker, T. Prescher, E. Schmidt, B. Sonntag & H.E. Wetzel, Phys. Rev. A 33 (1986) 3891. (Xe4d)
- BQB81** S. Baroni, A. Quattropani and A. Baldereschi, Chem. Phys. Lett. 79 (1981) 509. (Ne1s, Ar1s)
- BRB04** M. Barbatti, A.B. Rocha, C.E. Bielschowsky, Generalized oscillator strength for core excitations of nitrous oxide, Chemical Physics, 299 (2004) 83
- BRB05** M. Barbatti, A.B. Rocha and C.E. Bielschowsky, Phys. Rev. A 72 (2005) 032711. (CO<sub>2</sub>-C1s, O1s; C<sub>4</sub>H<sub>6</sub>-C1s)
- BRK00** A.A. Borovik, H.J. Rojas and G.C. King, Meas. Sci. Tech. 11 (2000) N42. (K2p)
- BR&92** S. Bodeur, C. Reynaud, K. Bisson, P. Millie, I. Nenner, U. Rockland and H. Baumgartel, AIP Conf. Proc. 258 (1992) 300. (SF<sub>6</sub>, SF<sub>5</sub>Cl, H<sub>2</sub>S - S1s)
- BR&95** C.P.J. Barty, F. Raksei, C. Rose-Petrucci, K.J. Schafer, K.R. Wilson, V.V. Yakovlev, K. Yamakawa, J. Zhiming, A. Ikhlef, C.Y. Cote and J.C. Kieffer, S.P.I.E. Proc 2521 (1995) 246. (SF<sub>6</sub> - S1s)
- BS85** A. Barth and J. Schirmer, J. Phys. B 18 (1985) 867. (N<sub>2</sub>-N1s, CO-C1s,O1s)
- BS87** C.E. Brion and K.H. Sze, Electron-Molecule Scattering and Photoionisation, Proc. XV ICPEAC (Brighton, 1987) (Plenum, 1988) (ClF<sub>3</sub>-Cl2p,F1s; NO<sub>2</sub> - N1s,O1s)
- BS90** U. Becker and D.A. Shirley, Phys. Scripta T31 (1990) 56. (Ne1s, Kr3d, Xe3d, N<sub>2</sub>-N1s, CO-C1s)

- BS96** U. Becker and D.A. Shirley, "Partial Cross-sections and Angular Distributions" in VUV and Soft X-ray Photoionization, U. Becker, D.A. Shirley, eds. (Plenum, NY, 1996) 135. (Ar1s, Ar2p, Eu4d, Mn3p, Xe4d; C<sub>60</sub>-C1s)
- BSS93a** J.D. Bozek, N. Saito and I.H Suzuki, J. Chem. Phys.98 (1993) 4652. (N<sub>2</sub>O - N1s,O1s)
- BSS93b** J.D. Bozek, N. Saito and I.H Suzuki, Proc. VUV-10 (World Scientific, 1993) (CF<sub>2</sub>Cl<sub>2</sub> - Cl2p, F1s]
- BSS94** J.D. Bozek, N. Saito and I.H. Suzuki, J. Chem. Phys. 100 (1994) 393. (CO - C1s, O1s)
- BSS95** J.D. Bozek, N. Saito and I.H. Suzuki, Phys. Rev.A 51 (1995) 4563. (CO<sub>2</sub> - C1s, O1s)
- BST80** H.G. Bennewitz, W.H.E. Schwarz and K.H. Thunemann, Chem. Phys. 52 (1980) 227. (TeF<sub>4</sub>-Te4d)
- BSW77** R. Bruhn, B. Sonntag and H.W. Wolff, Proc. 5th Int. Vac. UV Rad. Phys. Conf. (Montpellier, 1977) I-20. (Fe3p)
- BSW78** R. Bruhn, B. Sonntag and H.W. Wolff, Phys. Lett. A 69 (1978) 9. (Mn3p)
- BSW79** R. Bruhn, B. Sonntag and H.W. Wolff, J. Phys. B 12 (1979) 203. (Fe3p, Co3p, Ni3p, Cu3p)
- BS&69** S.M. Blokhin, A.P. Sadovskii, G.N. Dolenko and V.M. Bertenev, J. Struct. Chem. 10 (1969) 722 [Zh. Struk. Khim. 10 (1969) 833]. (Cl<sub>2</sub>, HCl, CCl<sub>4</sub>, CHCl<sub>3</sub>, CH<sub>3</sub>Cl - Cl1s)
- BS&74** S. Bodeur, C. Senemaud, C. Bonnelle and J.P. Connerade, Proc. 4th Int. Vac. UV Rad. Phys. Conf. (Hamburg, 1974) 94. (O<sub>2</sub> - O1s)
- BS&82** R. Bruhn, E. Schmidt, H. Schroder and B. Sonntag, J. Phys. B 15 (1982) 2807. (Cr3p)
- BS&88** C E Brion, K H Sze, W Zhang, J M Li, X M Tong, "Inner-Shell Excitation Of SO<sub>2</sub> And NO<sub>2</sub> By High Resolution Electron Energy Loss Spectroscopy-- Comparison With Multichannel Quantum Defect Theory," Proc. SPIE 911 (1988) 46, doi: 10.1117/12.945474 (SO<sub>2</sub> – S2p,O1s, S1s; NO<sub>2</sub> – N1s, O1s)
- BS&89a** U. Becker, D. Szostak, M. Kupsch, H.G. Kerkoff, B. Langer, and R. Wehlitz, J. Phys. B 22 (1989) 749. (Xe4d)
- BS&89b** U. Becker, D. Szostak, H.G. Kerkoff, M. Kupsch, B. Langer, R. Wehlitz, A. Yagashita and T. Hayaishi, Phys. Rev. A 39 (1989) 3902. (Xe4d,4p)
- BS&97** O. Bjorneholm, S. Sundin, S.Svensson, R.R.T. Marinho, A. Naves de Brito, F.Kh. Gel'mukhanov and H. Agren, Phys. Rev. Lett. 79 (1997) 3150. (HCl - Cl2p)
- BS&02a** B.H. Boo, N. Saito, I.H. Suzuki and I. Koyano, J. El. Spec. 123 (2002) 73. (CBr<sub>4</sub> – Br3d, C1s)
- BS&02b** B.H. Boo, N. Saito, I.H. Suzuki and I. Koyano, J. Mol. Struct. 610 (2002) 17. (C<sub>4</sub>GeH<sub>12</sub> – Ge3d,3p,3s; C1s)
- BS&12** R. B. Bernini, L. B. G. da Silva, F. N. Rodrigues, L. H. Coutinho, A. B. Rocha and G. G. B. de Souza, J. Chem. Phys. 136, 144307 (2012) (CH<sub>3</sub>)<sub>2</sub>S, CH<sub>3</sub>)<sub>2</sub>S<sub>2</sub> - S 2p)
- BT92** I.M. Band and M.B. Trzhaskovskaya, J. Phys. B 25 (1992) L145 (U5d, Th5d)

- BT97** I.M. Band and M.B. Trzhaskovskaya, J. Phys. B 30 (1997) 5185. (Ba4d)
- BT&87** J.D. Bozek, K.H. Tan, G.M. Bancroft and J.S. Tse, Chem. Phys. 138 (1987) 33. (SiCl<sub>4</sub>, Si(CH<sub>3</sub>)<sub>4</sub> - Si2p,2s, Cl2p)
- BT&92** J.D. Bozek, K.H. Tan, G.M. Bancroft and K.J. Fu, Chem. Phys. 158 (1992) 171 (Si(CH<sub>3</sub>)<sub>x</sub>F<sub>4-x</sub> - Si2p)
- BW&76** A.L. Bennani, H.F. Wellenstein, A. Diguet, B. Nuguyen and A.D. Barlas, Chem. Phys. Lett. 41 (1976) 470. (CH<sub>4</sub> - C1s)
- BW&99** M. Banndorf, W.B. Westerveld, J. van Eck, J. van der Weg and H.G.M. Heideman, J. Phys. B32 (1999) 2503. (CO - C1s, O1s)
- BY&93** M. Byong-Soo, Y. Yoshinari, T. Watabe, Y. Tanaka, C. Takayanagi, T. Takayanagi, K. Wakiya and H. Suzuki, J. Phys.Soc. Jpn. 62 (1993) 1183. (Xe4d)
- BZ&67** V.I. Barinovskii, T.M. Zimkina, V.A. Fomichev and B.E. Dzevitski, Theor. Exp. Chem. 3 (1967) 260 [Teor. i Eksp. Khim. 3 (1967) 354]. (SF<sub>6</sub>-S2p)
- C30** W.W. Colvert, Phys. Rev. 36 (1930) 1619. (Ar2p, Ne1s, SO<sub>2</sub>-S2p, Cl<sub>2</sub>-Cl2p)
- C37** B. Cioffari, Phys. Rev. 51 (1937) 630. (HBr,Br<sub>2</sub>,IBr-Br1s; IBr,I<sub>2</sub>-I1s)
- C64** J.W. Cooper, Phys. Rev. Lett. 13 (1964) 762. (Xe4d)
- C69** H.U. Chun, Phys. Lett. A 30 (1969) 445. (CH<sub>4</sub> - C1s)
- C73** K. Codling, Rep. Prog. Phys. 36 (1973) 541. (Ar2p, N<sub>2</sub>-N1s, SiH<sub>4</sub>-Si2p, review)
- C76** J.P. Connerade, Proc. Roy. Soc. London A 347 (1976) 581. (Xe4p)
- C78** J.P. Connerade, Contemp. Phys. 19 (1978) 415. (review of atomic photo- absorption; Ba4d)
- C82a** J.P. Connerade, J. Phys. B 15 (1982) L881. (Ba4d)
- C82b** J.P. Connerade, J. Phys. C 15 (1982) L367. (Cs4d - theory)
- C82c** F. Combet-Farnoux, Phys. Rev. A 25 (1982) 287. (Xe4d, Cu3p, La4d)
- C83** J.P. Connerade, J. Phys. B 16 (1983) L257. (Ba4d)
- C84** J.P. Connerade, J. Phys. B 17 (1984) L165. (Ba4d, Cd3d, Eu4d, Kr3d, Mn3p, Xe4d)
- C86** F. Combet-Farnoux, Z. Phys. D 2 (1986) 337. (Cu3p)
- C88** J.W. Cooper, Phys. Rev. A 38 (1988) 3417. (Ar1s)
- C89** J.W. Cooper, Phys. Rev. A 39 (1989) 3714. (Ar2p)
- C90** K.F. Chung, Phys. Rev. A 42 (1990) 5732. (Be1s)
- C93** J.W. Cooper, Phys. Rev. A 47 (1993) 1841. (Ar2p, Ne1s, Kr3d, Xe3d,4d)

- C95** L.S. Cederbaum, J. Chem. Phys. 103 (1995) 562. (C<sub>2</sub>H<sub>4</sub> - C1s)
- C02** Ahmet Cengiz, Radiation Physics and Chemistry, 65 (2002) 33. (N<sub>2</sub>)
- C05** Chong, D.P. , Density Functional Calculation of K-Shell Spectra of Small Molecules J. Electron Spectrosc. Rel. Phenom. 148 (2005) 115 (Ne1s, HF-F1s, H<sub>2</sub>O-O1s, NH<sub>3</sub> – N1s, CH<sub>4</sub> –C1s, CO – C1s, O1s)
- C07** D.P. Chong, Chem. Phys. Lett. 441 (2007) 209-212. (N<sub>2</sub>O – N1s, O1s)
- CAC89** A. Cesar, H. Agren and V. Carravetta, Phys. Rev. A 40 (1989) 187. (H<sub>2</sub>O - O1s)
- CA&87** T.X. Carroll, S.E. Anderson, L. Ungier and T.D. Thomas, Phys. Rev. Lett. 58 (1987) 867. (NO-N1s)
- CA&95** V. Carravetta, H. Ågren, L.G. M. Pettersson and O. Vahtras, J. Chem. Phys. 102 , 5589 (1995) (C<sub>n</sub>H<sub>n</sub>-C1s)
- CA&99** M. Corenco, L. Avaldi, R. Camilloni, K.C Prince, M. de Simone, J. Karvonen, R. Colle and S. Simonucci, Phys. Rev A 59 (1999) 2494. (Ne1s)
- CB80** F. Combet-Farnoux and M. Ben Amar, Phys. Rev. A 21 (1980) 1975. (Ni 3p)
- CBS87** J.P. Connerade, M.A. Baig and M. Sweeney, J. Phys. B 20 (1987) L771. (Ca3p)
- CB&95** G. Cooper, G.R. Burton, W.F. Chan and C.E. Brion, Chem. Phys. 196 (1995) 293. (SiH<sub>4</sub> - Si2p)
- CB&01** E.J. Cardosa, F. Burmeister, O.Bjorneholm and A. Naves de Brito, VUV-13 abstracts (2001) CS<sub>2</sub>, SO<sub>2</sub> – S1s)
- CC82** S. Canuto and M.R. Chacon, Chem. Phys. 87 (1984) 17. (BeF<sub>2</sub>-Be1s, F1s)
- CC85** M.R. Chacon and S. Canuto, Chem. Phys. Lett. 120 (1985) 86. (HF-F1s)
- CC86** P.K. Carroll and J.T. Costello, Phys. Rev. Lett. 57 (1986) 1581. (Th5d)
- CC94** M.K. Chen and K.T. Chung, Phys. Rev. A 49 (1994) 1675. (Li1s)
- CCM88** I. Cacelli, V. Carravetta and R. Moccia, Chem. Phys. 120 (1988) 51. (H<sub>2</sub>S-S2p)
- CC&81** R. Cambi, G. Ciullo, A. Sgamellotti, F. Tarentelli and M. F. Guest, Chem. Phys. Lett. 83 (1981) 320. (BeH<sub>2</sub>-Be1s)
- CC&82** R. Cambi, G. Ciullo, A. Sgamellotti, F. Tarentelli and M. F. Guest, Chem. Phys. Lett. 91 (1982) 178. (NH<sub>2</sub>-N1s)
- CC&89** J.W. Cooper, C.W. Clark, C.L. Cromer, T.B. Lucarto, B.F. Sonntag, E.T. Kennedy and J.T. Costello, Phys. Rev. A 39 (1989) 6074. (Mn. Mn<sup>+</sup> - Mn3p; Cr3p)
- CC&92** W.F. Chan, G. Cooper, X. Guo, G.R. Burton and C.E. Brion, Phys. Rev. A 46 (1992) 149. (Ar2p, Kr3d, Xe4d)
- CC&95** S.C. Chung, C.I. Chen, P.C. Tseng, H.F. Lin, T.E. Dann, Y.F. Song, L.R. Huang, C.C. Chen, J.M. Chuang, K.L. Tsang and C.N. Chang, Rev. Sci. Inst. 66 (1995) 1655. (Ne1s, Ar2p; N<sub>2</sub>-N1s, CO - C1s,O1s; O<sub>2</sub> - O1s)
- CC&11** P.A. Crozier and S. Chenna, Ultramicroscopy, 111 (2011) 177. (CO<sub>2</sub>, Cl - C1s, O 1s)

- CD78** B.E. Cole and R.N. Dexter, J. Quant. Spectrosc. Rad. Transfer 19 (1978) 303. ( $\text{CCl}_x\text{F}_{4-x}$ ,  $x=0-4$ ,  $\text{CHClF}_2$ ,  $\text{CHCl}_2\text{F}$ ,  $\text{C}_2\text{F}_6$ ,  $\text{C}_2\text{Cl}_2\text{F}_4$  - Cl2p)
- CD96** J.P. Connerade and V.K. Dolmatov, J. Phys. B 29 (1996) L831. (Mn3p)
- CDM76** J.P. Connerade, B. Drerup and M.W.D. Mansfield, Proc. Roy. Soc. London A 348 (1976) 235. (Pb4f)
- CD&90** B. Carre, P. D'Oliveira, M. Ferray, P. Fournier, F. Gounard, D. Cubaynes, J.M. Bizau and F.J. Willeumier, Z. Phys. D 15 (1990) 117. (Na2p)
- CD&96** D. Cubaynes, S. Diehl, L. Journel, B. Rouvellou, J.-M. Bizau, S. Al Moussalam, F.J. Willeumier, N. Berrah, L. VoKy, P. Faucher, A. Hibbert, C. Blancard, E. Kennedy, T.J. Morgan, J. Bozek and A.S. Schlachter, Phys. Rev. Lett. 77 (1996) 2194. (Li1s)
- CEK76** P.H. Citrin, P. Eisenberger and B.M. Kincaid, Phys. Rev. Lett. 36 (1976) 1346. (CBr<sub>4</sub>, Br<sub>2</sub> - Br1s)
- CE&92** J.T. Costello, D. Evans, R.B. Hopkins, E.T. Kennedy, L. Kiernor, M.W.D. Mansfield, J.P. Mosnier, M.H. Sayyad and B.F. Sonntag, J. Phys. B 25 (1992) 5055. (Al2p)
- CE&09** Emiliano Corte 's, † Mauricio F. Erben, et al., Dissociative Photoionization of Methyl Thiocyanate, CH<sub>3</sub> SCN, in the Proximity of the Sulfur 2p Edge, J. Phys. Chem. A 113 (2009) 564. (CH<sub>3</sub>SCN – S2p)
- CF83** K.T. Cheng and C. Froese-Fischer, Phys. Rev. A 28 (1983) 2811, 2820 (Xe, Cs<sup>+</sup>, Ba<sup>2+</sup>, etc - 4d)
- CF&83** R. Camilloni, E. Fainelli, G. Petracelli and G. Stefani, in *EXAFS and Near Edge Structure* (1983, Springer-Verlag, Berlin) 174. (N<sub>2</sub>-N1s G.O.S.)
- CF&84a** R. Camilloni, E. Fainelli, G. Petracelli, G. Stefani, F. Moracci and R. Platania, Lect. Notes in Chemistry 35 (1984) 172. (N<sub>2</sub>, NO, N<sub>2</sub>O -N1s; BF<sub>3</sub>-B1s)
- CF&84b** C.T. Chen, W.K. Ford, R.A. DiDio, E.W. Plummer and W. Eberhardt, NSLS Report (1984) 163. (CO-C1s)
- CF&85** N. Correia, A. Aores-Riveros, H. Agren, K. Helenelund, L. Asplund and U. Gelius, J. Chem. Phys. 83 (1985) 2035. (CO-C1s,O1s)
- CF&87** R. Camilloni, E. Fainelli, G. Petracelli and G. Stefani, J. Phys. B 20 (1987) 1839. (N<sub>2</sub>, NO, N<sub>2</sub>O -N1s)
- CF&90** C.D. Caldwell, M. Flemming, M.O. Krause, P. Van der Meulen, C. Pau and A.F. Starace, Phys. Rev A 41 (1990) 542. (Be1s)
- CGM71** J.P. Connerade, W.R.S. Garton and M.W.D. Mansfield, Astrophys. J. 165 (1971) 203. (Na2p, Na2s)
- CG&80** D.T. Clark, M.F. Guest, A. Sgamellotti and F. Tarantelli, Chem. Phys. 52 (1980) 11. (CH<sub>2</sub>-C1s)
- CG&88** T.A. Carlson, P. Gerard, M.O. Krause, G.V. Wald, J.W. Taylor, F.A. Grimm and B.P. Pullen, J. El. Spectrosc. 47 (1988) 227. (SiCl<sub>4</sub> - Si2p,Cl2p; CH<sub>x</sub>Cl<sub>4-x</sub>,  $x=0-3$  - Cl2p)
- CG&97a** A. Cesar, F.Kh. Gel'mukhanov, Y. Luo, H. Agren, P. Skytt, P. Glans, J. Guo, K. Gunnelin and J. Nordgren, J. Chem. Phys. 106 (1997) 3439. (CO<sub>2</sub> - O1s)
- CG&97b** V.Carravetta, F.Kh. Gel'mukhanov, H. Agren, S. Sundar, S.J. Osbore, A. Naves de Brito, O. Bjorneholm, A.

Ausmees and S. Svensson, Phys. Rev. A 56 (1997) 4665. (CO - C1s)

- CG&03** M.L. Gordon, G. Cooper, C. Morin, T. Araki, C.C. Turci, K. Kaznatcheev, and A. P. Hitchcock, Inner shell spectroscopy of the peptide bond: comparison of the C 1s, N 1s and O 1s spectra of glycine, glycyl-glycine and glycyl-glycyl-glycine, J. Phys. Chem A 107 (2003) 6144-6159. ( $\text{C}_2\text{H}_5\text{NO}_2$ ,
- CG&04** G. Cooper, M. Gordon, D.Tulumello, C.C. Turci, K. Kaznatcheev and A.P. Hitchcock, J. Electron Spectroscopy 137-140 (2004) 795. ( $\text{C}_2\text{H}_5\text{NO}_2$ ,  $\text{C}_3\text{H}_7\text{NO}_2$ ,  $\text{C}_4\text{H}_8\text{N}_2\text{O}_4$ ,  $\text{C}_6\text{H}_6$ ,  $\text{C}_9\text{H}_{11}\text{NO}_2$  - C 1s;  $\text{C}_2\text{H}_5\text{NO}_2$ ,  $\text{C}_4\text{H}_8\text{N}_2\text{O}_4$  - N1s, O1s)
- CG&16** R.C. Couto, Marco Guarise, et al., Anomalously strong two-electron one-photon X-ray decay transitions in CO caused by avoided crossing, Scientific Reports 6 (2016) 20947. (CO – O1s RIXS)
- CH86** J.P. Connerade and J. Hormes, Z. Phys. D 4 (1986) 3 (Ar1s, H<sub>2</sub>S, SCl<sub>2</sub>-S1s)
- CH98** D.P. Chong and C.H. Hu, J. Electron Spectrosc. 94 (1998) 181. ( $\text{C}_5\text{H}_8\text{O}_2$  - O1s)
- CH07** G. Cooper and A.P. Hitchcock, (2007) unpublished. ( $\text{C}_7\text{H}_8$ ,  $\text{C}_{10}\text{H}_8$  C1s)
- CHW77** K. Codling, J.R. Hamley and J.B. West, J. Phys. B 10 (1977) 353. (Na2p)
- CHW78** K. Codling, J.R. Hamley and J.B. West, J. Phys. B 11 (1978) 1713. (Cd4d)
- CH&73** F.J. Comes, R. Haensel, U. Nielsen and W.H.E. Schwarz, J. Chem. Phys. 58 (1973) 516. (XeF<sub>2</sub>, XeF<sub>4</sub> - Xe4d)
- CH&85** T.C. Chang C.S. Hsue, P.A. Ruttink and W.H.F. Schwarz, Chem. Phys. 93 (1985) 405. (HF-F1s, H<sub>2</sub>O-O1s, NH<sub>3</sub>-N1s)
- CH&97** R. Chauvistre, J. Hormes, E. Hartmann, N. Etzenbach, R. Hosch and J. Hahn, Chem. Phys. 223 (1997) 293. (R-S<sub>n</sub>-R, (n=2): R=Me, iPr, t-Bu, n-Bu, C<sub>6</sub>H<sub>5</sub>, C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub>, CH<sub>3</sub>CH=CHCH<sub>2</sub>, Me<sub>2</sub>C=CMeCH<sub>2</sub>; (n=3,4) t-Bu, n-Bu, Me<sub>2</sub>C=CMeCH<sub>2</sub> - S 1s)
- CH&01** H. S. Chakraborty, D. L. Hansen, O. Hemmers, P.C. Deshmukh, P. Focke, I. A. Sellin, C. Heske, D.W. Lindle, and S. T. Manson, Phys. Rev. A 63 (2001) 042708. (Kr3d, Kr3p, Kr3s)
- CIB90** G. Cooper, T. Ibuki and C.E. Brion, Chem. Phys. 140 (1990) 147. (SiH<sub>4</sub> - Si2p,2s)
- CJ99** R.G. Cavell and A. Jürgensen, J. El. Spec. 101-103 (1999) 125. (Br<sub>3</sub>P, CCl<sub>2</sub>H<sub>3</sub>P, CCl<sub>2</sub>H<sub>3</sub>OP, CCl<sub>2</sub>H<sub>3</sub>PS, C<sub>2</sub>CIH<sub>6</sub>PO<sub>2</sub>S, C<sub>3</sub>H<sub>9</sub>P, C<sub>3</sub>H<sub>9</sub>O<sub>4</sub>P, C<sub>3</sub>H<sub>9</sub>O<sub>3</sub>P, C<sub>3</sub>H<sub>9</sub>O<sub>3</sub>PS, C<sub>6</sub>H<sub>15</sub>P, Cl<sub>3</sub>OP, Cl<sub>3</sub>P, Cl<sub>3</sub>PS, F<sub>3</sub>PS, F<sub>3</sub>OP, PF<sub>5</sub>, F<sub>3</sub>P, H<sub>3</sub>P, - P1s)
- CKS80** P.K. Carroll, E.T. Kennedy and G.O. Sullivan, Appl. Optics 19 (1980) 1454. (CH<sub>3</sub>I - I4d, CCl<sub>4</sub> - Cl1s, Cl2p)
- CK&85** S.H. Chou, F.W. Kutsley, D.E. Ellis, G.K. Shenoy, T.I. Morrison and P.A. Montano, Phys. Rev. B 31 (1985) 1069. (FeCl<sub>2</sub>-Fe1s,Cl2p; KrF<sub>2</sub>-Kr1s)
- CKJ88** C.D. Caldwell, M.O. Krause and J.Jiminez Mier, Phys. Rev. A. 37 (1988) 2408. (Ga3d)
- CK&91a** J.T. Costello, E.T. Kennedy, B.F. Sonntag and C.W. Clark, Phys. Rev. A 43 (1991) 1441. (Cr,Cr<sup>+</sup>-Cr3p; Mn,Mn<sup>+</sup>-Mn3p)
- CK&91b** J.T. Costello, E.T. Kennedy, B.F. Sonntag and C.L. Cromer, J. Phys. B 24 (1991) 5063. (W4f,Pt4f)

- CK&95** J.M. Chen, R. Klausen, S.C. Yang and C.R. Wen, Chem. Phys. Lett. 246 (1995) 285. (SiCl<sub>4</sub> - Si2p)
- CK&98a** J.T. Costello, E.T. Kennedy, J.P. Mosnier, M.H. Sayyad and C. McGuiness, J. Phys. B 31 (1998) L547. (Si2p)
- CK&98b** J.T. Costello, E.T. Kennedy, J.P. Mosnier and M.H. Sayyad, J. Phys. B 31 (1998) 677. (Al2p, Si2p)
- CK&99** C.D. Caldwell, M.O. Krause, R.D. Cowan, A. Menzel, S.B. Whitfield, S. Hallinen, S.P. Frigo and M.C. Seversen, Phys. Rev. A 59 (1999) R926. (Cl2p)
- CL&97** J.M. Chen, K.T. Lu, R.G. Liu, J.W. Lay and Y.C. Liu, J. Chem. Phys. 106 (1997) 9105. (C<sub>2</sub>Cl<sub>2</sub>H<sub>6</sub>Si -Si2p)
- CL&05** J.M. Chen, K.T. Lu, J.M. Lee, S.C. Ho, H.W. Chang and Y.Y. Lee, J. El. Spec. 144-147 (2005) 171. (Si(CH<sub>2</sub>)Cl<sub>2</sub> – Cl2p, Si2p)
- CM64** K. Codling and R.P. Madden, Phys. Rev. Lett. 12 (1964) 106. (Kr3d, Xe4d)
- CM65** K. Codling and R.P. Madden, Appl. Opt. 4 (1965) 1431. (Kr3d, Xe4d)
- CM73** J.P. Connerade and M.W.D. Mansfield, Proc. Roy. Soc. London A 335 (1973) 87. (Hg4f, Hg5s)
- CM74a** J.P. Connerade and M.W.D. Mansfield, Proc. Roy. Soc. London A 339 (1974) 533. (Zn3s)
- CM74b** J.P. Connerade and M.W.D. Mansfield, Proc. Roy. Soc. London A 341 (1974) 267. (Ba3d)
- CM75a** J.P. Connerade and M.W.D. Mansfield, Proc. Roy. Soc. London A 343 (1975) 415. (Kr3d)
- CM75b** J.P. Connerade and M.W.D. Mansfield, Proc. Roy. Soc. London A 344 (1975) 435. (T14f)
- CM76a** J.P. Connerade and M.W.D. Mansfield, Proc. Roy. Soc. London A 348 (1976) 239. (Cs4d, Cs3d)
- CM76b** J.P. Connerade and M.W.D. Mansfield, Proc. Roy. Soc. London A 348 (1976) 539. (Rb3d, Rb3p)
- CM77a** J.P. Connerade and M.W.D. Mansfield, Proc. Roy. Soc. London A 352 (1977) 557. (Cd3d, Rb3d, Rb3p, Kr3d, Sr3d, Sr3p)
- CM77b** J.P. Connerade and M.W.D. Mansfield, Proc. Roy. Soc. London A 356 (1977) 135. (Se<sub>2</sub> - Se3d)
- CM82** J.P. Connerade and M.W.D. Mansfield, Phys. Rev. Lett. 15 (1982) 131. (Ba4d - theory)
- CMM76** J.P. Connerade, M.W.D. Mansfield and M.A.P. Martin, Proc. Roy. Soc. London A 350 (1976) 405. (Mn3p)
- CMS89** C.T. Chen, Y. Ma and F. Sette, Phys. Rev. A 40 (1989) 6737. (N<sub>2</sub>-N1s)
- CMT73** J.P. Connerade, M.W.D. Mansfield, K. Thimm, Chem. Phys. 1 (1973) 256. (N<sub>2</sub> - N1s)
- CMT74** J.P. Connerade, M.W.D. Mansfield and K. Thimm, Proc. Roy. Soc. London A 337 (1974) 293. (Cd3d)
- CM&72** J.P. Connerade, M.W.D. Mansfield, K. Thimm and I. Pollard, Phys. Rev. A 6 (1972) 1955. (Cd3d)
- CM&80** J.P. Connerade, M.W.D. Mansfield, M. Cukier and M. Pantelouris, J. Phys. B 13 (1980) L235. (UF<sub>4</sub>-U5d)

- CM&88a** T.A. Carlson, D.R. Mullins, C.E. Beall, B.W. Yates, J.W. Taylor, B.P. Pullen, D.W. Lindle and F.A. Grimm, Phys. Rev. Lett. 60 (1988) 1382 (Kr3d).
- CM&88b** T.A. Carlson, D.R. Mullins, C.E. Beall, B.W. Yates, J.W. Taylor, B.P. Pullen and F.A. Grimm, J. Chem. Phys. 89 (1988) 4490 (SiCl<sub>4</sub>-Si2p)
- CM&89** T.A. Carlson, D.R. Mullins, C.E. Beall, B.W. Yates, J.W. Taylor, and D.W. Lindle, Phys. Rev. A 39 (1989) 1170 (Ar2p, Kr3d, Xe4d)
- CM&91** J.T. Costello, J.P. Mosnier, E.T. Kennedy, P.K. Carroll and G. O'Sullivan, Phys. Scripta T34 (1991) 77. (Th5d, U5d, Cr3p, Cr<sup>+</sup>-3p, Mn3p, Mn<sup>+</sup>-3p)
- CM&98** S.Y. Chen, C.I. Ma, D.M. Hanson, K. Lee and D.Y. Kim, J. Electron Spectrosc. 93 (1998) 61. (N<sub>2</sub>O-N1s)
- CM&01** A. Cummings, C. McGuiness, G. O'Sullivan, J.T. Costello, J.P. Moesnier and E.T. Kennedy, Phys. Rev. A 63 (2001) 22702. (Cs4d)
- CM04** Z. Chen and A.Z. Msezane, Phys. Rev A 70 (2004) 032714. (C2s, Na2p )
- CNS73** F.J. Comes, U. Nielsen and W.H.E. Schwarz, J. Chem. Phys. 58 (1973) 2230. (I<sub>2</sub> - I4d)
- CP75** T.N. Chang and R.T. Poe, Phys. Rev. A 11 (1975) 191. (Li1s)
- CP84** J.P. Connerade and M. Pantelouris, J. Phys. B 17 (1984) L173. (Gd, GdF<sub>3</sub> - Gd4d)
- CPA01** Vincenzo Carravetta, Oleksandr Plashkevych and Hans Ågren, Chem. Phys. 263 (2001) 231. (CO- C1s, O1s; C<sub>4</sub>H<sub>6</sub> – C1s; C<sub>5</sub>H<sub>2</sub>N<sub>4</sub>, C<sub>6</sub>H<sub>5</sub>N, C<sub>6</sub>H<sub>7</sub>N, -C1s, N1s)
- CP&72** B. Cadioli, U. Pincelli, E. Tosatti, U. Fano and J.L. Dehmer, Chem. Phys. Lett. 17 (1972) 15. (BF<sub>3</sub>)
- CP&77** A.M. Cantu, W.H. Parkinson, G. Tondello and G.P. Tozz, J. Opt. Soc. Am. 67 (1977) 1030. (Li1s)
- CP&80** J.P. Connerade, M. Pantelouris, M.A. Baig, M.A.P. Martin and M. Cukier, J. Phys. B 13 (1980) L357. (ThF<sub>4</sub>-Th5d, LaF<sub>3</sub>-La4d)
- CP&90** D. Coulman, A. Puschmann, U. Hofer, H.P. Steinruck, W. Wurth, P. Feulner and D. Menzel, J. Chem. Phys. 93 (1990) 58. (H<sub>2</sub>O - O1s)
- CP&98** V. Carravetta, G. Polzonetti, G. Iucci, M.V. Russo, G. Paolucci, M. Barnaba, Chem Phys Lett 288 (1998) 37. (C<sub>8</sub>H<sub>6</sub> – C1s)
- CP&07** D. Céolin, M. N. Piancastelli, R. Guillemin, W. C. Stolte, S.-W. Yu, O. Hemmers, and D. W. Lindle, J. Chem. Phys. 126 (2007) 084309. (CH<sub>3</sub>Cl - C1s, Cl 2p)
- CR&00** N.A. Cherepkov, G. Rascev, J. Adachi, Y. Hikosaka, K. Ito, S. Motoki, M. Sano, K. Soejima and A. Yagashita, J. Phys. B 33 (2000) 4213. (CO – C1s, O1s)
- CS77** T.C. Chang and W.H.E. Schwarz, Theor. Chim. Acta (Berl.) 44 (1977) 45. (Li1s)
- CS89** C.T. Chen and F. Sette, Rev. Sci. Inst. 60 (1989) 1616 (N<sub>2</sub>-N1s; CO-C1s)

- CS90** C.T. Chen and F. Sette, Phys. Scripta T31 (1990) 119. ( $N_2$ -N1s;  $C_2H_4, C_2D_4$ ,  $C_6H_6, C_6D_6$ ,  $CCl_2F_2$ ,  $CClF_3$  - C1s)
- CS96** A. Cummings and G. O'Sullivan, Phys. Rev. A 54 (1996) 323. (Br3d)
- CS01** A. Cummings and G. O'Sullivan, J. Phys. B 34 (2001) 199. (Cs4d)
- CS&20** S Carniato, P Selles, et al., Single photon simultaneous K-shell ionization/excitation in  $C_6H_6$ : experiment and theory, J. Phys. B: At. Mol. Opt. Phys. 53 (2020) 244010 ( $C_6H_6$  – C1s)
- CSB89** G. Cooper, K.H. Sze and C.E. Brion, J. Am. Chem. Soc. 111 (1989) 5051. (CO - C1s,O1s;  $Ni(CO)_4$  - C1s, O1s, Ni3p)
- CSB90** G. Cooper, K.H. Sze and C.E. Brion, J. Am. Chem. Soc. 112 (1990) 4221. (M(CO)6, M=Cr, Mo, W - C1s, O1s)
- CS&86** T.A. Carlson, W.A. Svensson, M.O. Krause, T.A. Whitley, F.A. Grimm, G.V. Wald, J.W. Taylor and B.P. Pullen, J. Chem. Phys. 84 (1986) 122. ( $SiCl_4$  - Si2p)
- CS&00** N.A. Cherepkov, S.K. Semenov, Y. Hikosaka, K. Ito, S. Motoki and A. Yagashita, Phys. Rev. Lett. 84 (2000) 250. ( $N_2$  – N1s)
- CT88** T.X. Carroll and T.D. Thomas, J. Chem. Phys. 89 (1988) 5983 (O2-O1s).
- CT89** T.X. Carroll and T.D. Thomas, J. Chem. Phys. 90 (1989) 3479. (CO,  $CO_2$ , COS - O1s)
- CT90** T.X. Carroll and T.D. Thomas, J. Chem. Phys. 92 (1990) 7171. (O<sub>2</sub>-O1s)
- CT91** T.X. Carroll and T.D. Thomas, J. Chem. Phys. 94 (1991) 11. (CO<sub>2</sub> - C1s,O1s)
- CT92** T.X. Carroll and T.D. Thomas, J. Chem. Phys. 97 (1992) 894. (NO - N1s)
- CT06** D.P. Chong and Y. Takahata, Chem. Phys. Lett. 418 (2006) 286. ( $H_2CO$  – C1s)
- CTS82** A.M. Cantu, G.P. Tozzi and N. Spector, J. Opt. Soc. Am. 72 (1982) 729. (Al2p)
- CT&74** J.P. Connerade, D. Tracy, M.W.D. Mansfield and K. Thimm, Proc. 4th Int. Vac. UV Rad. Phys. Conf. (Hamburg, 1974) 243. (Ba4d)
- CT&12** D. Céolin, O. Travnikova, Z. Bao, F.F. Guimarães, M.S. da Costa, Y.Velkov, N. Sisourat, S. Carniato, M. Simon, M.N. Piancastelli, J. El. Spec. 185 (2012) 252. ( $CH_2CCl_2$  - C1s)
- CU05** R.R. Cooney, S.G. Urquhart, J. Phys. Chem. B, 108 (2005) 18185. ( MANY SPECIES !!)
- CV&98** D. Cubaynes, L. VoKy, F.J. Wuilleumier, B. Rouvellou, A. Hibbert, P. Faucher, J.M. Bizau, L. Journel, H.E. Saraph and F. Bely-Dubau, Phys. Rev. A 57 (1998) 4432. (Na2p)
- CWB94** G. Cooper, Z. Wenzhu and C.E. Brion, Can. J. Phys. 72 (1994) 1093. (IF<sub>5</sub> - I4d, I3d, F1s)
- CW&92** D. Cubric, A.A. Wills, J. Comer and M.A. MacDonald, J. Phys. B 25 (1992) 5069. (Kr3d)
- CZ&91** G. Cooper, E.B. Zarate, R.K. Jones and C.E. Brion, Chem. Phys. 150 (1991) 251. (SO<sub>2</sub> - S2p,2s)

- D68** R.D. Deslattes, Phys. Rev. Lett. 20 (1968) 483. (Xe3d)
- D69** R.D. Deslattes, Phys. Rev. 186 (1969) 1. (Ar2p)
- D72** J.L. Dehmer, J. Chem. Phys. 56 (1972) 4496. (potential barriers - review; H<sub>2</sub>S, SF<sub>5</sub>CF<sub>3</sub>, SF<sub>6</sub>-S1s; BF<sub>3</sub>-B1s; CS<sub>2</sub>, H<sub>2</sub>S, SO<sub>2</sub>, SF<sub>6</sub>-S2p; SiCl<sub>4</sub>, SiF<sub>4</sub>-Si2p)
- D86a** L.C. Davis, J. Appl. Phys. 59 (1986) R25. (Ni3p)
- D86b** R.D. Deslattes, Aust. J. Phys. 39 (1986) 845. (Ar1s; HCl, CH<sub>3</sub>Cl - Cl1s; H<sub>2</sub>S - S1s)
- D92a** J. Delwiche, AIP Conf. Proc. 258 (1992) 292. (SiF<sub>4</sub>, SiCl<sub>43</sub> - Si2p; C<sub>6</sub>F<sub>6</sub> - Cl1s, F1s)
- D92b** V.K. Dolmatov, J. Phys. B 25 (1992) L692. (Mn4s)
- D93a** V.K. Dolmatov, J. Phys. B 26 (1993) L79. (Mn3p)
- D93b** V.K. Dolmatov, J. Phys. B 26 (1993) L393. (Cr3p)
- DA&93** J. Doppelfeld, N. Anders, B. Esser, F. von Busch, H. Scherer and A. Zinz, J. Phys. B 26 (1993) 445. (Ar1s)
- DBH83** S. Daviel, C.E. Brion and A.P. Hitchcock, Rev. Sci. Inst. 55 (1984) 182. (N<sub>2</sub>-N1s; HCl-Cl2p, review)
- DBK91** M. Deutsch, G. Brill and P. Kizler, Phys. Rev. A 43 (1991) 2591. (Xe1s)
- DB&96** Th. Dohrmann, A. von dem Borne, A. Verweyen, B. Sonntag, M. Wedowski, K. Godehusen and P. Zimmermann, J. Phys. B 29 (1996) 5699. (Cr3p)
- DB&98** C. Dezarnaud-Dandine, F. Bournel, M. Tronc, D. Jones and A. Modelli, J. Phys. B 31 (1998) L497. (CH<sub>3</sub>)<sub>2</sub>S<sub>x</sub> x=1-3 - Si1s)
- DC76** P.W. Deutsch and L.A. Curtiss, Chem. Phys. Lett. 39 (1976) 588. (CH<sub>4</sub>, NH<sub>3</sub>, H<sub>2</sub>O, HF)
- DCT98** N.V. Dobrodey, L.S. Cederbaum and F. Tarantelli, Phys. Rev. B 58 (1998) 2316. (NiN<sub>2</sub> - N1s)
- DCZ83** J.W. Davenport, G.J. Cosgrove and A. Zangwill, J. Chem. Phys. 78 (1983) 1095. (Li<sub>2</sub>-Li1s, Na<sub>2</sub>-Na1s)
- DC&90** J.P. Doering, M.A. Copley, J.W. Cooper and J.H. Moore, Phys. Rev. A 41 (1990) 535. (Ar2p)
- DC&96** S. Diehl, D. Cubaynes, J.-M. Bizau, L. Journel, B. Rouvellou, S. Al Moussalam, F.J. Wuilleumier, E.T. Kennedy, N. Berrah, C. Blanchard, T.J. Morgan, J. Bozek, A.S. Schlachter, L. VoKy, P. Faucher and A. Hibbert, Phys. Rev. Lett. 76 (1996) 3915. (Li1s)
- DC&97a** S. Diehl, D. Cubaynes, E.T. Kennedy, F.J. Wuilleumier, J.-M. Bizau, L. Journel, L. VoKy, P. Faucher, A. Hibbert, C. Blanchard, N. Berrah, T.J. Morgan, J. Bozek and A.S. Schlachter, J. Phys. B 30 (1997) L595. (Li1s)
- DC&97b** S. Diehl, D. Cubaynes, F.J. Wuilleumier, J.-M. Bizau, L. Journel, E.T. Kennedy, C. Blanchard, L. VoKy, P. Faucher, A. Hibbert, N. Berrah, T.J. Morgan, J. Bozek and A.S. Schlachter, Phys. Rev. Lett. 79 (1997) 1241. (Li1s)
- DC&99** R.Darcy, J.T. Costello, C. McGuiness and G. O'Sullivan, J. Phys.B 32 (1999) 4859.(Sb4d)

- DD75** J.L. Dehmer and D. Dill, Phys. Rev. Lett. 35 (1975) 213. (N<sub>2</sub>-N1s)
- DD76a** J.L. Dehmer and D. Dill, J. Chem. Phys. 65 (1976) 5327.(N<sub>2</sub>-N1s)
- DD76b** J.L. Dehmer and D. Dill, Proc. 2nd Int. Conf. on Inner Shell Ionization Phenomenon, Freiburg, W. Mehlhorn and R. Brehm, eds., (1976) 221. (N<sub>2</sub>-N1s)
- DD79** J.L. Dehmer and D. Dill, *Electron-Molecule and Photon-Molecule Collisions* (T. Rescigno,ed.; Plenum, 1979) 225. (N<sub>2</sub>-N1s; CO-C1s,O1s)
- DDH82** W.R. Daasch, E.R. Davidson and A.U. Hazi, J. Chem. Phys. 76 (1982) 6031. (CO<sub>2</sub>-O1s)
- DF76** L.C. Davis and L.A. Feldkamp, Sol. St. Comm. 19 (1976) 413. (Cr,Mn,Fe,Co,Ni-3p)
- DF81** L.C. Davis and L.A. Feldkamp, Phys. Rev. A 24 (1981) 1862. (Cu3p)
- DFL92** P. Decleva, G. Fronzoni and A. Lisini, Chem. Phys. 168 (1992) 51. (Ni(CO)<sub>4</sub>, Ni(C<sub>3</sub>H<sub>5</sub>)<sub>2</sub> - Ni2p; Pd(C<sub>3</sub>H<sub>5</sub>O<sub>2</sub> - Pd2p; Fe(CO)<sub>2</sub>(NO)<sub>2</sub> - Fe2p; Cr(NO)<sub>4</sub> - Cr2p)
- DF&89** C. Dzionk, W. Fielder, M. von Lucke and P. Zimmermann, Phys. Rev. Lett. 62 (1989) 878 (Dy4d).
- DF&94** P. Decleva, G. Fronzoni, A. Lisini and M. Stener, Chem. Phys. 186 (1994) 1. (TiX<sub>4</sub>, X=F,Cl,Br - Ti1s, Ti2p; VOX<sub>3</sub>, X=F,Cl - V1s, V2p; CrO<sub>2</sub>X<sub>2</sub>, X=F,Cl - Cr1s, Cr2p; MnO<sub>3</sub>X, X=F,Cl - Mn1s, Mn2p)
- DF&00** D. Duflot, J.P. Flament, J. Heinesch and M.J Hubin-Franskin, J El. Spec. 113 (2000) 79. (C<sub>6</sub>H<sub>6</sub> – C1s)
- DF&03** D. Duflot, J.P. Flament, I.C. Walker, J. Heinesch and M.J Hubin-Franskin, J Chem. Phys. 118 (2003) 1137. (C<sub>3</sub>H<sub>4</sub>O – C1s, O1s)
- DF&08** D. Duflot, J.P. Flament, A. Giuliani, J. Heinesch and M.J Hubin-Franskin, Int. J. Mass. Spec. (2008) in press. (C<sub>2</sub>H<sub>4</sub>O<sub>2</sub> – C1s, O1s)
- DG86** A.K. Dozier and P.C. Gibbons, Phys. Rev. A 32 (1985) 1981. (Xe4d)
- DGT92** C. Dezarnaud, F. Guillot and M. Tronc, J. Phys. B 25 (1992) L123 (Xe2p,2s).
- DG&86** J.P. Doering, A. Gedanken, A.P. Hitchcock, P. Fischer, J.A. Moore, J.K. Olthoff, J. Tossell, K. Raghavachari and M.B. Robin, J. Am. Chem. Soc. 108 (1986) 3602. (B<sub>3</sub>N<sub>3</sub>H<sub>6</sub>-B1s,N1s; C<sub>6</sub>H<sub>6</sub>,C<sub>6</sub>H<sub>12</sub>-C1s)
- DH86a** M. Deutsch and M. Hart, J. Phys. B 19 (1986) L303. (Kr1s)
- DH86b** M. Deutsch and M. Hart, Phys. Rev. A 34 (1986) 5168. (Kr1s)
- DH&86** G. Dujardin, L. Hellner, D. Winkoun and M.J. Besnard, Chem. Phys. 105 (1986) 291. (CH<sub>3</sub>I-I4d)
- DH&89** G. Dujardin, L. Hellner, B.J. Olsson, M.J. Besnard-Ravage and A. Doderich, Phys. Rev. Lett. 62 (1989) 745. (SO<sub>2</sub> - S2p)
- DH&98** D. Duflot, C. Hannay, J.P. Flament and M.J. Hubin-Franskin, J. Chem. Phys. 109 (1998) 5308. (C<sub>3</sub>N<sub>2</sub>H<sub>4</sub>, C<sub>4</sub>H<sub>5</sub>N - C1s, N1s)

- DH&02** M. Drescher, M. Hentschel, R. Kienberge, M. Uiberacker, V. Yakovlev, A. Scrinzi, Th. Westerwalbesloh, U. Kleineberg U. Heinzmann and F. Krausz, *Nature* 419 (2002) 803. (Kr 3d)
- DH&09** D. Dowek, A. Houas, R. Guillemin, C. Elkharrat, J.C. Houver, W.B. Li, F. Catoire, L. Journel, M. Simon and R.R. Lucchese *Eur. Phys. J. Spec. Top.* 169 (2009) 85. (N<sub>2</sub>O - N1s)
- DJ&92** H.J. Dietrich, R. Jung, E. Waterstradt and K. Muller-Dethlefs, *Ber. Bun. Physik. Chem.* 96 (1992) 1179. (CO<sub>2</sub>, (CO<sub>2</sub>)<sub>n</sub> - C1s)
- DK73** P.W. Deutsch and A.B. Kunz, *J. Chem. Phys.* 59 (1973) 1155. (CH<sub>4</sub>, SiH<sub>4</sub>)
- DK75** P.W. Deutsch and A.B. Kunz, *J. Chem. Phys.* 62 (1975) 4069. (CH<sub>4</sub>-C1s; Ne1s)
- DK92** M. Deutsch and P. Kitzler, *Phys. Rev. A* 45 (1992) 2112 (Xe1s, Kr1s).
- DK94** G. Dawber and G.C. King, *J. Phys. B* 27 (1994) L685. (CO - C1s)
- DK&82** G.H.F. Diercksen, W.P. Kaemer, T.N. Rescigno, C.F. Bender, B.V. McKoy, S.R. Langhoff and P.W. Langhoff, *J. Chem. Phys.* 76 (1982) 1043. (H<sub>2</sub>O - O1s)
- DL86** K.G. Dyall and R.E. LaVilla, *Phys. Rev. A* 34 (1986) 5123. (Ar1s)
- DLR82** A. Duguet, A. Lahman-Bennani and M. Rouault, *J. Chem. Phys.* 76 (1982) 5178. (Ar1s)
- DL&83** R.D. Deslattes, R.E. LaVilla, P.L. Cowan and A. Henins, *Phys. Rev. A* 27 (1983) 923. (Ar1s)
- DM98** V.K. Dolmatov and S.T. Manson, *J. Phys. B* 31 (1998) 999. (Mn3p)
- DMD92** M. Deutsch, N. Maskil and W. Drube, *Phys. Rev. A* 46 (1992) 3963 (Ar1s).
- DM&92** M. Domke, T. Mandel, A. Puschmann, C. Xue, D.A. Shirley, G. Kaindl, H. Petersen and P. Kuske, *Rev. Sci. Inst.* 63 (1992) 80 (Ar2p, Kr3d, Xe4d, N<sub>2</sub>-N1s, CO, O<sub>2</sub> - O1s)
- DO&96** J.M. Durand, J. Olivier-Fourcade, J.C. Jumes, M. Womes, C.M. Teodorescu, A. Elafif, J.M. Esteva and R.C. Karnatak, *J. Phys. B* 29 (1996) 5773. (S<sub>2</sub> - S1s)
- DQB90** D.M. Dickinson, C.A. Quarles and C.E. Blount, *J. El. Spectr.* 53 (1990) 195. (N<sub>2</sub> - N1s)
- DP&95** M. Domke, R. Püttner, K. Schulz and G. Kaindl, *Phys. Rev. A* 52 (1995) 1147. (SiCl<sub>4</sub> - Si2p)
- DR83** V. Dose and G. Reusing, *J. El. Spectrosc.* 32 (1983) 257. (NH<sub>3</sub>, NO, N<sub>2</sub>, N<sub>2</sub>O, NF<sub>3</sub> - N1s by ion yield)
- DRK94** M. Domke, G. Remmers and G. Kaindl, *Nucl. Inst. Meth. B* 87 (1994) 173. (N<sub>2</sub>, NO - N1s; CO, CH<sub>4</sub>, CD<sub>4</sub> - C1s; CO - O1s)
- DR&89** R. Dudde, M.L.M. Rocco, E.E. Koch, S. Bennstorff and W. Eberhardt, *J. Chem. Phys.* 91 (1989) 20. (C<sub>5</sub>H<sub>5</sub>N, C<sub>4</sub>H<sub>4</sub>N<sub>2</sub>, C<sub>3</sub>H<sub>3</sub>N<sub>3</sub> - N1s)
- DSD76** D. Dill, J. Segal and J.L. Dehmer, *J. Chem. Phys.* 65 (1976) 3158. (CO-C1s, O1s; N<sub>2</sub>-N1s)
- DS&80** D. Dill, J.R. Swanson, S. Wallace and J.L. Dehmer, *Phys. Rev. Lett.* 45 (1980) 1393. (CO-C1s, O1s; N<sub>2</sub>-N1s)

- DS&91** A. Dadouch, S. Stranger, M.Y. Adam, L. Hellner, G. Dujardin and F. Combet-Farnoux, Phys. Rev. A 43 (1991) 1648. (Cu3p)
- DS&92** A. DiCicco, S. Stizza, A. Filippini, F. Boscherini and S. Mobilio, J. Phys. B 25 (1992) 2309 (SiX<sub>4</sub>, x=Cl,F,CH<sub>3</sub> - Si1s)
- DS&05** D. Duflot, K. Sidhoum, J.-P. Flament, A. Giuliani, J. Heinesch and M.-J. Hubin-Franskin, Eur. Phys. J. D 35 (2005) 239. (C<sub>3</sub> H<sub>3</sub>N<sub>3</sub> - C1s, N1s)
- DS&21** Simon Dörner, Lucas Schwob et al., Probing Structural Information of Gas-Phase Peptides by Near-Edge X-ray Absorption Mass Spectrometry, J. Am. Soc. Mass Spectrom. 32 (2021) 670–684. (C<sub>28</sub>H<sub>37</sub>N<sub>5</sub>O [LeuEnk+H]; C<sub>27</sub>H<sub>35</sub>N<sub>5</sub>O<sub>7</sub>S MetEnk+H], ENK = Tyr-Gly-Gly-Phe) - C1s, N1s, O1s)
- DT02** A.T. Domondon and X.M. Tong, Phys. Rev. A 65 (2002) 032718. (I4d)
- DTH90** C. Dezarnaud, M. Tronc and A.P. Hitchcock, Chem. Phys. 142 (1990) 455. (RSH, R=Me, Et, Ph); RSR (R=Me,Et), PhSMe - S1s; CH<sub>3</sub>SH - C1s, S2p, S2s)
- DTM91** C. Dezarnaud, M. Tronc and A. Modelli, Chem. Phys. 156 (1991) 129. (CH<sub>3</sub>SH, (CH<sub>3</sub>)<sub>2</sub>S, C<sub>2</sub>H<sub>5</sub>SH, (C<sub>2</sub>H<sub>5</sub>)<sub>2</sub>S, C<sub>6</sub>H<sub>5</sub>SH, C<sub>6</sub>H<sub>5</sub>SCH<sub>3</sub>, CH<sub>3</sub>SCN, CH<sub>3</sub>SNC, SCl<sub>2</sub> - S1s)
- DV82** A.Yu. Dukhnyakov and A.S. Vinogradov, Opt. Spectrosc. 53 (1982) 502 [Opt. Spek. 53 (1982) 841]. (SiF<sub>4</sub>-F1s)
- DYM86** G. Doggett, F.N. Yousif and J.A.D. Matthew, Mol. Phys. 57 (1986) 1297. (Li, LiH-Li1s)
- DX&90** M. Domke, C. Xue, A. Puschmann, T. Mandel, E. Hudson, D.A. Shirley and G. Kaindl, Chem. Phys. Lett. 173 (1990) 122. (erratum: Chem. Phys. Lett. 174 (1990) 668. (CO - C1s, O1s)
- E64** D.L. Ederer, Phys. Rev. Lett. 13 (1964) 760. (Xe4d)
- E87** W. Eberhardt, Phys. Scripta T17 (1987) 28. (CO, Fe(CO)<sub>5</sub>-C1s)
- EA&91** F.J. Esposto, P. Aebi, T. Tyliszczak, A.P. Hitchcock, M. Kasrai, J.D. Bozek, T.E. Jackman and S.R. Rolfe, J. Vac. Sci. Tech A 9 (1991) 1663. (BF<sub>3</sub> - B1s)
- EA&97** B. Esser, U. Ankerhold, N. Anders and F. von Busch, J. Phys. B 30 (1997) 1191. (COS, CS<sub>2</sub> - S1s)
- EB&88** W. Eberhardt, S. Bernstorff, H.W. Jochims, S.B. Whitfield and B. Crasemann, Phys. Rev. A 38 (1988) 3808 (Ar2p)
- EB&18** Egorov, D.; Bari, S. Near-Edge Soft X- ray Absorption Mass Spectrometry of Protonated Melittin. J. Am. Soc. Mass Spectrom. 2018, 29, 2138. (C<sub>131</sub>H<sub>229</sub>N<sub>39</sub>O<sub>31</sub> - C1s, N1, O1s)
- EC&85** W. Eberhardt, C.T. Chen, W.K. Ford, E.W. Plummer and H.R. Moser, *Dissociation Induced by Electronic Transitions II*, Springer Series in Surface Science 4 (1985) 50. (CO, Fe(CO)<sub>5</sub>, Fe<sub>3</sub>(CO)<sub>12</sub>, Cr(CO)<sub>6</sub>-C1s)
- ED&90** W. Eberhardt, R. Dudde, M.L.M. Rocco, E.E. Koch and S. Bernstorff, J. Electron Spectrosc. 51 (1990) 373. (N<sub>2</sub>, C<sub>6</sub>H<sub>5</sub>N, N<sub>2</sub>O - N1s)
- EF&00** I.G. Eustatiu, J. T. Francis, T. Tyliszczak, C.C. Turci, A.L.D. Kilcoyne and A.P. Hitchcock, Chem. Phys. 257 (2000) 235. (SF<sub>6</sub> – S2p, S2s, F1s)

- EG&83** J.M. Esteva, B. Gauthe, P. Dhez and R.C. Karnatak, *J. Phys. B* 16 (1983) L263. (Ne1s)
- EH&76** W. Eberhardt, R.P. Haelbich, M. Iwan, E.E. Koch and C. Kunz, *Chem. Phys. Lett.* 40 (1976) 180. ( $\text{CH}_4$ ,  $\text{C}_2\text{H}_6$ ,  $\text{C}_2\text{H}_2$ ,  $\text{C}_2\text{H}_4$ ,  $\text{C}_6\text{H}_6$ , - C1s)
- EH&96** P. Erman, P.A. Hatherly, A. Karawajczyk, U. Köble, E. Rachlew-Kallne, M. Stankiewicz and K.Y. Franzen, *J. Phys. B* 29 (1996) 1501. (NO-N1s)
- EH&98** I.G. Eustatiu, B. Huo, S.G. Urquhart and A.P. Hitchcock, *J. Electron Spectrosc.* 94 (1998) 243. (o,m,p- $\text{C}_7\text{H}_8$  - C1s)
- EH99** L.E. Ennis and A.P. Hitchcock, *J. Chem. Phys.* 111 (1999) 3468. ( $\text{HBO}$ ,  $\text{H}_3\text{B}_3\text{O}_3$ - B1s, O1s;  $\text{HBS}$  – B1s, S2p;  $\text{H}_2\text{S}$  – S2p)
- EKK78** W. Eberhardt, G. Kalkoffen and C. Kunz, *Phys. Rev. Lett.* 41 (1978) 156. (Kr3d, Xe4d)
- EK&83** J.M. Esteva, R.C. Karnatak, J.C. Fuggle and G.A. Sawatzky, *Phys. Rev. Lett.* 50 (1983) 910. (La3d)
- EK&95a** P. Erman, A. Karawajczyk, E. Rachlew-Kalne and C. Strömholm, *J. Phys. B* 28 (1995) 2069. (CO - C1s)
- EK&95b** A. Elafif, R.C. Karnatak, J.M. Esteva, C.M. Teodoresiu, M. Womes and E. Bouisset, *Physica B* 208 (1995) 115. (NaBr - Na1s; KBr - K1s)
- EK&95c** P. Erman, A. Karawajczyk, E. Rachlew, M. Stankiewicz and K.Y. Franzen, MAX report (1995) 170. (COS-C1s)
- EK&96** P. Erman, A. Karawajczyk, U. Köble, E. Rachlew-Kallne, and K.Y. Franzen, *Phys. Rev. A* 53 (1996) 1407. (CO-C1s)
- EK&97a** P. Erman, A. Karawajczyk, E. Rachlew, M. Stankiewicz and K.Y. Franzen, *Phys. Rev A* 56 (1997) 2705. (COS - S2p, C1s)
- EK&97b** P. Erman, A. Karawajczyk, E. Rachlew, M. Stankiewicz and K.Y. Franzen, *J. Chem. Phys.* 107 (1997) 10827. (COS - S2p, C1s)
- EK&97c** P. Erman, A. Karawajczyk, E. Rachlew, M. Stankiewicz and K.Y. Franzen, *Acta Phys. Polonica A* 91 (1997) 769. (COS - C1s, O1s, S2p)
- EK&97d** C. Engemann, G. Kohring, A. Pantelouris, J. Hormes, S. Grimme, S.D. Peyerimhoff, J. Clade, F. Frick and M. Jansen, *Chem. Phys.* 221 (1997) 189. ( $\text{P}_4\text{O}_6$ ,  $\text{P}_4\text{O}_7$ ,  $\text{P}_4\text{O}_6\text{S}$ ,  $\text{P}_4\text{O}_6\text{Se}$  - P1s)
- ELM70** D.L. Ederer, T. Lucarto and R.P. Madden, *Phys. Rev. Lett.* 25 (1970) 1537. (Li1s)
- ELS74** D.L. Ederer, T.B. Lucarto and E.B. Soloman, Proc. 4th Int. Vac. UV Rad. Phys. Conf. (Hamburg, 1974) 245. (Ba4d)
- EL&75** D.L. Ederer, T.B. Lucarto, E.B. Soloman, R.P. Madden and J. Sugar, *J. Phys. B* 8 (1975) L21. (Ba4d)
- EL&98** L.E. Ennis, J.F. Lehmann, A.P. Hitchcock, B. Cook and W.J. Leigh, (1998) unpublished. ( $\text{C}_6\text{H}_{10}$ ,  $\text{C}_8\text{H}_{14}$  - C1s)
- EM74** J.M. Esteva and G. Mehlman, *Astrophys. J.* 193 (1974) 747. (Mg 2p)

- EP&87** W. Eberhardt, E.W. Plummer, I.W. Lyo, R. Murphy, R. Carr and W.K. Ford, J. Phys. 48 (1987) C9-679. (N<sub>2</sub> - N1s)
- ER&92** W. Eberhardt, J.E. Rubensson, K.J. Randall, J. Feldhaus, A.L.D. Kilcoyne, A.M. Bradshaw, Z. Xu, P.D. Johnson and Y. Ma, Phys. Scripta T 41 (1992) 143 (N<sub>2</sub>-N1s)
- ES84** W. Eberhardt and T.K. Sham, Proc. of S.P.I.E. (1984) 143. (CO, CH<sub>2</sub>ClCHCl<sub>2</sub>, CH<sub>3</sub>COOH, (CH<sub>3</sub>)<sub>2</sub>CO,C<sub>6</sub>H<sub>6</sub>,C<sub>6</sub>H<sub>5</sub>Cl-C1s)
- ES&83a** W. Eberhardt, T.K. Sham, R. Carr, S. Krummacher, M. Strongin, S.L. Weng and D. Wesner, Phys. Rev. Lett. 50 (1983) 1038. (CO, (CH<sub>3</sub>)<sub>2</sub>CO - C1s)
- ES&83b** W. Eberhardt, J. Stöhr, J. Feldhaus, E.W. Plummer and F. Sette, Phys. Rev. Lett. 51 (1983) 2370. (N<sub>2</sub>-N1s)
- ES&84** W. Eberhardt, T.K. Sham, R.G. Carr, S. Krummacher, M. Strongin, S.L. Weng and D. Wesner, NSLS Report (1984). ((CH<sub>3</sub>)<sub>2</sub>CO-C1s)
- ES&16** D. Egorov, L. Schwob, et al, Near edge X-ray absorption mass spectrometry of gas phase proteins: the influence of protein size, Phys.Chem.Chem.Phys., 18 (2016) 26213. (proteins -C1s)
- ETH99** I.G. Eustatiu, T. Tyliszczak and A.P. Hitchcock, Chem. Phys. Lett. 300 (1999) 676. (SF<sub>6</sub> - S2p, S2s)
- ET&00** I.G. Eustatiu, T. Tyliszczak, A.P. Hitchcock, C.C. Turci, A.B. Rocha and C.E. Bielschowsky, Phys. Rev. A 61 (2000) 042505. (CO<sub>2</sub> - C1s, O1s)
- ET&07** I.G. Eustatiu, T. Tyliszczak, G. Cooper, A. P. Hitchcock, C.C. Turci, A.B. Rocha, M. Barbatti, and C.E. Bielschowsky, J. Electron Spectrosc. Rel. Phenom. 156-158 (2007) 145. (CS<sub>2</sub> - C1s, S2p)
- EUH98** L.E. Ennis, S.G. Uruquhart and A.P Hitchcock, (1998) unpublished. (C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>,C<sub>3</sub>H<sub>8</sub>O<sub>2</sub> - C1s, O1s)
- EU&98** L.E. Ennis, S.G. Uruquhart and A.P Hitchcock, (1998) unpublished. (C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>,C<sub>3</sub>H<sub>8</sub>O<sub>2</sub> - C1s, O1s)
- F68** V.A. Fomichev, Sov. Phys. Solid State 9 (1968) 2496 [Fiz. Tverd. Tela 9 (1967) 3167]. (BF<sub>3</sub> - B1s)
- F72** U. Fano, Comments At. Mol. Phys. 3 (1972) 75. (review)
- F95** R.F. Fink, J. El. Spec. 76 (1995) 295. (N<sub>2</sub>, N<sub>2</sub>O – N1s; N<sub>2</sub>O – O1s)
- F97** R.F. Fink, J. Chem.Phys. 106 (1997) 4038. (NO – N1s, O1s)
- FA91** A. Flores-Riveros and H. Agren, Phys. Scripta 44 (1991) 442 (CO,CO<sub>2</sub> - C1s, O1s)
- FA98** A. Filippioni and P D. Angelo, J. Chem. Phys. 109 (1998) 5356. (Br<sub>2</sub> - Br1s; GeCl<sub>4</sub> – Ge1s; BBr<sub>3</sub> – Br1s)
- FB70** V.A. Fomichev and R.L. Barinskii, J. Struct. Chem. 11 (1970) 810 [Zh. Struk. Khim. 11 (1970) 875]. (BF<sub>3</sub>, BCl<sub>3</sub> - B1s, Cl2p)
- FB02** R. Feng and C.E. Brion, Chem. Phys. 284 (2002) 615. (C<sub>4</sub>H<sub>10</sub>O – C1s)
- FBN90** J.L. Ferrer, S. Bodeur and I. Nenner, J. El. Spectr. 52 (1990) 711. (Si(CH<sub>3</sub>)<sub>x</sub>Cl<sub>4-x</sub>, x=0-4; Si1s; X=0-3 Cl1s)

- FB&94** F. Federmann, O. Björneholm, A. Beutler and T. Möller, Phys. Rev. Lett. 73 (1994) 1549. (Ne<sub>n</sub>-Ne<sub>n</sub>-Ne1s)
- FB&00** R. Feifel, F Burmeister et al. Phys. Rev. Lett. 85 (2000) 3133. (HCl – Cl2p)
- FB&01** A De Fanis, H-J Beyer, K J Ross and J B West, J. Phys. B 34 (2001) 199. (Cs4d)
- FB&02** R. F. Fink F. Burmeister, R. Feifel, M. Bässler, O. Björneholm, L. Karlsson, C. Miron, and M.-N. Piancastelli, S. L. Sorensen, H. Wang, K. Wiesner, and S. Svensson, Phys Rev. A 70 (2002) 034705. (HCl, DCl – Cl2p)
- FB&03a** R. Flesch, I.L. Bradenau, A.A. Pavylchev and E. Ruhl, Bessy Ann. Rep. (2003) 78. (Ar<sub>n</sub>-Ar2p, N<sub>2</sub>-N1s)
- FB&03b** R. Flesch, I.L. Bradenau, A.A. Pavylchev and E. Ruhl, Bessy Ann. Rep. (2003) 76. (C<sub>6</sub>H<sub>6</sub>- C1s, C<sub>5</sub>H<sub>5</sub>N - N1s)
- FB&14** Fronzoni G, Baseggio O, Stener M, Hua W, Tian G, Luo Yet al Vibrationally resolved high-resolution NEXAFS and XPS spectra of phenanthrene and coronene. J Chem Phys 141 (2014) 044313. (C<sub>14</sub>H<sub>10</sub>, C<sub>24</sub>H<sub>12</sub> – C1s)
- FB&07** V. Feyer, P. Bolognesi, M. Coreno, K.C. Prince and L. Avaldi, J. El. Spec. 161 (2007) 17. (N<sub>2</sub>-N1s)
- FC68** U. Fano and J. W. Cooper, Rev. Mod. Phys. 40 (1968) 441. (atoms - theory, review)
- FCB99** R Feng, G. Cooper and C.E. Brion, Chem. Phys. 244 (1999) 127. (H<sub>2</sub>S – S2p)
- FCB00** R Feng, G. Cooper and C.E. Brion, Chem. Phys. 252 (2000) 359. (COS – C1s, S2p)
- FCH05** R. Feng, R.G. Cavell and A.P. Hitchcock, J. Electron Spectrosc. 144-147 (2005) 231 (SO<sub>2</sub> - S2p, S2s)
- FCM96** I.W. Fomunung, Z. Chen and A.Z Msezane, Phys. Rev. A 53 (1996) 806. (CO<sub>2</sub> - C1s; SF<sub>6</sub> - S2p)
- FD95** A. Filippini and A. DiCicco, Phys. Rev. B 52 (1995) 15,135. (Br<sub>2</sub> - Br1s; CS<sub>2</sub> - S1s)
- FDL93** G. Fronzoni, P. Decleva and A. Lisini, Chem. Phys. 174 (1993) 57. [Ni(CO)<sub>4</sub>-Ni1s; Fe(CO)<sub>5</sub>, Fe(C<sub>5</sub>H<sub>5</sub>)<sub>2</sub>- Fe1s; Cr(CO)<sub>6</sub>,Cr(NO)<sub>4</sub>, CrO<sub>2</sub>Cl<sub>2</sub>-Cr2p]
- FD&93** G. Fronzoni, P. Decleva, A. Lisini and M.Ohno J. Electron Spectrosc. 62 (1993) 245. [Ni(CO)<sub>4</sub>-Ni2p; Fe(CO)<sub>5</sub>, Fe(C<sub>5</sub>H<sub>5</sub>)<sub>2</sub>- Fe2p; Cr(CO)<sub>6</sub>-Cr2p]
- FE&86** J.L. Feldman, W.T. Elam, A.C. Ehrlich, E.F. Skelton, D.D. Dominguez, D.D.L. Chung and F.W. Lytle, Phys. Rev. B 33 (1986) 7961. (Br<sub>2</sub>-Br1s)
- FE&94** J.T. Francis, C. Enkvist, S. Lunell and A.P. Hitchcock, Can. J. Phys. 72 (1994) 879. (CO, C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>4</sub>, C<sub>6</sub>H<sub>6</sub> - C1s)
- FE&99** K.Y. Franzen, P. Erman, A. Karawajczyk, E.Rachlew, P.A. Hatherly and M.Stankiewicz, J. Chem. Phys. 110 (1999) 3621. (CS<sub>2</sub> – C1s, S2p)
- FE&04** R.F. Fink, A. Eschner, M. Magnuson, O. Björneholm, I. Hjelte, C. Miron, M. Bassler, S. Svnesson, M. Novella Piancastelli and S.L. Sorensen, Max Lab Annual Report 2004, 178. COS-S2p.
- FE&06** R. F. Fink, A. Eschner, et al., Long-lived highly excited sulphur atoms produced by an ultrafast dissociation of 2p-1s\*-excited OCS molecules“ J. Phys. B 39 (2006) L269 (OCS – S2p)

- FF&96** H. Feist, M. Feldt, et al., Phys. Rev. A 53 (1996) 760. (Fe3p, Co3p, Ni3p)
- FG&02** R. Feifel, F. Gel'mukhanov, A. Baev, H. Ågren, M.N. Piancastelli, M. Bässler, C. Miron, S. L. Sorensen, A. Naves de Brito, O. Björneholm, L. Karlsson, and S. Svensson, Phys. Rev. Lett. 89 (2002) 103002. (N<sub>2</sub> - N1s)
- FH92** J.T. Francis and A.P. Hitchcock, J. Phys. Chem. 96 (1992) 6598. (C<sub>6</sub>H<sub>4</sub>O<sub>2</sub>, C<sub>6</sub>H<sub>6</sub>O, C<sub>6</sub>H<sub>6</sub>O<sub>2</sub> - C1s, O1s)
- FH94** J.T. Francis and A.P. Hitchcock, J. Phys. Chem. 98 (1994) 3650. (C<sub>6</sub>H<sub>10</sub>O, 1,2;-1,3;-1,4-C<sub>6</sub>H<sub>8</sub>O<sub>2</sub> - C1s, O1s)
- FH&87** T.A. Ferrett, P.A. Heiman, H.G. Kerkhoff, U.E. Becker, D.W. Lindle and D.A. Shirley, Chem. Phys. Lett. 138 (1987) 607. (SO<sub>2</sub>-S2p)
- FH&96** M. Fujisawa, A. Harasawa, A. Agui, M. Watanabe, A. Kakizaki, S. Shin, T. Ishii, T. Kita, T. Harada, Y. Saitoh and S. Suga, Rev. Sci. Inst. 67 (1996) 345. (Ar2p, N<sub>2</sub> - N1s)
- FH&97** A. Farhat, M. Humphrey, B. Langer, N. Berrah, J.D. Bozek and D. Cubaynes, Phys. Rev. A 56 (1997) 501. (Ar2p)
- FH&16** Thomas Fransson, Yoshihisa Harada, Nobuhiro Kosugi, Nicholas, Besley, Bernd Winter, John J. Rehr, Lars G. M. Pettersson and Anders Nilsson, Chem. Rev. 116 (2016), 7551. (H<sub>2</sub>O - O1s)
- FH&20** F. Frati, M. O.J.Y. Hunault, and F.M.F.de Groot. "Oxygen K-edge X-ray Absorption Spectra." Chemical Reviews 120 (2020) 4056. (CO, NO, O<sub>2</sub> - O1s)
- FKA99** R.F. Fink, M. Kivikopolo and H. Aksela, J. Chem. Phys. 111 (1999) 10034. (HCl - Cl2p)
- FKH94** J.T. Francis, N. Kosugi and A.P. Hitchcock, J. Chem. Phys. 101 (1994) 10429. (CO - C1s)
- FK&00** R. Feifel, L. Karlsson et al. MaxLab Report (2000) 156. (CO - C1s)
- FK&02** R. Feifel, L. Karlsson, M.-N. Piancastelli, R.F. Fink, M. Bässler, O. Björneholm, K. Wiesner, C. Miron, H. Wang, A. Giertz, S. L. Sorensen, A. Naves de Brito, S. Svensson, Phys. Rev A 65 (2002) 052701. (CO - C1s)
- FL96** G. Fronzoni and A. Lisini, Chem. Phys. 207 (1996) 1. (n-C<sub>n</sub>H<sub>2n</sub>, n=3-6 - C1s)
- FL00** X.W. Fan and K.T. Leung, Phys. Rev. A 62 (2000) 062703. (Ar2p)
- FL01** X.W. Fan and K.T. Leung, J. Chem. Phys. 115 (2001) 2603. (SiF<sub>4</sub> - Si2p)
- FL02** X.W. Fan and K.T. Leung, J. El. Spec. 132 (2002) 287. (C<sub>2</sub>ClH<sub>5</sub> - C1s, Cl2p)
- FL&86** T.A. Ferrett, D.W. Lindle, P.A. Heiman, H.G. Kerkhoff, U.E. Becker and D.A. Shirley, Phys. Rev. A 34 (1986) 1916. (SF<sub>6</sub>-S1s)
- FL&87** T.A. Ferrett, D.W. Lindle, P.A. Heiman, W.D. Brewer, U.E. Becker, H.G. Kerkhoff and D.A. Shirley, Phys. Rev. A 36 (1987) 3172. (Li1s)
- FL&88** T.A. Ferrett, D.W. Lindle, P.A. Heiman, M.N. Piancastelli, P.H. Kobrin, H.G. Kerkhoff, U.E. Becker, W.D. Brewer and D.A. Shirley, J. Chem. Phys. 89 (1988) 4726. (SF<sub>6</sub>-S2p)
- FM92** Z. Felfli and S.T. Manson, Phys. Rev. Lett. 68 (1992) 1687 (Li1s)

- FM&96** E. Fainelli, F. Marocci, R. Platania and L. Avaldi, J. Chem. Phys. 104 (1996) 3227. (NO - N1s)
- FM&98** E. Fainelli, F. Marocci, R. Platania and L. Avaldi, J. Electron Spectrosc. 87 (1998) 169. (SF<sub>6</sub> - S2p, F1s)
- FM&01** E. Fainelli, F. Marocci, R. Platania and L. Avaldi, J. Electron Spectrosc. 119 (2001) 81. (CCl<sub>4</sub> – Cl2p)
- FM&04** R. Friedleinm L. Minkov, F. Gel'mukhanov, W. Osikowicz, C. Seuss, G. Ohrwall, S.L. Sorensen, H. Agren aand W.R. Salaneck, Max Lab annual report 2004, 180. (C<sub>10</sub>H<sub>8</sub>, C<sub>12</sub>H<sub>10</sub> – C1s)
- FN67** P. Feldman and R. Novick, Phys. Rev 160 (1967) 143. (Li1s)
- FN&06** S. Fritzsche, J. Nikkinen, S.-M. Huttula, H. Aksela, M. Huttula and S. Aksela, MAXLab 2005-06 Annual Report (2006) 220. (Ar2p)
- FP11** R. Feifel and M.N. Piancastelli, J. El. Spec. 183 (2011) 10. (H<sub>2</sub>O - O 1s)
- FPH97** G. Faraci, A.R. Pennisi and J.L. Hazemann, Phys. Rev. B 56 (1997) 12553. (Kr1s)
- FPR05** R. Flesch, J. Plenge, E. Rühl, Int J Mass Spec 249-250 (2006) 68. (ClO<sub>2</sub> – Cl2p, O1s)
- FPS95a** D.L. Foulis, R.F. Pettifer and P. Sherwood, Europhys. Lett. 29 (1995) 647. (Cl<sub>2</sub> - Cl1s)
- FPS95b** D.L. Foulis, R.F. Pettifer and P. Sherwood, Physica B 209 (1995) 68. (HCl - Cl1s)
- FP&80** H. Friedrich, B. Pittel, P. Rabe, W.H.E. Schwarz and B. Sonntag, J. Phys. B 13 (1980) 25. (SiF<sub>4</sub> - Si2p)
- FP&88** T.A. Ferrett, M.N. Piancastelli, D.W. Lindle, P.A. Heiman and D.A. Shirley, Phys. Rev. A 38 (1988) 701. (SiF<sub>4</sub> - Si2p, 2s)
- FP&01** R . Flesch, A.A. Pavlychev, J.J. Neville, J. Blumberg, M. Kuhlmann, W. Tappe, F. Senf, O. Schwarzkopf, A.P. Hitchcock, and E. Rühl, Phys. Rev. Lett. 86 (2001) 3767. ((N<sub>2</sub>)<sub>n</sub> – N1s)
- FP&09** V. Feyer, O. Plekan, M. Coreno, K.C. Prince, V. Caravetta, J. Phys. Chem. A 113 (2009) 10726. (C<sub>2</sub>H<sub>5</sub>NO<sub>2</sub>, C<sub>4</sub>H<sub>7</sub>N<sub>2</sub>O<sub>3</sub> – N 1s)
- FP&10** Feyer V,Plekan O,Richter R, Coreno M, de Simone M, Prince KC et al Tautomerism in cytosine and uracil: a theoretical and experimental X-ray absorption and resonant auger study. J Phys Chem A 114 (2010) 10270. (C<sub>4</sub>H<sub>4</sub>N<sub>2</sub>O<sub>2</sub>, C<sub>4</sub>H<sub>5</sub>N<sub>3</sub>O – C1s, N1s, O1s)
- FP&11** Feyer V, Plekan O, Kivim A, Prince KC, Moskovskaya TE, Zaytseva IL et al ) Comprehensive core-level study of the effects of isomerism halogenation, and methylation on the tautomeric equilibrium of cytosine. J Phys Chem A 115 (2011) 7722. (C<sub>4</sub>H<sub>4</sub>FN<sub>3</sub>O, C<sub>4</sub>H<sub>5</sub>N<sub>3</sub>O C<sub>5</sub>H<sub>7</sub>N<sub>3</sub>O – C1s, N1s, O1s)
- FR&87** J. Feldhaus, A. Reimer, J. Schirmer, A,M, Bradshaw, H.G. Kerkoff, B. Langler, D. Szostak, R. Wehlitz and W. Braun, J. Phys. 48 (1987) C9-773. (CO-C1s,O1s; N<sub>2</sub>-N1s)
- FSD99** G. Fronzoni, M. Stener and P. DeCleva, Chem. Phys. 248 (1999) 127. (ClF, ClF<sub>3</sub> – Cl2p, Cl1s)
- FSL91** R.E. Farren, J.A. Sheehy and P.W. Langhoff, Chem. Phys. Lett. 177 (1991) 307. (C<sub>2</sub>H<sub>x</sub>, x=2,4,6 - C1s)
- FS&79** H. Friedrich, B. Sonntag, P. Rabe, W. Butscher and W.H.E. Schwarz, Chem. Phys. Lett. 64 (1979) 360.

- (SiH<sub>4</sub>-Si2p; PH<sub>3</sub>- P2p)
- FS&95** L. Ferrand-Tanaka, M. Simon, R. Thissen, M. Lavollée and P. Morin, Rev. Sci. Inst. 66 (1995) 1587. (N<sub>2</sub>O - N1s)
- FS&96** L. Ferrand-Tanaka, M. Simon, R. Thissen, M. Lavollée and P. Morin, Rev. Sci. Inst. 67 (1996) 358. (N<sub>2</sub>O - N1s)
- FS&98** G. Fronzoni, M. Stener, P. Decleva and G.De Altı, Chem. Phys. 232 (1998) 9. (HCl - Cl2p, Cl1s)
- FS&00** R.F. Fink, S.L Sorensen, A. Naves de Brito, A. Ausmees and S. Svensson, J. Chem. Phys. 112 (2000) 6666. (C<sub>2</sub>H<sub>4</sub> – C1s)
- FS&02** A. De Fanis, N. Saito, H. Yoshida, Y. Senba, Y. Tamenori, H. Ohashi, H. Tanaka, and K. Ueda, Phys. Rev. Lett. 89 (2002) 243001. (Ne1s)
- FTD76** U. Fano, C.E. Theodosiou and J.L. Dehmer, Rev. Mod. Phys. 48 (1976) 49. (review - electron optical effects of atomic fields)
- FT&93** A. Filipponi, T.A. Tyson, K.O. Hodgson and S. Mobilio, Phys. Rev. 48 (1993) 1328. (SiH<sub>4</sub>, SiCl<sub>4</sub>, Si(CH<sub>3</sub>)<sub>4</sub>, SiF<sub>4</sub> - Si1s)
- FT&95** J.T. Francis, C.C. Turci, T. Tyliszczak, G.G.B. de Souza, N. Kosugi and A.P. Hitchcock, Phys. Rev. A 52 (1995) 4665. (SF<sub>6</sub> - S2p, S2s, F1s)
- FT&99** B.O. Fisher, M.K. Thomas, P.A. Hatherly, K Codling, M Stankiewicz, A Karawajczyk and M. Roper, J. Phys. B. 32(1999) 4437. (SO<sub>2</sub> – O1s, S2p)
- FZ&70** V.A. Fomichev, T.M. Zimkina, A.S. Vinogradov and A.M. Evdokimov, J. Struct. Chem. 11 (1970) 626 [Zh. Struk. Khim. 11 (1970) 676]. [SiCl<sub>x</sub>(CH<sub>3</sub>)<sub>4-x</sub> - Si2p]
- G51** H. Glaser, Phys. Rev. 82 (1951) 616. (GeCl<sub>4</sub>-Ge1s)
- G70** E. Gilberg, Z. Phys. 236 (1970) 2. (HCl - Cl1s)
- G77** E.S. Gluskin, Proc. VUV-5 (Montpellier, 1977) I-117. (Cl<sub>2</sub> - Cl2p)
- G82** T. Gustafsson, Proc. 8th Int. Conf. Atom. Phys., (Goteborg, Sweden,1982) 355. (N<sub>2</sub>-N1s)
- G83** S.J. Gurman, J. Phys. C 16 (1983) 2987. (N1s)
- G91** T.A. Green, *Boron Rich Solids*, AIP Conf. Proc. 231 (1991) 42. (C<sub>2</sub>B<sub>10</sub>H<sub>12</sub> - B1s)
- G94** F.M.F. de Groot, J. El. Spec. 67 (1994) 529. (review; FeCp<sub>2</sub> - Fe2p)
- G00** T.W Gorczyca, Phys. Rev. A 61 (2000) 024702-1. (Ne1s)
- GA95** F.Kh. Gel'mukhanov and H. Agren, J. Phys. B 28 (1995) 3699. ((CH<sub>2</sub>)<sub>n</sub>, n=2,4,11)
- GA97** F.Kh. Gel'mukhanov and H. Agren, Phys. Rev A 56 (1997) 2676. (CO - C1s, O1s)
- GA&80** A. Gerwer, C. Asaro, B.V. McKoy and P.W. Langhoff, J. Chem. Phys. 72 (1980) 713. (O<sub>2</sub> - O1s)

- GA&97** A. Gottwald, S. Anger, J.M. Bizau, D. Rosenthal and M. Richter, Phys. Rev. A 55 (1997) 3941. (Ca3d)
- GA&05a** A V Golovin, J Adachi, S Motoki, M Takahashi and A Yagishita, J. Phys. B 38 (2005) L63. (COS –S2p, C1s, O1s)
- GA&05b** A V Golovin, J Adachi, S Motoki, M Takahashi and A Yagishita, J. Phys. B 38 (2005) 3755. (COS –S2p, C1s, O1s)
- GB81** M. Galan and C.F. Bunge, Phys. Rev. A 23 (1981) 1624. (Li1s)
- GB&83** L.J. Garvin, E.R. Brown, S.L. Carter and H.P. Kelly, J. Phys. B 16 (1983) L269. (Mn3p)
- GB&11** M.F. Gharaibeh, J.M. Bizau, J.Phys. B 44 (2011) 172208. (N-N1s)
- GBP82** D.C. Griffin, C. Bottcher and M.S. Pindzola, Phys. Rev. A 25 (1982) 1374. (Ti2p, Zr3p, Hf4p)
- GC&88** F.A. Grimm, T.A. Carlson, J. Jimenez Mier, B. Yates, J.W. Taylor and B.P. Pullen, J. EL. Spect. 47 (1988) 257. (N<sub>2</sub>O - N1s,O1s)
- GC&92** X. Guo, G. Cooper, W.F. Chan, G.R. Burton and C.E. Brion, Chem. Phys. 161 (1992) 471 (SiF<sub>4</sub> - Si2p, Si2s)
- GC&02** A.V. Golovin and N.A. Cherepkov, J. Phys. B 35 (2002) 3191. (CO-C1s,O1s)
- GC&03** M.L. Gordon, G. Cooper, C. Morin, T. Araki, C.C. Turci, K. Kaznatcheev, and A. P. Hitchcock, Inner shell spectroscopy of the peptide bond: comparison of the C 1s, N 1s and O 1s spectra of glycine, glycyl-glycine and glycyl-glycyl-glycine, J. Phys. Chem A 107 (2003) 6144. (C<sub>2</sub>H<sub>5</sub>NO<sub>2</sub>, C<sub>4</sub>H<sub>8</sub>N<sub>2</sub>O<sub>3</sub> C<sub>6</sub>H<sub>16</sub>N<sub>2</sub>O<sub>5</sub> - C1s, N1s, O1s.)
- GC&04** G. Cooper, M. Gordon, D.Tulumello, C.C. Turci, K. Kaznatcheev and A.P. Hitchcock, Inner shell excitation of glycine, glycyl-glycine, alanine and phenylalanine, J. Electron Spectroscopy 137-140 (2004) 795-799. (C<sub>2</sub>H<sub>5</sub>NO<sub>2</sub>, C<sub>4</sub>H<sub>8</sub>N<sub>2</sub>O<sub>3</sub> C<sub>3</sub>H<sub>7</sub>NO<sub>2</sub> , C<sub>8</sub>H<sub>9</sub>NO<sub>2</sub> - C1s, N1s, O1s; C<sub>6</sub>H<sub>6</sub>-C1s)
- GDT97** F. Guillot, C. Dezarnaud-Dandine and M. Tronc, Chem. Phys. 224 (1997) 281. (GeCl<sub>4</sub>, SnCl<sub>4</sub>, AsCl<sub>3</sub>, PCl<sub>3</sub> - Cl 2p ; GeCl<sub>4</sub> - Ge2p; SnCl<sub>4</sub> - Sn2p; AsCl<sub>3</sub> - As2p; PCl<sub>3</sub> - P1s)
- GD&95** F. Guillot, C. Dezarnaud-Dandine, M. Tronc, A. Lisini, P. Decleva and G. Fronzini, Chem. Phys. 191 (1995) 289. (Mo(CO)<sub>6</sub>, MoF<sub>6</sub> - Mo2p, Mo1s)
- GD&96** F. Guillot, C. Dezarnaud-Dandine, M. Tronc, A. Modelli, A. Lisini, P. Decleva and G. Fronzini, Chem. Phys. 205 (1996) 359. (GeH<sub>4</sub>, GeCl<sub>4</sub>, GeMe<sub>3</sub>Cl - Ge 2p; GeCl<sub>4</sub> - Ge3p,Cl2p,Cl1s)
- GD&15** R. Guillemin, P. Decleva, M. Stener, C. Bomme, T. Marin, L. Journel, T. Marchenko, R.K. Kushawaha, K. Jänkälä, N. Trcera, K.P. Bowen, D.W. Lindle, M.N. Piancastelli & M. Simon, Nature Comm 6 (2015) 6166 (CS<sub>2</sub> - S1s)
- GE&89** J. Gus, D.E. Ellis, E. Alp, L. Soderholm and G.K. Shenoy, Phys. Rev. B 39 (1989) 6125. (UCl<sub>4</sub> - U3d, U3p)
- GE&92** J.A. de Gouw, J. van Eck, J. van der Weg and H.G. Herdenan, J. Phys. B 25 (1992) 2007.(Ar2p)
- GE&94** J.A. de Gouw, J. van Eck, A.Q. Wollrabe, J. van der Weg and H.G.M. Heidemann, J.Phys. B 27 (1994) 3915. (Ar2p, Kr3d)

- GE&95** J.A. de Gouw, J. van Eck, J. van der Weg and H.G.M. Heidemann, J.Phys. B 28 (1995) 1761. (Ar2p)
- GGL72** F.A. Gianturco, C. Guidotti and U. Lamanna, J. Chem. Phys. 57 (1972) 840. (SF<sub>6</sub> - S2p, S1s)
- GG&96** P. Glans, K. Gunnelin, P. Skytt, J.H. Guo, N. Wassdahl, J. Nordgren, H. Agren, F. Kh. Gel'mukhanov, T. Warwick and E. Rotenberg, Phys. Rev. Lett. 76 (1996) 2448. (O<sub>2</sub> - O1s)
- GG&98a** K. Gunnelin, P. Glans, P. Skytt, J.H. Guo, J. Nordgren, H. Agren, Phys. Rev. A 57 (1998) 864. (CO<sub>2</sub> - O1s)
- GG&98b** A. Gottwald, Ch. Gerth, M. Groen, M. Richter and P. Zimmermann, J.Phys. B 31 (1998) 3875. (Pr4d, Nd4d)
- GG&99** K. Gunnelin, P. Glans, J.E. Rubensson, C. Sathe, J. Nordgren, Y. Li, F. Gel'mukhanov and H. Agren, Phys. Rev. Lett. 83 (1999) 1315. (C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>4</sub>, C<sub>2</sub>H<sub>6</sub> – C1s)
- GH01** M.L. Gordon and A.P. Hitchcock, unpublished (C<sub>3</sub>H<sub>6</sub>NO<sub>2</sub>, C<sub>8</sub>H<sub>9</sub>NO<sub>2</sub> - C1s, N1s, O1s)
- GHF81** E. Gilberg, M.J. Hanus and B. Foltz, Rev. Sci. Inst. 52 (1981) 662. (Ar 2p)
- GH&94** F.M.F. de Groot, Z.W. Hu, M.F. Lopez, G. Kaindl, F. Guillot and M. Tronc, J. Chem. Phys. 101 (1994) 6570. (MoF<sub>6</sub> - Mo2p)
- GK86** P.W. Goalwin and A.B. Kunz, Phys. Rev. B 34 (1986) 2140. (CH<sub>4</sub>-C1s)
- GKM77a** E.S. Gluskin, A.A. Krasnoperova and L.N. Mazalov, J. Struct. Chem. 18 (1977) 156 [Zh. Struk. Khim. 18 (1977) 185]. (SF<sub>6</sub> - S2p)
- GKM77b** E.S. Gluskin, A.A. Krasnoperova and L.N. Mazalov, J. Struct. Chem. 18 (1977) 529 [Zh. Struk. Khim. 18 (1977) 665]. (Cl<sub>2</sub> - Cl2p)
- GK&91** F.X. Gadea, H. Koppel, J. Schirmer, L.S. Cederbaum, K.J. Randall, A.M. Bradshaw, Y. Ma, F. Sette and C.T. Chen, Phys. Rev. Lett 66 (1991) 883. (C<sub>2</sub>H<sub>4</sub> - C1s)
- GM98** Z.W. Gortel and D. Menzel, Phyas. Rev. A 58 (1998) 3699. (O<sub>2</sub> – O1s)
- GM00** T.W. Garcyyca and B.M. McLaughlin, J. Phys.B 33 (2000) L859. (O1s)
- GMK77** F.K. Gel'mukhanov, L.N. Mazalov and A.V. Kondratenko, Chem. Phys. Lett. 46 (1977) 133. (CO-C1s,O1s)
- GMT85** J.C. Giordan, J.H. Moore and J.A. Tossell, J. Am. Chem. Soc. 107 (1985) 5600. (C<sub>6</sub>H<sub>6</sub>-C1s)
- GM&75** E.S. Gluskin, L.N. Mazalov, A.P. Sadovskii and D.A. Zhogolev, J. Struct. Chem. 16 (1975) 972 [Zh. Struk. Khim. 16 (1975) 1061]. (N<sub>2</sub>O-N1s)
- GM&76** E.S. Gluskin, L.N. Mazalov, A.A. Krasnoperova, V.A. Kochubei, S.I. Mishnev, A.N. Shrinskii, E.M. Trahtenberg and G.M. Tumaikin, Bull. Acad. Sci. USSR Phys. Ser. 40 (1976) No. 2, p.1 [Izv. Akad. Nauk. SSSR Fiz. Ser. 40 (1976) 226]. (Kr3d, SiCl<sub>4</sub> - Si2p, POCl<sub>3</sub> - P2p)
- GM&04** A.C.O. Guerra, J.B. Maciel, C.C. Turci, R.C. Bilodeau and A. P. Hitchcock, , Can. J. Chem. 82 (2004) 1052. (CO - C1s, O1s)
- GM&06** A.C.O. Guerra, J.B. Maciel, C.C. Turci, H. Ikeura-Sekiguchi and A. P. Hitchcock, Chemical Physics 326

(2006) 589. (DCO<sub>2</sub>H, HCO<sub>2</sub>D, D<sub>2</sub>CO, CH<sub>2</sub>O<sub>2</sub> - C1s)

- GN&83** M.M. Gofman, V.I. Nefedov, V.L. Kraizman and R.V. Vedrinski, J. Electron Spectrosc. 32 (1983) 59. (N<sub>2</sub>-N1s; CO-C1s,O1s; SF<sub>6</sub>-S2p,F1s)
- GOI97** T. Gejo, K. Okada and T. Ibuki, Chem. Phys. Lett. 272 (1997) 497. (O<sub>3</sub> - O1s)
- GP&98** E.Gedat, R. Puttnoy, M. Domke and G. Kaindl, J. Chem. Phys. 109 (1998) 4471. (SO<sub>2</sub> – S2p)
- GR&03** K. Godehusen, T. Richter, P. Zimmermann and M. Martins, J. Phys. B 36 (2003) L387. (Cr3p)
- GR&12** González-Magaña, O.; Reitsma e al., Near-edge X-ray absorption mass spectrometry of a gas-phase peptide. J. Phys. Chem. A 116 (2012) 1074. (C<sub>26</sub>H<sub>36</sub>N<sub>3</sub>O<sub>7</sub> – C1s).
- GSL0** Guillemin R, Stolte WC, Lindle D, WFragmentation of formic acid following photo- excitation around the carbon K edge. J Phys B Atomic Mol Phys 42 (2009) 125101. (CH<sub>2</sub>O<sub>2</sub>-C1s)
- GSM73** E.S. Gluskin, A.P. Sadovskii and L.N. Mazalov, J. Struct. Chem. 14 (1973) 685 [Zh. Struk. Khim. 14 (1973) 739]. (NO, N<sub>2</sub>, N<sub>2</sub>O - N1s)
- GSS83** F.A. Gianturco, E. Semprini and F. Stefani, Nuovo Cimento D 2 (1983) 687. (BF<sub>3</sub>-B1s)
- GS&96** P. Glans, P. Skytt, K. Gunnelin, J.H. Guo and J. Nordgren, J. Electron Spectrosc. 82 (1996) 192. (N<sub>2</sub>-N1s)
- GS&05** R. Guillemin, W. C. Stolte, L. T. N. Dang, S.-W. Yu, and D. W. Lindle, J. Chem. Phys. 122 (2005) 094318. (H<sub>2</sub>S – S2p)
- GT91** R.J. Gould and Y.D. Jung, Astrophys. J. 373 (1991) 271. (C,N,O,Ne,Mg,Si,S,P - 1s)
- GTM98** Z.W. Gortel, R. Techima and D. Menzel, Phys. Rev. A 58 (1998) 1225. (N<sub>2</sub>-N1s; CO-C1s, O1s)
- GTM99** Z.W. Gortel, R. Techima and D. Menzel, Phys. Rev. A 60 (1999) 2159. (HCl – Cl2p)
- GT&03a** M.L.Gordon, D.Tulumello, G. Cooper,A.P. Hitchcock, P. Glatzel, O.C. Mullins and U. Bergmann, J. Phys. Chem. B (2003) (submitted). (C<sub>6</sub>H<sub>6</sub>, C<sub>10</sub>H<sub>8</sub>, C<sub>14</sub>H<sub>10</sub>, C<sub>14</sub>H<sub>10</sub>, C<sub>18</sub>H<sub>12</sub>, C<sub>18</sub>H<sub>12</sub> - C1s)
- GT&03b** T Gejo, Y Takata, T Hatsui, M Nagasono, H Oji, N Kosugi, E Shigemasa, Chem. Phys. 289 (2003) 15. (Ar2p, N<sub>2</sub> - N1s; NO<sub>2</sub>-N1s, O1s; SO<sub>2</sub>, O<sub>2</sub>-O1s)
- GT&11** Y.K. Gao, .a Traeger, K. Kotsisw and V. Staemmler, Phys. Chem. Chem. Phys.13 (2011) 10709 (C<sub>3</sub>H<sub>7</sub>NO<sub>2</sub> - C1s, N1s, O1s)
- GV95** Z.W. Gortel and J.P. de Villiers, Chem. Phys. Lett. 245 (1995) 41. (N<sub>2</sub> - N1s)
- GYA96** F.Kh. Gel'mukhanov, L. Yang and H. Agren, J. Chem. Phys. 105 (1996) 5224. (H(C<sub>2</sub>H<sub>2</sub>)<sub>n</sub>H, n=1-10 - C1s)
- GW09** A. Ganesan and F. Wang, J. Chem. Phys.,131 (2009) 044321. (C<sub>3</sub>H<sub>7</sub>NO<sub>2</sub>, C<sub>6</sub>H<sub>6</sub>, C<sub>8</sub>H<sub>10</sub>O<sub>2</sub>, C<sub>8</sub>H<sub>11</sub>N – C 1s; C<sub>8</sub>H<sub>11</sub>NO<sub>2</sub> – C1s, N1s, O1s)
- GZ&20** A. Guarnaccio, T. Zhang, et al., PPT Isolated Molecule and Its Building Block Moieties Studied by C 1s and O 1s Gas Phase X-ray Photoelectron and Photoabsorption Spectroscopies : J. Phys. Chem. C 124 (2020) 9774. (C<sub>12</sub>H<sub>8</sub>S – C 1s; C<sub>18</sub>H<sub>15</sub>PO – C1s, O1s; C<sub>32</sub>H<sub>28</sub>P<sub>2</sub>O<sub>2</sub>(PPT) – C1s, O1s)

- H31** J.D. Hanawalt, Phys. Rev. 37 (1931) 715. (As, AsCl<sub>3</sub>, AsH<sub>3</sub>, As<sub>2</sub>O<sub>3</sub> -As1s; AsBr<sub>3</sub>, Br<sub>2</sub>, HBr – Br 3d; Hg, HgCl<sub>2</sub> – Hg1s; Kr2p, Se<sub>8</sub>, SeO<sub>2</sub>-Se 2p; Xe2pZn – Zn1s) - ADD TO TABLE, check edges, in papers-op\gas
- H72** J.E. Hansen, J. Phys. B 5 (1972) 1083. (La4d)
- H77a** J.B. Hastings, Proc. VUV-5 (Montpellier, 1977) I-61. (Ar1s)
- H77b** P.J. Hay, J. Am. Chem. Soc. 99 (1977) 1013. (SF<sub>6</sub> - S2p, F1s)
- H86a** I. Harrison, PhD thesis (1986), University of Manchester (SF<sub>6</sub>-S2p)
- H86b** A.P. Hitchcock, Proc. EXAFS IV, J. Phys. (Paris) 47 C-8 (1986) 575. (C<sub>3</sub>H<sub>6</sub>, C<sub>3</sub>H<sub>8</sub>, C<sub>4</sub>H<sub>8</sub>, C<sub>4</sub>H<sub>10</sub>, C<sub>5</sub>H<sub>8</sub>-C1s; CF<sub>3</sub>OOCF<sub>3</sub>-C1s,O1s,F1s; C<sub>4</sub>H<sub>4</sub>S, C<sub>4</sub>H<sub>8</sub>S-C1s,S2p,S1s)
- H87** R.G. Hayes, J. Chem. Phys. 86 (1987) 1683. (CS<sub>2</sub>-C1s,S2p)
- H89** A.P. Hitchcock, Ultramicroscopy, 28 (1989) 165. (review - N<sub>2</sub>, N<sub>2</sub>O, - N1s; CO,CH<sub>4</sub>, CH<sub>3</sub>OH, C<sub>6</sub>H<sub>12</sub>, C<sub>6</sub>H<sub>6</sub>, C<sub>6</sub>F<sub>6</sub> - C1s)
- H90a** A.P. Hitchcock, Phys. Scripta T31 (1990) 159. (**Review:** Ne1s; NH<sub>3</sub>, N<sub>2</sub>H<sub>4</sub>, N<sub>2</sub> - N1s; PCL<sub>3</sub> - Cl2p; C<sub>2</sub>H<sub>6</sub>, C<sub>2</sub>H<sub>3</sub>F<sub>3</sub>, CF<sub>4</sub>, C<sub>2</sub>F<sub>6</sub>, C<sub>2</sub>F<sub>4</sub>, C<sub>6</sub>F<sub>6</sub>, CO, Mn(CO)<sub>5</sub>Br, Fe(CO)<sub>5</sub>, Co<sub>2</sub>(CO)<sub>8</sub>, Ni(CO)<sub>4</sub>, MCp<sub>2</sub> (M = Fe,Co,Ni), C<sub>5</sub>H<sub>6</sub> - C1s; CF<sub>3</sub>O<sub>2</sub>CF<sub>3</sub> - O1s)
- H90b** D.M. Hanson, Adv. Chem. Phys. 77 (1990) 1. (review; O<sub>2</sub>-O1s; N<sub>2</sub>O-N1s, O1s)
- H92a** A.P. Hitchcock, unpublished. (C<sub>2</sub>Cl<sub>3</sub>H, C<sub>2</sub>Cl<sub>2</sub>H<sub>4</sub> - C1s, Cl2p; C<sub>7</sub>H<sub>5</sub>N - C1s, N1s; NO - N1s)
- H92b** A.P. Hitchcock, *Collision Processes of Ions, Positrons, Electrons and Photons with Matter*, Proc. ELAF-91 (World Sci., 1992) 104. (CO, Fe(CO)<sub>5</sub>, C<sub>7</sub>H<sub>10</sub>, C<sub>7</sub>CoH<sub>5</sub>O<sub>2</sub>, C<sub>8</sub>H<sub>12</sub>, C<sub>8</sub>H<sub>9</sub>F<sub>3</sub>, C<sub>8</sub>Co<sub>2</sub>O<sub>8</sub>, C<sub>9</sub>H<sub>10</sub>O<sub>2</sub>, C<sub>10</sub>CoH<sub>10</sub> - C1s)
- H98** G.H. Ho, Chem. Phys. 226 (1998) 101. (CCl<sub>4</sub> - Cl2p)
- H00** A.P. Hitchcock, J. El. Spec. 112 (2000) 9. (review; HBO, HBS – B1s; HBS, H<sub>2</sub>S – S2p; CO-C1s; C<sub>6</sub>H<sub>6</sub>N<sub>2</sub>O<sub>2</sub> – C1s; C<sub>9</sub>H<sub>10</sub>O<sub>2</sub>, C<sub>10</sub>H<sub>10</sub>O<sub>4</sub> – C1s; SF<sub>6</sub> – S2p; CO<sub>2</sub> – C1s)
- H01** A.P. Hitchcock (2001) unpublished (C<sub>3</sub>H<sub>6</sub>O<sub>3</sub> - C1s, O1s)
- H04** U, Hergenhan, J. Phys. B 37 (2004) R89. (CO<sub>2</sub> – O 1s)
- H14** A.P. Hitchcock (2014) unpublished (C<sub>2</sub>ClF<sub>3</sub> – Cl2p, C1s)
- H19** A.P. Hitchcock (2019) unpublishtd. (CCl<sub>2</sub>F<sub>2</sub>, C<sub>2</sub>F<sub>2</sub>H<sub>4</sub> – C1s, F1s, Cl2p)
- H31** J. D. Hanawalt, The Dependence of X-Ray Absorption Spectra Upon Chemical and Physical State, Phys. Rev. 37 (1931) 715. (As,AsCl<sub>3</sub>, As<sub>2</sub>O<sub>3</sub>, AsH<sub>3</sub> – As1s; HBr, Br<sub>2</sub>, AsBr<sub>3</sub> – Br1s, Hg, HgCl<sub>2</sub> - Hg2p; Kr – Kr2p; Se<sub>8</sub>, SeO<sub>2</sub> – Se1s; Xe 2p)
- HA&95** P.A. Hatherly, J. Adachi, E. Shigemasa and A. Yagashita, J. Phys. B 28 (1995) 2643 (CO - C1s, O1s)
- HA&97** M.J. Hubin-Franksin, H. Aouni, D. Duflot, F. Motte-Tollet, C. Hannay, L.F. Ferreira and G. Tourillon, J. Chem. Phys. 106 (1997) 35. (C<sub>2</sub>H<sub>3</sub>CN, C<sub>4</sub>H<sub>2</sub>N<sub>2</sub>, C<sub>4</sub>H<sub>5</sub>N - C1s, N1s)

- HA&98a** D.L. Hansen, M.E. Arrasate, J. Cotter, G.R. Fisher, K.T. Leung, J.C. Levin, R. Martin, P. Neill, R.C.C. Perera, I.A. Sellin, M. Simon, Y. Uehara, B. Vanderford, S.B. Whitfield and D.W. Lindle, Phys. Rev. A 57 (1998) R2608. (HCl - Cl 1s)
- HA&98b** D.L. Hansen, G.B. Armen, M.E. Arrasate, J. Cotter, G.R. Fisher, K.T. Leung, J.C. Levin, R. Martin, P. Neill, R.C.C. Perera, I.A. Sellin, M. Simon, Y. Uehara, B. Vanderford, S.B. Whitfield and D.W. Lindle, Phys. Rev. A 57 (1998) R4090. (HCl - Cl 1s)
- HA&98c** D.L. Hansen, M.E. Arrasate, J. Cotter, G.R. Fisher, O. Hemmers, K.T. Leung, J.C. Levin, R. Martin, P. Neill, R.C.C. Perera, I.A. Sellin, M. Simon, Y. Uehara, B. Vanderford, S.B. Whitfield and D.W. Lindle, Phys. Rev. A 58 (1998) 3757. (HCl, DCl - Cl 1s; H<sub>2</sub>S, D<sub>2</sub>S - S 1s)
- HA&04** K Hosaka, J Adachi, et al. , J. Phys. B 37 (2004) L49. (NO – N1s)
- HA&06** K Hosaka, J Adachi, A V Golovin, M Takahashi, T Teramoto, N Watanabe, A Yagishita, S K Semenov and N A Cherepkov, J. Phys. B 39 (2006) L25. (N<sub>2</sub>-N1s)
- HB71** W. Hayes and F.C. Brown, J. Phys. B 4 (1971) L85. (BF<sub>3</sub>,BCl<sub>3</sub> - B1s)
- HB72** W. Hayes & F.C. Brown, Phys. Rev. A 6 (1972) 21. (SiH<sub>4</sub> - Si2p; GeH<sub>4</sub> - Ge2p; HCl - Cl2p; PH<sub>3</sub> -P2p; H<sub>2</sub>S - S2p)
- HB77** A.P. Hitchcock and C.E. Brion, J. El. Spectrosc. 10 (1977) 317. (C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>4</sub>, C<sub>2</sub>H<sub>6</sub>, C<sub>6</sub>H<sub>6</sub> - C1s)
- HB78a** A.P. Hitchcock and C.E. Brion, J. El. Spectrosc. 13 (1978) 193. (CH<sub>3</sub>X, (X=F,Cl,Br,I) - C1s, F1s, Cl2p, Br3d, I4d)
- HB78b** A.P. Hitchcock and C.E. Brion, J. El. Spectrosc. 14 (1978) 417. (CH<sub>x</sub>Cl<sub>4-x</sub> (x=0-4) - C1s, Cl2p)
- HB78c** A.P. Hitchcock and C.E. Brion, Chem. Phys. 33 (1978) 55. (SF<sub>6</sub> - S2p, S2s, F1s)
- HB79a** A.P. Hitchcock and C.E. Brion, J. El. Spectrosc. 15 (1979) 401. HCN -C1s, N1s)
- HB79b** A.P. Hitchcock and C.E. Brion, Chem. Phys. 37 (1979) 319 (HCN, C<sub>2</sub>N<sub>2</sub> - C1s, N1s)
- HB79c** A.P. Hitchcock and C.E. Brion, J. El. Spectrosc. 17 (1979) 139. (CH<sub>3</sub>X, X=F,Cl,Br,I - C1s)
- HB80a** A.P. Hitchcock and C.E. Brion, J. El. Spectrosc. 18 (1980) 1. (CO -C1s,O1s; N<sub>2</sub> - N1s; O<sub>2</sub> - O1s)
- HB80b** A.P. Hitchcock and C.E. Brion, J. El. Spectrosc. 19 (1980) 231. (H<sub>2</sub>CO, CH<sub>3</sub>CHO, (CH<sub>3</sub>)<sub>2</sub>CO - C1s, O1s)
- HB80c** A.P. Hitchcock and C.E. Brion, J. Phys. B. 13 (1980) 3269. (Nels)
- HB81a** A.P. Hitchcock and C.E. Brion, J. El. Spectrosc. 22 (1981) 283. (C<sub>2</sub>H<sub>2</sub>-C1s)
- HB81b** A.P. Hitchcock and C.E. Brion, J. Phys. B. 14 (1981) 4399. (HF, F<sub>2</sub> - F1s)
- HBC96** A.P. Hitchcock, C.E. Brion and R.G. Cavell, unpublished. (PF<sub>3</sub>, CF<sub>3</sub>PCl<sub>2</sub>, PCl<sub>3</sub> - P2p, Cl2p, F1s)
- HBK71** W. Hayes, F.C. Brown and A.B. Kunz, Phys. Rev. Lett. 27 (1971) 774. (SiH<sub>4</sub>,SiF<sub>4</sub> - Si2p; GeH<sub>4</sub> - Ge3p)
- HBT87** A.P. Hitchcock, S. Bodeur and M. Tronc, Chem. Phys. 115 (1987) 93. (SCl<sub>2</sub>, S<sub>2</sub>Cl<sub>2</sub>, SOCl<sub>2</sub>, SO<sub>2</sub>Cl<sub>2</sub> - S1s,

Cl1s)

- HBT89** A.P. Hitchcock, S. Bodeur and M. Tronc, Physica 158 (1989) 257. ( $\text{S}(\text{CH}_3)_2$ ,  $\text{S}_2(\text{CH}_3)_2$ ,  $\text{SO}_2\text{F}_2$ ,  $\text{SOFCl}$ ,  $\text{SO}_2\text{Cl}_2$  - S1s)
- HBW78** A.P. Hitchcock, C.E. Brion and M.J. Van der Wiel, J. Phys. B 11 (1978) 3245. ( $\text{SF}_6$  - S2p)
- HBW79** A.P. Hitchcock, C.E. Brion and M.J. Van der Wiel, Chem. Phys. Lett. 66 (1979) 213. ( $\text{CO}_2$  - C1s;  $\text{N}_2\text{O}$ -N1s)
- HB&84** A.P. Hitchcock, S. Beaulieu, T. Steel, J. Stöhr and F. Sette, J. Chem. Phys. 80 (1984) 3927. ( $\text{CH}_4$ ,  $\text{C}_2\text{H}_6$ ,  $\text{C}_4\text{H}_6$ ,  $\text{C}_4\text{H}_8$ ,  $\text{C}_4\text{F}_8$ -C1s)
- HB&89** J.E. Hansen, J. Brilly, E.T. Kennedy and G.O. Sullivan, Phys. Rev. Lett. 63 (1989) 1934. ( $\text{Xe}$ ,  $\text{Cs}^+$ ,  $\text{Ba}^{2+}$ ,  $\text{La}^{3+}$  - 3d)
- HB&90** W. Habenicht, H. Barter, K. Muller-Dethlefs and E.W. Schlag, Phys. Scripta 41 (1990) 814. ( $\text{N}_2\text{O}$  - N1s)
- HB&91** W. Habenicht, H. Barter, K. Muller-Dethlefs and E.W. Schlag, J. Chem. Phys. 95 (1991) 6774. ( $\text{CF}_2\text{CH}_2$ ,  $\text{CF}_3\text{CH}_3$  - C1s)
- HB&97** Y.F. Hu, G.M. Bancroft, et al., Phys. Rev. A 56 (1997) R3342. (HBr - Br3d)
- HC96** C.H. Hu and D.P. Chong, Chem. Phys. Lett. 262 (1996) 729. ( $\text{CO}$ ,  $\text{C}_2\text{H}_2$ ,  $\text{C}_2\text{H}_4$ ,  $\text{C}_6\text{H}_6$  - C1s;  $\text{CH}_2\text{O}$  - C1s, O1s; CHFO,  $\text{CF}_2\text{O}$  - C1s, O1s, F1s)
- HC&87a** J. Hormes, R. Chauvistre, U. Kuetgens, U. Fischer and J. Ruppert, J. Phys. (Paris) 48 C-9 (1987) 1113. ( $(\text{CH}_3)_x\text{SiCl}_{4-x}$ ,  $x=0-4$  - Si1s)
- HC&87b** W. Habenicht, L.A. Chewter, M. Sander, K. Muller-Dethlefs and E.W. Schlag, J. Phys. 48 (1987) C9-741. ( $\text{CF}_2\text{CH}_2$ ,  $\text{CF}_3\text{COCH}_3$ ,  $\text{CF}_3\text{CH}_2\text{NH}_2$  - C1s)
- HC&95** P.A. Hatherly, K. Codling, M. Stankiewicz and M. Roper, J. Phys. B 28 (1995) 3249. ( $\text{CO}_2$  - C1s, O1s)
- HC&96** P.A. Hatherly, K. Codling, M. Stankiewicz and M. Roper, J. Electron Spectrosc. 79 (1996) 407. ( $\text{CO}_2$  - C1s, O1s)
- HC&99** D.L. Hansen, J. Cotter, G.R. Fisher, K.T. Leung, R. Martin, P. Neill, R.C.C. Perera, M. Simon, Y. Uehara, B. Vanderford, S.B. Whitfield and D.W. Lindle, J. Phys.B 32 (1999) 2629. ( $\text{CH}_3\text{Cl}$  - Cl 1s)
- HC&00** N. Haack, G. Ceballos, H. Werde, K. Baberschke, D. Arvanitis, A.L. Ankudinov and J.J. Rehr, Phys.Rev. Lett. 84 (2000) 614. ( $\text{C}_2\text{H}_2$ ,  $\text{C}_2\text{H}_4$ ,  $\text{C}_2\text{H}_6$  - Cs)
- HD&91** A.P. Hitchcock, R.S. DeWitte, J.M. Van Esbroeck, P. Aebi, C.L. French, R.T. Oakley and N.P.C. Westwood, J. Electron Spectrosc. 57 (1991) 165. ( $\text{C}_6\text{H}_4\text{N}_2\text{S}_x$ ,  $x=1-3$  - C1s, N1s, S2p, S2s, S1s)
- HD&92** G. Hagerow, W. Denzer, H.W. Jochims and H. Baumgartel, Chem. Phys. Lett. 195 (1992) 267 (BF<sub>2</sub>Cl, BFCl<sub>2</sub> - B1s)
- HD&99** C. Hannay, D. Duflot, J.P. Flament and M.J. Hubin-Franksin, J. Chem. Phys. 110 (1999) 5600. ( $\text{C}_5\text{H}_5\text{N}$ ,  $\text{C}_4\text{H}_4\text{N}_2$  - C1s, N1s)
- HE90** R.G. Hayes and W. Eberhardt, Phys. Scripta 41 (1990) 449. (CS<sub>2</sub>, C<sub>4</sub>H<sub>4</sub>S - S2p)

- HE91** R.G. Hayes and W. Eberhardt, J. Chem. Phys. 94 (1991) 397. ( $\text{C}_2\text{H}_4\text{S}$ ,  $\text{C}_4\text{H}_8\text{S}$  - S2p,C1s)
- HE&98** A.P. Hitchcock, I.G. Eustatiu, J.T. Francis and C.C. Turci, J. Electron Spectrosc. 88-91 (1998) 77. ( $\text{SF}_6$  - S2s;  $\text{C}_7\text{H}_8$  - C1s)
- HE&01** A.P. Hitchcock, L.E. Ennis, J.F. Lehmann and M.K. Denk, J. Electron Spectrosc. 114-116 (2001) 1037. ( $\text{C}_5\text{H}_{10}\text{N}_2$  ,  $\text{C}_{10}\text{H}_{20}\text{N}_2$  ,  $\text{C}_{10}\text{H}_{22}\text{N}_4$  – C1s, N1s; HBO-B1s, O1s, HBS-B1s, S2p;  $\text{H}_2\text{S}$ -S2p )
- HF15** A.P. Hitchcock and ???, unpublished (NO – N1s, O1s – rerun as earlier were wrong)
- HFK75** J.E. Hansen, A.W. Fliflet and H.P. Kelly, J. Phys. B 8 (1975) L127. (Ba4d)
- HFM87** A.P. Hitchcock, P. Fischer and R. McLaren, *Giant Resonances in Atoms, Molecules and Solids*, Proc. NATO ASI Ser. B: Physics 151 (1987) 281. ( $\text{CH}_4$ ,  $\text{CF}_4$  - C1s;  $\text{C}_n\text{F}_{2n+2}$ , n=2-6, C1s,F1s;  $\text{C}_2\text{HF}_{4-x}$ , x=0-4,  $\text{C}_6\text{HF}_{6-x}$ , x=0-6 - C1s)
- HF&87** A.P. Hitchcock, P. Fischer, A. Gedanken and M.B. Robin, J. Phys. Chem. 91 (1987) 531. ( $\text{C}_6\text{H}_x\text{F}_{6-x}$ ,x=0,6 - C1s, F1s)
- HF&91** A. Hiraya, K. Fukui, P.K. Tseng, T. Murata and M. Watanabe, J. Phys. Soc. Jpn., 60 (1991) 1824. (Ne1s)
- HF&93** A.P. Hitchcock, J.T. Francis, S.G. Urquhart, W. Leigh, E. Ruhl and N. Kosugi, unpublished. (O<sub>2</sub> - O1s)
- HF&00** T. Hyaishi, Y. Fujita, M. Izumisawa, T. Tanaka, E. Murakami, E. Shigemasa, A. Yagashita and Y. Morioka, J. Phys. B 33 (2000) 37. (Kr1s)
- HG76** M.J. Hanus and E. Gilberg, J. Phys. B 9 (1976) 137. ( $\text{C}_2\text{H}_5\text{Cl}$ ,  $\text{C}_2\text{H}_3\text{Cl}$ ,  $\text{CH}_3\text{Cl}$ ,  $\text{CF}_2\text{Cl}_2$  - Cl1s)
- HG&97** F. Heiser, O. Gessner, J. Viefhaus, K. Wieliczek, R. Hentges and U. Becker, Phys. Rev. Lett. 79 (1997) 2435. (CO - C1s)
- HHS86** A.P. Hitchcock, J.A. Horsley and J. Stöhr, J. Chem. Phys. 85 (1986) 4835. ( $\text{C}_4\text{H}_4\text{S}$ ,  $\text{C}_4\text{H}_8\text{S}$  - C1s, S2p, S2s, S1s)
- HH99** A. Hibbert and J.E. Hansen, J. Phys. B 32 (1999) 4133. (Ca3p)
- HH13** R. Hayes, A.P. Hitchcock (unpublished). ( $\text{C}_8\text{H}_8\text{O}$  -  $\text{C}_6\text{H}_5\text{CO}(\text{CH}_3)$  – C1s, O1s)
- HH14** R. Hayes, A.P. Hitchcock (unpublished). ( $\text{C}_2\text{H}_6\text{O}_2\text{S}$ ,  $\text{CH}_4\text{O}_3\text{S}$ -C1s, O1s, S2p; $\text{C}_2\text{F}_3\text{H}_3\text{O}_3\text{S}$ -C1s, F1s, O1s, S2p)
- HH&93** O. Hemmers, F. Heiser, J. Eiben, R. Wehlitz and U. Becker, Phys. Rev. Lett. 71 (1993) 987. (CO-C1s)
- HH&94** O. Hemmers, F. Heiser, J. Eiben, R. Wehlitz and U. Becker, Nucl. Inst. Meth. B 87 (1994) 209. (CO-C1s)
- HH&95** C. Hannay, J. Heinesch, U. Kleyens and M.J. Hubin-Franskin, Meas. Sci. Tech. 6 (1995) 1140. ( $\text{SF}_6$  - S2p)
- HH&96** C. Hennig, K.H. Hallmeier, A. Bach, S. Bender, R. Franke, J. Hormes and R. Szargan, Spectrochim. Acta 52 (1996) 1079. ( $\text{C}_3\text{H}_5\text{NO}$ ,  $\text{C}_3\text{H}_3\text{SO}$ ,  $\text{C}_4\text{H}_5\text{N}$ ,  $\text{C}_4\text{H}_7\text{N}$  – N1s)
- HH&98** C.W. Hutchings, A.P. Hitchcock, A.T. Wen, S.D. Hwang, J.A. Glass, J.T. Spencer, X.F. Hu, G.M. Bancroft and P.A. Dowben, J. Electron Spectrosc. 94 (1998) 187. ( $\text{C}_3\text{H}_9\text{P}$ ,  $\text{C}_8\text{H}_{18}\text{PCl}$ ,  $\text{PCl}_3$  - P2p, P2s, Cl2p, Cl2s)

- HH&99** O. Hemmers, F. Heiser, J. Viefhaus, K. Wieliczek and U. Becker, J. Phys. B 32 (1999) 3769. (CO – C1s)
- HI86** A.P. Hitchcock and I. Ishii, Proc. EXAFS IV, J. Phys. (Paris) 47 C-8 (1986) 199. (CF<sub>4</sub>,C<sub>6</sub>H<sub>6</sub>,C<sub>6</sub>H<sub>12</sub>-C1s; CO,CO<sub>2</sub>-C1s,O1s - EXELFS)
- HI87** A.P. Hitchcock and I. Ishii, J. Electron Spectrosc. 42 (1987) 11. (CH<sub>4</sub>, C<sub>2</sub>H<sub>6</sub>, C<sub>3</sub>H<sub>8</sub>, iso,n-C<sub>4</sub>H<sub>10</sub>, n-,iso-,neo-C<sub>5</sub>H<sub>12</sub>, C<sub>6</sub>H<sub>14</sub> - C1s)
- HI88a** A.P. Hitchcock and I. Ishii, unpublished. (C<sub>5</sub>H<sub>8</sub>O-C1s,O1s; C<sub>10</sub>H<sub>16</sub> (adamantine)-C1s; C<sub>10</sub>F<sub>16</sub>-C1s,F1s (perfluoro-adamantine); CH<sub>3</sub>CCH, C<sub>10</sub>H<sub>22</sub>O-C1s (decyl alcohol), C<sub>5</sub>H<sub>10</sub>O - tetrahydropyran)
- HI88b** A.P. Hitchcock and I. Ishii, unpublished. (COS - C1s,S2p,O1s; CO<sub>2</sub>-O1s; CF<sub>4</sub> -C1s, F1s; EXELFS: see also **HI86, HW&90**)
- HIR89** A.P. Hitchcock, I. Ishii and M.B. Robin, unpublished (N<sub>2</sub>H<sub>4</sub>-N1s; N<sub>2</sub>F<sub>4</sub> - N1s, F1s; CF<sub>3</sub>NO-C1s,N1s, O1s,F1s)
- HJ&87** G. Hagerow, H.W. Joachim, S. Bernstorff and H. Baumgartel, BESSY report (1987) 161. (BF<sub>3</sub> - B1s)
- HJ&02** A.P. Hitchcock, S. Johnston, T. Tyliaszczak, C.C. Turci, M. Barbatti, A.B. Rocha and C.E. Bielschowsky, J. Electron Spectrosc. Rel. Phe. 123 (2002) 303. (C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>2</sub> – C1s)
- HK83** J.B. Hastings and V.O. Kastroun, Nucl. Inst. Meth. 208 (1983) 815. (Kr1s)
- HK86** I. Harrison and G.C. King, J. Phys. B 19 (1986) L447. (CO-C1s)
- HK87** I. Harrison and G.C. King, J. Electron Spectr. 43 (1987) 155. (C<sub>2</sub>H<sub>4</sub>, CO<sub>2</sub>, COS, CS<sub>2</sub>-C1s; N<sub>2</sub>O-N1s)
- HKA88** I. Harrison, G.C. King and L. Avaldi, J. Phys. B 21 (1988) 4015. (CO-C1s)
- HKR86** J. Hormes, U. Kuettgens and I. Ruppert, Abstr.-EXAFS IV (1986). (SCl<sub>2</sub>-S1s)
- HK&69a** R. Haensel, G. Keitel. P. Schreiber and C. Kunz, Phys. Rev. 188 (1969) 1375. (Kr3d, Xe4d - solid, gas)
- HK&69b** R. Haensel, G. Keitel. P. Schreiber and C. Kunz, Phys. Rev. Lett. 22 (1969) 398. (Xe4d - solid, gas)
- HK&71** R. Haensel, G. Keitel, N. Kosuch, U. Nielsen and P. Schreiber, J. Phys. 32 (1971) C4-236. (Ar2p)
- HK&92** B.A. Hammel, D.R. Kania, F. Rogers, C.A. Iglesias, R.W. Lee, J.F. Seeley, C.N. Brown and J.M. Edwards, Europhysics Lett. 20 (1992) 319. (C1s)
- HK&98** A. Hiltunen, T. Kyisil, J. Mursu, O.P. Sairanen, H. Aksela and S. Aksela, J. El. Spec. 87 (1998) 203. (Ar2p)
- HK&01** U. Hergenhann, O. Kuegler, A. Rüdel, E.E. Rennie and A.M. Bradshaw, J. Phys. Chem. A 105 (2001) 5704. (N<sub>2</sub> – N1s)
- HK&07** Y. Hikosaka, T. Kaneyasu, Y. Tamenori and E. Shigemasa, J. El. Spec. 156-158 (2007) 284. (CO<sub>2</sub>-C1s, O1s)
- HL81** M.H. Hecht and I. Lindau, Phys. Rev. Lett. 47 (1981) 821. (Ba4d)
- HLD91** A.P. Hitchcock, S. Lee and P.T. Dowben, (1991) unpublished. (B<sub>5</sub>C<sub>19</sub>FeH<sub>17</sub>O<sub>2</sub>P, B<sub>5</sub>C<sub>12</sub>H<sub>18</sub>P - B1s, C1s, Fe2p,3p, P2p)

- HLS05** Y Hikosaka, P Lablanquie and E Shigemasa, J. Phys. B. 38 (2005) 3597. (N<sub>2</sub>-N1s)
- HL&87** P.A. Heiman, D.W. Lindle, T.A. Ferrett, S.H. Liu, L.J. Medhurst, M.N. Piancastelli, D.A. Shirley, U.E. Becker, H.G. Kerkoff, B. Langler, D. Szostak and R. Wehlitz, J. Phys. B 20 (1987) 5005 (Ar2p, Kr3d, Xe4d)
- HL&88** A.P. Hitchcock, P. Lablanquie, P. Morin, E. Lizon A Lugrin, M. Simon, P. Thiry and I. Nenner, Phys. Rev. A 37 (1988) 2448. (CO-C1s,O1s)
- HL&92** D.M. Hanson, D.A. Lapiano-Smith, K. Lee, C.J. Ma and D.Y. Kim, Chem. Phys. 162 (1992) 439 (O<sub>2</sub>-O1s)
- HL&04** Y Hikosaka, P Lablanquie, F Penent, J.G Lambourne, R.I Hall, T Aoto and K Ito, J. El. Spec. Rel. Phen. 137-140 (2004) 287. (H<sub>2</sub>S – S2p)
- HM94** A.P. Hitchcock and D.C. Mancini, J. Electron Spectrosc. 67 (1994) 1. (C<sub>2</sub>H<sub>2</sub> - C1s; CF<sub>4</sub> - C1s, F1s)
- HMS90** W. Habenicht, K. Muller-Dethlefs and E.W. Schlag, J. Electron Spectr. 52 (1990) 697. (Ar2p, Ne1s)
- HM&84** T. Hayaishi, Y. Morioka, Y. Kageyoma, M. Watanake, I.H. Suzuki, A. Mikuni, G. Isoyama, S. Asaoka and M. Nakamura, J. Phys. 17 (1984) 3511. (Ar2p, Kr3d, Xe4d)
- HM&86** T. Hayaishi, Y. Morioka, T. Akahori, M. Watanabe, A. Yagashita and M. Nakamura, Z. Phys. D 4 (1986) 25. (Kr3p, Xe4p)
- HM&87** D. Haneschuck, M. Meyer P. Pahler, T. Prescher, M. Richter, B. Sonntag and H.E. Wenzel, J. Phys. 48 (1987) C9-539. (La4d)
- HM&88** T. Hayaishi, E. Murakami, A. Yagashita, F. Koike, Y. Morioka and J.E. Hansen, J. Phys. B 21 (1988) 3203. (Ar2p)
- HM&89** A.P. Hitchcock, P. Morin, E. Lizon a Lugrin, M. Simon and I. Nenner, unpublished (CH<sub>3</sub>CN - C1s,N1s; CF<sub>3</sub>OOCF<sub>3</sub> - C1s,O1s,F1s)
- HM&90** D.M. Hanson, C.I. Ma, K. Lee, D. Lapiano-Smith and D.Y. Kim, J. Chem. Phys. 93 (1990)9200. (N<sub>2</sub>O - N1s)
- HM&91a** T. Hayaishi, E. Murakami, Y. Morioka, H. Aksela, S. Aksela, E. Shigemasa and A. Yagashita, Phys. Rev. A 44 (1991) R2771. (Kr3d, Xe4d)
- HM&91b** P.A. Heimann, L.J. Medhurst, M.R.F. Siggel, D.A. Shirley, C.T. Chen, Y. Ma and F. Sette, Chem. Phys. Lett. 183 (1991) 234. (CH<sub>4</sub>, CD<sub>4</sub> - C1s)
- HM&92a** T. Hayaishi, E. Murakami, Y. Morioka, H. Aksela, S. Aksela, E. Shigemasa and A. Yagashita, J. Phys. B 26 (1992) 4119. (Ar2p)
- HM&92b** T. Hayaishi, E. Murakami, Y. Morioka, E. Shigemasa and A. Yagashita, Photon Factory Ann. Rep. (1992) 36. (Ne1s)
- HM&93** A.P. Hitchcock, M.J. McGlinchey, A.L. Johnson, W.K. Walter, M. Perez-Jigato, D.A. King, D. Norman, E. Ruhl, C. Heinzel and H. Baumgartel, J.C.S. Faraday Trans 89 (1993) 3331 . (Co<sub>3</sub>(CO)<sub>9</sub>-C-X, X=Cl, OCH<sub>3</sub> - C1s, Co2p, Co3p, Cl2p, O1s)
- HM&95a** T. Hayaishi, E. Murakami, Y. Morioka, E. Shigemasa, A. Yagashita and F. Koike, J. Phys. B 28 (1995) 1411.

(Ne1s)

- HM&95b** T. Hayaishi, E. Murakami, E. Shigemasa, A. Yagashita, F. Koike and Y. Morioka, J. Phys. B 28 (1995) 5261. (Ar1s)
- HM&96** T. Hayaishi, E. Murakami, Y. Lu, E. Shigemasa, A. Yagashita, F. Koike and Y. Morioka, Phys. Rev. A 54 (1996) 4064. (Xe2p)
- HM&02** T Hayaishi, T Matsui, H Yoshii, A Higurashi, E Murakami, A Yagishita, T Aoto, T Onuma and Y Morioka , J. Phys. B 35 (2002) 141. (Xe4p)
- HM&08** M Hoshino, R Montuoro, R R Lucchese, A De Fanis, U Hergenhahn, G Prümper, T Tanaka, H Tanaka and K Ueda, J.Phys. B 41 (2008) 085105. (NO – N1s)
- HN86** A.P. Hitchcock and D.C. Newbury, (1986) unpublished. (CHF<sub>3</sub> - C1s, F1s)
- HN02** A.P. Hitchcock and J.J. Neville, Chemical Applications of Synchrotron Radiation, Part I: Dynamics and VUV Spectroscopy, Advanced Series in Physical Chemistry Vol 12A, (World Scientific, Singapore, 2002) 154. (review; PF<sub>3</sub>-P1s; SPF<sub>3</sub>- P2p,P1s; COS-S1s; H<sub>2</sub>O – O1s)
- HNK04** T Hatsui, Mitsuru Nagasono, Nobuhiro Kosugi, J. El. Spec. Rel. Phen. 137-140 (2004) 435. (Ar2p)
- HN&86** A.P. Hitchcock, D.C. Newbury, I. Ishii, J. Stöhr, J.A. Horsley, R.D. Redwing, A.L. Johnson and F. Sette, J. Chem. Phys. 85 (1986) 4849. (C<sub>3</sub>H<sub>6</sub>, C<sub>4</sub>H<sub>8</sub>, C<sub>5</sub>H<sub>8</sub>, C<sub>6</sub>H<sub>10</sub>, C<sub>5</sub>H<sub>10</sub>, C<sub>6</sub>H<sub>12</sub>, C<sub>8</sub>H<sub>8</sub> - C1s)
- HN&98** A.P. Hitchcock, J.J. Neville, A. Jürgensen and R.G. Cavell, J. Electron Spectrosc. 88-91 (1998) 71. (PF<sub>3</sub>, SPF<sub>3</sub> - P2p)
- HPB77** A.P. Hitchcock, M. Pocock and C.E. Brion, Chem. Phys. Lett. 49 (1977) 125. (CH<sub>4</sub>, CD<sub>4</sub> - C1s)
- HP&78** A.P. Hitchcock, M. Pocock, C.E. Brion, M.S. Banna, D.C. Frost, C.A. McDowell and B. Wallbank, J. El. Spectrosc. 13 (1978) 345. (C<sub>6</sub>H<sub>5</sub>X (X=F, Cl, Br, I) - C1s, Cl2p, Br3d, I4d)
- HP&98** I. Hjelte, M.N. Piancastelli et al. MaxLab report (1998) 178. (H<sub>2</sub>O - O1s)
- HP&99** A. Hempelmann, M.N. Piancastelli, F. Heiser, O. Gesner, A. Rudel and U. Becker, J. Phys. B 32 (1999) 2677. (CH<sub>3</sub>OH – C1s, O1s)
- HP&01** I. Hjelte, M. N. Piancastelli, R. F. Fink, O. Björneholm, M. Bässler, R. Feifel, A. Giertz, H. Wang, K. Wiesner, A. Ausmees, C. Miron, S. L. Sorensen and S. Svensson „Evidence for ultra-fast dissociation of molecular water from resonant Auger spectroscopy” Chem. Phys. Lett. 334 (2001) 151 .
- HR87** F.L. Hutson and D.E. Ramaker, J. Chem. Phys. 87 (1987) 6824. (C<sub>2</sub>H<sub>4</sub>, C<sub>2</sub>H<sub>6</sub> - C1s)
- HR89** A.P. Hitchcock and E. Rühl, Physica B 158 (1989) 403. (C<sub>6</sub>H<sub>12-x</sub>, x=0,2,4,6; CH<sub>3</sub>CN, CH<sub>3</sub>NC, CH<sub>3</sub>SCN, CH<sub>3</sub>NCS - C1s; Mn(CO)<sub>5</sub>X, X=H, Br, Mn<sub>2</sub>(CO)<sub>10</sub> - C1s, O1s)
- HR96** A.P. Hitchcock and E. Rühl, (ICPEAC XIX) AIP Conf. Proc. 360 (1996) 89. (Ar<sub>n</sub>-Ar1s; (C<sub>2</sub>H<sub>2</sub>)<sub>n</sub> - C1s; C<sub>2</sub>B<sub>10</sub>H<sub>12</sub> - C1s, B1s)
- HR&96** A.P. Hitchcock, E. Rühl, A.L.D. Kilcoyne, T. Tyliszczak, P.A. Dowben, unpublished. (C<sub>2</sub>B<sub>10</sub>H<sub>12</sub> - C1s, B1s)

- HR&02** P.A. Hatherly, J. Rius i Riu, M. Stankiewicz, F.M. Quinn and L.J. Frasinski, *J. Phys. B* 35(2002) L77. (CO<sub>2</sub> - C1s)
- HS87** A.P. Hitchcock and J. Stöhr, *J. Chem. Phys.* 87 (1987) 3523. (CO<sub>2</sub>-C1s,O1s)
- HS90** A.P. Hitchcock and J. Stöhr, unpublished. (C<sub>3</sub>H<sub>4</sub>, C<sub>3</sub>H<sub>6</sub>, C<sub>3</sub>F<sub>3</sub>H, C<sub>2</sub>F<sub>3</sub>N, C<sub>6</sub>H<sub>6</sub>, C<sub>7</sub>H<sub>8</sub> - C1s; C<sub>8</sub>H<sub>12</sub>Si - C1s, Si2p)
- HS92** A.P. Hitchcock and D. Sutton, unpublished. (C<sub>12</sub>H<sub>15</sub>N<sub>2</sub>O<sub>2</sub>Re - Cp\*Re(CO)<sub>2</sub>N<sub>2</sub> - C1s, N1s, O1s, Re4f)
- HS&81** K.H. Hallmeier, R. Szargan, A. Meisel, E. Hartmann and E.S. Gluskin, *Spect. Chim. Acta* 37A (1981) 1049. (BF<sub>3</sub>-B1s,CF<sub>4</sub>-C1s,F1s; KBF<sub>4</sub>, NH<sub>4</sub>BF<sub>4</sub>, H<sub>3</sub>BO<sub>3</sub>, B<sub>2</sub>O<sub>3</sub>-B1s)
- HS&84a** H.W. Haak, G.A. Sawatsky, L Ungier, J.K. Gimzewski, and T.D. Thomas, *Rev. Sci. Inst.* 55 (1984) 696. (N<sub>2</sub>-N1s)
- HS&84b** A.P. Hitchcock, J. Stohr, (1984) unpublished (C<sub>4</sub>F<sub>6</sub> - C1s, F1s)
- HS&85** J.A. Horsley, J. Stöhr, A.P. Hitchcock, D.C. Newbury, A.L. Johnson and F. Sette, *J. Chem. Phys.* 83 (1985) 6099. (C<sub>6</sub>H<sub>6</sub>-C1s, C<sub>5</sub>H<sub>5</sub>N-C1s, N1s)
- HS&90** P.A. Heimann, F. Senf, W. McKinney, M. Howells, R.D. van Zee, L.J. Medhurst, T. Lauritzen, J. Chin, J. Meneghetti, W. Gath, H. Hogrefe and D.A. Shirley, *Phys. Scripta* T31 (1990) 127. N<sub>2</sub> - N1s; C<sub>2</sub>H<sub>4</sub> - C1s)
- HS&93** E. Hudson, D.A. Shirley, M. Domke, G. Remmers, A. Puschmann, T. Mandel, C. Xue and G. Kaindl, *Phys. Rev. A* 47 (1993) 361. (SF<sub>6</sub> - S2p, F1s)
- HS&94** E. Hudson, D.A. Shirley, M. Domke, G. Remmers, and G. Kaindl, *Phys. Rev. A* 49 (1994) 161. (H<sub>2</sub>S, D<sub>2</sub>S - S2p)
- HS&02** D L Hansen, W C Stolte, O Hemmers, R Guillemin and D W Lindle, *J. Phys. B* 35 (2002) L381. (CO-C1s, O1s)
- HT88** A.P. Hitchcock and M. Tronc, *Chem. Phys.* 121 (1988) 265. (SO<sub>2</sub>-S1s; SO<sub>2</sub>Cl<sub>x</sub>F<sub>2-x</sub> - S1s,Cl1s)
- HTB89** A.P. Hitchcock, G. Tourillon and W. Braun, *Can. J. Chem.* 67 (1989) 1819. (C<sub>4</sub>H<sub>4</sub>Se, C<sub>5</sub>H<sub>6</sub>Se - C1s, Se3d, Se3p,3s)
- HTM89** A.P. Hitchcock, M. Tronc and A. Modelli, *J. Phys. Chem.* 93 (1989) 3068. (CH<sub>3</sub>CN, CH<sub>3</sub>NC - C1s, N1s; CH<sub>3</sub>SCN, CH<sub>3</sub>NCS - C1s, N1s, S2p,2s)
- HT&89** A.P. Hitchcock, G. Tourillon, R. Garrett and N. Lazarz, *J. Phys. Chem.* 93 (1989) 7624. (C<sub>10</sub>H<sub>8</sub>, C<sub>10</sub>F<sub>8</sub> - azulene, naphthalene - C1s)
- HT&90** A.P. Hitchcock, G. Tourillon, G.P. Williams, C. Mahatsekake and C. Andrieu, *J. Phys. Chem.* 94 (1990) 2327. (C<sub>4</sub>H<sub>3</sub>S-X, X= H, Me, Et, Bu, Hx, Oc, De - C1s, S2p,2s)
- HT&93** A.P. Hitchcock, T. Tyliszczak, P. Aebi, J. Xiong, T.K. Sham, K.M. Baines, K.A. Mueller, X.H. Feng, J.M. Chen, B.X. Yang, Z.H. Lu, J.M. Baribeau and T.E. Jackman, *Surf. Sci.* 291 (1993) 349. (SiMe<sub>4</sub>, Si(GeMe<sub>3</sub>)<sub>4</sub>, Si(SiMe<sub>3</sub>)<sub>4</sub>, Ge(SiMe<sub>3</sub>)<sub>4</sub> - Si1s)
- HT&99** T. Hayaishi, T. Tanaka, H. Yoshii, E. Murakami, E. Shigemasa, A. Yagashita, F. Koike and Y. Morioka, *J. Phys. B* 32 (1999) 1507. (Kr2p)

- HT&00** C.F. Hague, M. Tronc, Y. Yanagida, A. Kotani, J.H. Guo and C.J. Sathe, Phys. Rev. A 63 (2000) 012511. (TiCl<sub>4</sub> – Ti2p)
- HUR92** A.P. Hitchcock, S.G. Urquhart and E.G. Rightor, J. Phys. Chem. 96 (1992) 8736. (Cl<sub>2</sub>CO, C<sub>8</sub>Cl<sub>2</sub>H<sub>4</sub>O<sub>2</sub> - C1s, O1s, Cl2p; C<sub>6</sub>H<sub>6</sub> - C1s; C<sub>7</sub>H<sub>6</sub>O, C<sub>8</sub>H<sub>6</sub>O<sub>2</sub>, C<sub>9</sub>H<sub>10</sub>O - C1s, O1s)
- HUR93** A.P. Hitchcock, S.G. Urquhart and E.G. Rightor, (1993) unpublished. (C<sub>6</sub>H<sub>5</sub>N(CH<sub>3</sub>)<sub>2</sub> - C1s, N1s)
- HU&97** A.P. Hitchcock, S.G. Urquhart, A.T. Wen, A.L.D. Kilcoyne, T. Tyliaszczak, E. Rühl, N. Kosugi, J.D. Bozek, J.T. Spencer, D.N. McIlroy and P.A. Dowben, J. Phys. Chem. B 101 (1997) 2267. (C<sub>2</sub>B<sub>10</sub>H<sub>12</sub> - C1s, B1s)
- HV&20** Georg Held,Federica Venturini, et al. Ambient-pressure endstation of the Versatile Soft X-ray (VerSoX) beamline at Diamond Light Source, J. Synchrotron Rad. 27 (2020) 1153, (CH<sub>4</sub> – C1s, N<sub>2</sub>-N1s, O<sub>2</sub>-O1s).
- HWR89** A.P. Hitchcock, A.T. Wen and E. Ruhl, unpublished. (M(Cp)<sub>2</sub> - V,Cr,Mn - C1s)
- HWR90a** A.P. Hitchcock, A.T. Wen and E. Ruhl, J. Electron Spectrosc. 51 (1990) 653. (CO, Mn(CO)<sub>5</sub>Br, Fe(CO)<sub>5</sub>, Ni(CO)<sub>4</sub>, Co<sub>2</sub>(CO)<sub>8</sub>, C<sub>6</sub>H<sub>8</sub>Fe(CO)<sub>3</sub> - C1s,O1s)
- HWR90b** A.P. Hitchcock, A.T. Wen and E. Ruhl, Chem. Phys. 147 (1990) 51. (Mn(CO)<sub>5</sub>Br - Mn2p; Fe(CO)<sub>5</sub>, FeCp<sub>2</sub>, C<sub>6</sub>H<sub>8</sub>Fe(CO)<sub>3</sub> - Fe2p,Fe3p; Co<sub>2</sub>(CO)<sub>8</sub>, CoCp<sub>2</sub>, CpCo(CO)<sub>2</sub> -Co2p,3p)
- HW&90** B.P. Hollebone, A.T. Wen, T. Tyliaszczak and A.P. Hitchcock, J. Elect. Spect. 51 (1990) 661. (CO<sub>2</sub>, CF<sub>4</sub>, C<sub>6</sub>H<sub>6</sub>, Fe(CO)<sub>5</sub>, CpCo(CO)<sub>2</sub> - C1s; EXELFS)
- HW&91** A.P. Hitchcock, A.T. Wen, S.G. Urquhart and E. Rightor, unpublished (C<sub>3</sub>H<sub>6</sub>O<sub>3</sub>, C<sub>12</sub>H<sub>10</sub>O<sub>3</sub> - C1s,O1s)
- HW&93** A.P. Hitchcock, A.T. Wen, S. Lee, J.A. Glass, Jr., J.T. Spencer and P.A. Dowben, J. Phys. Chem. 97 (1993) 8171. (B<sub>5</sub>H<sub>9</sub>, B<sub>10</sub>H<sub>14</sub> - B1s; B<sub>4</sub>C<sub>6</sub>H<sub>16</sub>, B<sub>9</sub>C<sub>2</sub>H<sub>11</sub>, B<sub>10</sub>C<sub>2</sub>H<sub>12</sub> - B1s, C1s)
- HW&94** F. Heiser, S.B. Whitfield, J. Viefhaus, U. Becker, P.A. Heimann and D.A. Shirley, J. Phys. 27 (1994) 19. (Ar1s)
- HW&95** O. Hemmers, S.B. Whitfield, N. Berrah, B. Langer, R. Wehlitz and U. Becker, J. Phys. B 28 (1995) L693. (CO - C1s)
- HYP97** A.N. Hopersky, V.A. Yavna and V.A. Popov, J. Phys. B 30 (1997) 5131. (Xe1s)
- HY&90a** T. Hayaishi, A. Yagashita, E. Shigemasa, J. Murakami and Y. Morioka, Phys. Scripta 41 (1990) 35. (Kr3d, Xe4d)
- HY&90b** T. Hayaishi, A. Yagashita, E. Shigemasa, Y. Morioka and T. Sasaki, J. Phys. B 23 (1990) 1633. (Kr3d)
- HZ96** T. Hayaishi and P. Zimmermann, *AIon Yield Spectroscopy with Soft X-rays@, in VUV and Soft X-ray Photoionization*, U. Becker, D.A. Shirley, eds. (Plenum, NY, 1996) 465. (Ar2p, Ce4d, Co3p, Cr3p, Dy4d, Fe3p, Kr3d, Mn3p, Ni3p, Sc2p, Ti3p, Xe4d)
- I01** K. Ito, J. El. Spec. 114-116 (2001) 15. (N<sub>2</sub> – N1s, CO – C1s, O1s)
- IA&00** K. Ito, J. Adachi, Y. Hikosato, S. Motoki, K. Soejima, A. Yagashita, G. Raseev and N.A. Cherepkov, Phys. Rev. Lett. 85 (2000) 46. (CO - O1s)

- IB&91** T. Imamura, C.E. Brion, I. Koyano, T. Ibuki and T. Masuoka, J. Chem. Phys. 94 (1991) 4936. (SiF<sub>4</sub> - Si2p)
- IC&08** V. Ilakovac, S. Carniato, J.-J. Gallet, E. Kukk, D. Horvatić, and A. Ilakovac, Phys. Rev. A 77 (2008) 012516. (C<sub>3</sub>H<sub>3</sub>N - N1s)
- IF&91** H. Ishikawa, K. Fujima, H. Adachi, E.M. Yauchi and T. Fujii, J. Chem. Phys. 94 (1991) 6740. (SiX<sub>4</sub>, X=H,F,Cl - Si2p)
- IH87** I. Ishii and A.P. Hitchcock, J. Chem. Phys. 87 (1987) 830. (HCONH<sub>2</sub> - C1s, N1s, O1s; HCOOH - C1s,O1s; HCOF - C1s,O1s,F1s)
- IH88** I. Ishii and A.P. Hitchcock, J. Electron Spectrosc. 46 (1988) 55. (CH<sub>3</sub>OH, HCOOH, CH<sub>3</sub>COOCH<sub>3</sub>, HCCCO<sub>2</sub>H, CH<sub>2</sub>CHCO<sub>2</sub>H, CH<sub>3</sub>CH<sub>2</sub>O<sub>2</sub>H, HCCCH<sub>2</sub>OH, CH<sub>2</sub>CHCH<sub>2</sub>OH, CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>OH -C1s,O1s)
- IH07** N. Iannuzzi and J. Hutter, Phys Chem Chem Phys 9 (2007) 599. (CO, CH<sub>3</sub>OH , C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>4</sub>, C<sub>2</sub>H<sub>8</sub>O<sub>2</sub>, C<sub>5</sub>H<sub>5</sub>N, C<sub>3</sub>H<sub>6</sub>O - C1s; C<sub>5</sub>H<sub>5</sub>N - N1s; CO, CH<sub>3</sub>OH , C<sub>2</sub>H<sub>8</sub>O<sub>2</sub>, C<sub>3</sub>H<sub>6</sub>O, H<sub>2</sub>O, H<sub>4</sub>O<sub>2</sub> - O 1s)
- IH&96** T. Ibuki, A. Hiraya, T.N. Olney and C.E. Brion, Chem. Phys. 203 (1996) 359. (BrCN - Br3d)
- IH&10** E. Itälä, D. T. Ha, K. Kooser, E. Rachlew, M. A. Huels and E. KukkJ. Chem. Phys.133 (2010) 154316 (C<sub>3</sub>H<sub>2</sub>N<sub>2</sub>OB<sub>r</sub>, C<sub>4</sub>H<sub>6</sub>N<sub>2</sub>O<sub>2</sub> - C1s)
- IH&11** E. Itälä, D.T. Ha, K. Kooser, M.A. Huels, E. Rachlew, E. Nõmmiste, U. Joost, E. Kukk, J. El. Spec. 184 (2011) 119. (C<sub>3</sub>H<sub>2</sub>N<sub>2</sub>OB<sub>r</sub>, C<sub>3</sub>H<sub>3</sub>N<sub>2</sub>O<sub>2</sub>, C<sub>4</sub>H<sub>6</sub>N<sub>2</sub>O<sub>2</sub> - C1s)
- IIS12a** L. Ishikawa, H. Iwayama and E. Shigemasa, UVSOR Annual report 2012, 61. (COS - S2p)
- IIS12b** H. Iwayama, L. Ishikawa and E. Shigemasa, UVSOR Annual report 2012, 65. (CF<sub>4</sub> - C1s)
- II&80** E. Ishiguro, S. Iwata, Y. Suzuki, A. Mikuni and T. Sasaki, Proc. VUV-6 (Charlottesville 1980) II-70. (BF<sub>3</sub>, BCl<sub>3</sub>, BBr<sub>3</sub> -B1s)
- II&82** E. Ishiguro, S. Iwata, Y. Suzuki, A. Mikuni and T. Sasaki, J. Phys. B 15 (1982) 1841. (BF<sub>3</sub>, BCl<sub>3</sub>, BBr<sub>3</sub> - B1s)
- II&87** E. Ishiguro, S. Iwata, A. Mikuni Y. Suzuki, H. Kanamon and T. Sasaki, J. Phys. B 20 (1987) 4725. (PH<sub>3</sub>, PF<sub>3</sub>, PCl<sub>3</sub>, PBr<sub>3</sub> - P2p,Cl2p)
- II&91** H. Ishii, Y. Iketaki, T. Watabe, T. Takayangi, K. Wakiya, H. Suzuki and F. Koike, Phys. Rev. A 43 (1991) 134. (Ar2p, Kr3d, Xe4d)
- II&00** Y. Itoh, A. Ito, M. Kitajima, T. Koizumi, T.M. Kojima, H. Sakai, M. Sano and N. Watanabe, J. Phys. B 34 (2001) 3493. (Xe4d)
- IKN78** S. Iwata, N. Kosugi and O. Nomura, J. Jpn. Appl. Phys. 17 S2 (1978) 109. (CO, C<sub>2</sub>H<sub>2</sub> -C1s; N<sub>2</sub> -N1s; CO -O1s)
- IK&95a** B.S. Itchkawitz, B. Kempgens, H.M. Köppe, J. Feldhaus, A.M. Bradshaw and W.B. Peatman, Rev. Sci. Inst. 66 (1995) 1531. (Ar2p, CF<sub>4</sub> - C1s)
- IK&95b** Y. Itoh, T. Koizumi, Y. Awaya, S.D. Kravis, M. Oura, M. Sano, T. Sekioka and F. Koike, J. Phys. B 28

(1995) 4733. ( $\text{Sr}^+ - 3d$ )

- IK&14** E. Itälä, K. Kooser, E. Rachlew, M. A. Huels and E. Kukk, J. Chem. Phys. 140 (2014) 234305 ( $\text{C}_2\text{H}_3\text{NO}_2 - \text{C}1s$ )
- IL&17** H. Iwayam, C. Léonard, et al, Different Time Scales in the Dissociation Dynamics of Core-Excited  $\text{CF}_4$  by Two Internal Clocks, Phys. Rev. Lett. 119 (2017) 203203. ( $\text{CF}_4-\text{C}1s$ )
- IM&87** R. McLaren, I. Ishii, A.P. Hitchcock and M.B. Robin, J. Chem. Phys. 87 (1987) 4344. ( $\text{H}_2\text{O}, \text{F}_2\text{O}, \text{CF}_3\text{OF}, \text{CF}_3\text{OOCF}_3, (\text{CH}_3)_3\text{COH}, (\text{CH}_3)_3\text{COOC(CH}_3)_3 - \text{C}1s, \text{O}1s, \text{F}1s$ )
- IM&88** I. Ishii, R. McLaren, A.P. Hitchcock, K.D. Jordan, H. Choi and M.B. Robin, Can. J. Chem. 66 (1988) 2104. ( $\text{C}_2\text{H}_6, \text{C}_6\text{H}_{12}, \text{C}_x\text{F}_{2x+2}, x=1-6; \text{c-C}_3\text{F}_6, \text{c-C}_4\text{F}_8, \text{C}_5\text{F}_{12}, \text{c-C}_5\text{F}_{10}, \text{c-C}_6\text{F}_{12} - \text{C}1s, \text{F}1s$ )
- IN&92** Y. Ito, H. Nakamatsu, T. Mukoyama, K. Omote, S. Yoshikado, M. Takahashi and S. Emura, Phys. Rev. A 46 (1992) 6083. ( $\text{Kr}1s$ )
- IP&12** H. Iwayama, M.N. Piancastelli, R. Guillemin, M. Simon and E. Shigemasa, UVSIR annual report 2012, 63. ( $\text{CCl}_4-\text{Cl}2p$ )
- IOG97** T. Ibuki, K. Okada and T. Gejo, I.M.S. Report (1997) 46. ( $\text{C}_7\text{F}_5\text{N} - \text{C}1s$ )
- IOW01** Y. Iketani, K. Ohtsuki and T. Watanabe, J. Phys. B 34 (2001) 1889. ( $\text{NO} - \text{N}1s, \text{O}1s$ )
- IO&99** T. Ibuki, K. Okada, T. Gejo and K. Saito, J.El. Spec. 101 (1999) 149. ( $\text{C}_2\text{Cl}_3\text{N} - \text{Cl}2p, \text{N}1s; \text{C}_7\text{F}_5\text{N} - \text{C}1s, \text{N}1s; \text{C}_4\text{H}_5\text{NO}_2, \text{C}_8\text{F}_3\text{H}_4\text{NO} - \text{N}1s, \text{O}1s$ )
- IO&00** T. Ibuki, K. Okada, K. Saito and T. Gejo, J.El. Spec. 107 (2000) 39. ( $\text{C}_3\text{H}_3\text{NO}_2, \text{C}_4\text{H}_5\text{NO}_2 - \text{N}1s, \text{O}1s$ )
- IO&12** S. Ishikawa, K. Okada, H. Iwayama, L. Ishikawa and E. Shigemasa, UVSOR Annual Report, 2012 58. ( $\text{C}_4\text{F}_6\text{H}_2 - \text{C}1s$ )
- ISN97** Y. Ito, Y. Sugita and Y Nara, J Vac. Sci. Tech. A 15 (1997) 2561. ( $\text{SiH}_4 - \text{Si}2p$ )
- IS&93** H. Ikeura, T. Sekiguchi, K. Tanaka, K. Obi, N. Ueno and K. Honma, Jap. J. Appl. Phys. 32 (1993) S2, 246. ( $\text{H}_2\text{O}-\text{O}1s$ )
- IS&05** T. Ibuki, Y. Shimada, R. Hashimoto, S. Nagaok, M. Hino, K. Okada, I.H. Suzuki, Y. Morishita and Y. Tamenori, Chem. Phys. 314 (2005) 119. ( $\text{CF}_3\text{SF}_5 - \text{C}1s, \text{F}1s, \text{S}1s$ )
- ITH17** H. Inui, O. Takahashi and A. Hiraya, Theoretical study on X-ray absorption spectra and bond dynamics for core excitation from valence excited benzoic acids, J. El. Spec. 220 (2017) 101 ( $\text{C}_7\text{H}_6\text{O}_2, \text{C}_8\text{H}_8\text{O}_2 - \text{O} 1s$ )
- ITK99** S. Itoh, S. Tanaka and Y. Kayanumo, Phys. Rev. A 60 (1999) 4488. ( $\text{CF}_4 - \text{C}1s$ )
- IV&98** Y. Ito, A.M. Vlaicu, T. Tochino, T. Mikoyano, M. Takahashi, S. Emura and Y. Azuma, Phys. Rev. A 57 (1998) 873. ( $\text{Xe}2p$ )
- JA&97** U. Johansson, J.N. Andersen, R. Nyholm and I.Lindau, MaxLab Report (1997) 184. ( $\text{Nes}; \text{N}_2 - \text{N}1s, \text{CO} - \text{C}1s, \text{O}1s$ )
- JC00** A. Jürgensen and R.G. Cavell, Chem. Phys. 257 (2000) 123. ( $\text{SO}_2, \text{NO}_2 - \text{O}1s$ )

- JC01** A. Jürgensen and R.G. Cavell, Chem. Phys. 273 (2001) 77. ( $\text{NH}_3$ ,  $\text{NF}_3$  – N1s;  $\text{PH}_3$ ,  $\text{PF}_3$  – P1s)
- JC&93** J. Jiminez-Lier, C.D. Caldwell, M.G. Flemming, S.B. Whitfield and P. van der Muelen, Phys. Rev. A 48 (1993) 442. (Sr4p)
- JC&96** L. Journel, D. Cubaynes, J.-M. Bizau, S. Al Moussalami, B. Rouvellou, F.J. Wiillaume, L. Vokoy, P. Faucher and A. Hibbert, Phys. Rev. Lett. 76 (1996) 30. (Li1s)
- JC&97** J. Johnson, J.N. Cutler, G.M. Bancroft, Y.F. Hu and K.H. Tan, J. Phys. B 30 (1997) 4899. ( $\text{Br}_2$ , HBr, DBr,  $\text{FBr}$ ,  $\text{CH}_3\text{Br}$ ,  $\text{CF}_3\text{Br}$  - Br3d)
- JC&03** J.D Bozek, S.E Canton, E Kukk and N Berrah, Chem. Phys. 289 (2003) 149. ( $\text{H}_2\text{CO}$  - C1s)
- JH&84** Y. Jugnet, F.J. Himpsel, Ph. Avouris and E.E. Koch, Phys. Rev. Lett. 53 (1984) 198. (CO-C1s,O1s)
- JG&93** E. Jannitti, M. Gaye, M. Mazzoni, P. Nicolosi and P. Villoresi, Phys. Rev. A 47 (1993) 4033. (C1s)
- JJ&91** T. Jaing-Chang, S. Jeng-Feng, F. Xiao-Song and C.Y. Bing, Chin. Soc. Bull. 36 (1991) 557. ( $\text{O}_2$ ,CO - O1s)
- JKC99** A. Jurgensen, N. Kosugi and R.G. Cavell, Chem. Phys. 247 (1999) 445. ( $\text{NSF}_3$  – S2p;  $\text{OPF}_3$  – P2p)
- JK&89** J. Jimenez-Mier, M.O. Krause, P. Gerard, B. Hermsmeier and C.S. Fadley, Phys. Rev. A 40 (1989) 3712. (Mn3p)
- JNT87** E. Jannitti, P. Nicolosi and G. Tondello, J. Phys 48 (1987) C9-219. (C1s)
- JNT90** E. Jannitti, P. Nicolosi and G. Tondello, Phys. Scripta 41 (1990) 458. (C1s)
- JN&95** E. Jannitti, P. Nicolosi and P. Villoresi and F. Xianping, Phys. Rev. A 51 (1995) 314. (C1s)
- JP58** G. Joos and K.H. Peter, Z. Phys. Chem. NF 18 (1958) 74. ( $\text{Cr}(\text{CO})_6$  - Cr1s;  $\text{Fe}(\text{C}_5\text{H}_5)_2$ ,  $\text{Fe}(\text{CO})_5$  - Fe1s)
- JS&90** R. Jing, R. Staub, H. Baiter, G. Reiser, W. Habenicht and K. Muller-Dethlefs, Ber. Bun. Phys. Chem. 94 (1990) 1318. ( $\text{C}_2\text{F}_3\text{H}_3$ ,  $\text{C}_2\text{F}_2\text{H}_2$  - C1s)
- JS&08** H. Jiang, J. Stewart-Ornstein, G. Cooper and A.P. Hitchcock, Inner Shell Excitation Spectroscopy of Amino Acids and Peptides: Part I - Selected Amino Acids, (unpublished) ( TO UPDATE N, O, S missing)
- JT94a** P. Jayes and R.J. Tarento, Phys. Rev. B 49 (1994) 5003; *ibid*, J. Phys. (Paris) 2 (1992) 1667. ( $\text{C}_{60}$ -C1s)
- JT94b** D. Ji and T.D. Thomas, J. El. Spec. 67 (1994) 233. ( $\text{C}_3\text{H}_6\text{O}_2$  - C1s, O1s)
- JV&06** K. Jakubowska, G. Vall-Ilosera, A. Kivimaki, M. Coreno, E.M. Garia, M. Stankiewicz and E. Rachlew, Max Lab Annual Report (2006) 232. ( $\text{CH}_4$  – C1s)
- JV&07** K. Jakubowska, G. Vall-Ilosera, A. Kivimaki, M. Coreno, E.M. Garia, M. Stankiewicz and E. Rachlew, J. Phys. B 40 (2007) 1489 ( $\text{CH}_4$  – C1s,  $\text{NH}_3$  – N1s)
- JW&02** T. Jahnke, Th. Weber, A.L. Landers, A. Knapp, S. Schössler, J. Nickles, S. Kammer, O. Jagutzki, L. Schmidt, A. Czasch, T. Osipov, E. Arenholz, A. T. Young, R. Diez Muiño, D. Rolles, F.J. García de Abajo, C. S.

- Fadley, M.A. Van Hove, S. K. Semenov, N.A. Cherepkov, J. Rösch, M.H. Prior, H. Schmidt-Böcking, C. L. Cocke, and R. Dörner, Phys. Rev. Lett. 88 (2002) 073002. (CO – C1s, N<sub>2</sub>- N1s)
- K77** A.A. Krasnoperova, Dissertation, Novosibirsk, 1977. (PCl<sub>3</sub>, PSCl<sub>3</sub>, POCl<sub>3</sub> - P2p, Cl2p)
- K84** G.C. King, Lect. Notes in Chem. 35 (1984) 162. (N<sub>2</sub>-N1s, Ar2p)
- K87** N. Kosugi, Springer Series in Solid State Science 81 (1987) 203. (N<sub>2</sub>-N1s, CO-C1s; Fe(CO)<sub>5</sub>-Fe1s)
- K88** M.O. Krause, Proc. SPIE 911 (1988) 23. (Ne1s, Kr3d, Mn3p, Be1s)
- K92** P. Kitzler, Phys. Lett. A 172 (1992) 66. (BF<sub>3</sub>-B1s; N<sub>2</sub>, N<sub>2</sub>O - N1s; O<sub>2</sub>, N<sub>2</sub>O - O1s; GeCl<sub>4</sub> - Ge1s; Br<sub>2</sub> - Br1s; summary of XANES studies)
- K96a** A. Karawajczyk, Phys. Scripta 53 (1996) 46. (N<sub>2</sub> - N1s)
- K96b** N. Kosugi, J. Electron Spectrosc. 79 (1996) 351. (N<sub>2</sub>O - O1s; CH<sub>4</sub>, CO<sub>2</sub> - C1s)
- K96c** M. Kutzner, "Many Electron Effects in Photoionization" in VUV and Soft X-ray Photoionization, U. Becker, D.A. Shirley, eds. (Plenum, NY, 1996) 1. (Mn3d, La4d)
- K02** N. Kosugi, Chemical Applications of Synchrotron Radiation, Part I: Dynamics and VUV Spectroscopy, Advanced Series in Physical Chemistry Vol 12A, (World Scientific, Singapore, 2002) 228. (CO, C<sub>2</sub>H<sub>2</sub>, COS, CS<sub>2</sub>, CH<sub>4</sub> – C1s; CO<sub>2</sub> –C1s, O1s; O<sub>2</sub> – O1s, N<sub>2</sub> – N1s; C<sub>4</sub>H<sub>4</sub>S, SO<sub>2</sub> – S1s)
- K04** N. Kosugi, J. El. Spec. Rel. Phen. 137-140 (2004) 335. (Ar2p; N<sub>2</sub> – N1s, C<sub>2</sub>H<sub>2</sub> – C1s, SF<sub>6</sub> – S2p)
- KAA96** E. Kukki, S. Aksela and H. Aksela, Phys. Rev. A 53 (1996) 3271. (Kr3d)
- KAR12** A. Kivimaki, M. Alagia and R. Richter, Chem. Phys. Lett. 531 (2012) 252. CO<sub>2</sub> – O 1s)
- KA&92a** N. Kosugi, J. Adachi, E. Shigemasa and A. Yagashita, J. Chem. Phys. 97 (1992) 8842. (NO - N1s, O1s)
- KA&92b** N. Kosugi, J. Adachi, E. Shigemasa and A. Yagashita, Photon Factory Ann. Rep. (1992) 40 (NO - N1s, O1s)
- KA&93** A. Kivimaki, H. Aksela, S. Aksela, A. Yagashita and E. Shigemasa, J. Phys. B 26 (1993) 3379. (HCl - Cl2p)
- KA&94** E. Kukki, S. Aksela, H. Aksela, et al., J. Phys. B 27 (1994) 1965. (Eu4d, Sm4d)
- KA&96a** E. Kukki, H. Aksela, O.-P. Sairanen, S. Aksela, A. Kivimaki, E. Nommiste, A. Ausmeer, A. Kikas, S.J. Osborne and S. Svensson, J. Chem. Phys. 104 (1996) 4475. (HCl, DCl - Cl2p)
- KA&96b** E. Kukki, H. Aksela, S. Aksela, F. Gel'mukhanov, H. Agren and S. Svensson, Phys. Rev. Lett. 76 (1996) 3100. (HCl - Cl2p)
- KA&96c** T. Koizumi, Y. Awaya et al. J. Electron Spectrosc. 79 (1996) 289. (Xe4d, Ba4d, Eu4d)
- KA&96d** E. Kukki, H. Aksela, O.-P. Sairanen, E. Nommiste, S. Aksela, S.J. Osborne, A. Ausmees and S. Svensson, Phys. Rev. A 54 (1996) 2121. (HCl, DCl – Cl 2p)
- KA&97a** B. Kassahlke, P. Averkamp, S. Frigo, P. Feulner and W. Berthold, Phys. Rev. B 55 (1997) 10854. (N<sub>2</sub> -N1s)

- KA&97b** E. Kukki, H. Aksela, A. Kivimaki, J. Jouhainen, E. Nommiste and S. Aksela, Phys. Rev. A 56 (1997) 1481. (Kr3d)
- KA&00** H. Kjeldsen, P. Andersen, F. Folkmann, H. Knudsen, B. Kristensen, J.B. West and T. Andersen, Phys. Rev. A 62 (2000) 020702. (I4d)
- KA&01** H. Kjeldsen, P. Andersen, F. Folkmann, B. Kristensen and T. Andersen, J. Phys. B 34 (2001) L353. (Li1s)
- KA&02a** H. Kjeldsen, P. Andersen, F. Folkmann, J.E. Hansen, M. Katajima and T. Andersen, J. Phys. B 35 (2002) 2845. (Ba4d, Cs4d, I4d, Xe4d)
- KA&02b** A. Kodre, I. Arcon, J.P. Gomilsek, R. Preseren and R. Frahm, J. Phys. B 35 (2002) 3497. (Kr1s, Rb1s)
- KA&02c** B. Kristensen, T. Andersen, F. Folkmann, H. Kjeldsen, and J. B. West, Phys. Rev. A 65 (2002) 022706. (S2p)
- KA&03** A Kivimäki, J Alvarez Ruiz, P Erman, P Hatherly, E Melero Garcia, E Rachlew, J Rius i Riu and M Stankiewicz, J. Phys. B: At. Mol. Opt. Phys. 36 (2003) 781. (SF<sub>6</sub> – S2p)
- KA&10** A. Kivimäki, J. Alvarez-Ruiz, M. Coreno, M. Stankiewicz, G. Fronzoni, M. Stener and P. Decleva, Chemical Physics, 375 (2010) 101, CF<sub>3</sub>SF<sub>5</sub>, SF<sub>6</sub> – S2p)
- KA&11** A Kivimäki, J Alvarez-Ruiz, T J Wasowicz, C Callegari, M de Simone, M Alagia, R Richter and M Coreno, J. Phys. B. 44 (2011) 165103. (CO<sub>2</sub> – O1s)
- KBB00** E. Kukk, J.D. Bozek and N. Berrah, Phys. Rev. A 62 (2000) 032708. (CO<sub>2</sub> – C1s)
- KBH90** N. Kosugi, S. Bodeur and A.P. Hitchcock, J. Electron Spectrosc. 51 (1990) 103. (SF<sub>4</sub>, SF<sub>6</sub> - S2p, S2s, F1s, S1s)
- KB&93a** S. Krummacher, M. Biermann, M. Neeb, A. Liebsch and W. Eberhardt, Phys. Rev. B 48 (1993) 8424. (C<sub>60</sub>-C1s)
- KB&93b** S. Krummacher, M. Biermann, M. Neeb, A. Liebsch, W. Eberhardt, H. Kuzmany, J. Fink, M. Mehring and S. Roth, Proc. El. Prop. of Fullerenes (Springer-Verlag, 1993) 95. (C<sub>60</sub>-C1s)
- KB&96** N. Kosugi, C.E. Brion, R.G. Cavell and A.P. Hitchcock, Chem. Phys. Lett. (sub., Aug 1996) (PF<sub>3</sub> - P2p)
- KB&97a** S. Kakar, O. Bjorneholm, J. Weigelt, A.R.B. de Castro, L. Trager, R. Frahm, T. Möller, A. Knop and E. Rühl, Phys. Rev. Lett. 78 (1997) 1675. (Ar<sub>n</sub> - Ar1s)
- KB&97b** S. Kakar, O. Bjorneholm, J.O. Loefkan, F. Fearman, A.V. Soldatov and T. Möller, Z. Phys. D 40 (1997) 84. (CH<sub>4</sub>)<sub>n</sub> - C1s, Ne<sub>n</sub> - Ne1s)
- KB&99** E. Kukk, J.D. Bozek, W.T. Cheng, R.F. Fink, A.A. Willis and N. Berrah, J. Chem.Phys. 111 (1999) 9642. (CO – C1s)
- KB&18** Thomas Kierspel, Cedric Bomme, et al., Photophysics of indole upon X-ray absorption, Phys. Chem. Chem. Phys. 20 (2018) 20205. (C<sub>8</sub>H<sub>7</sub>N – N1s)
- KC87a** M.O. Krause and C.D. Caldwell, Phys. Rev. Lett. 59 (1987) 2736. (Be1s)
- KC87b** M.O. Krause and C.D. Caldwell, J. Phys. 48 (1987) 473. (Be1s)

- KCF83** M.O. Krause, F. Cerrina and A. Fahlman, Phys. Rev. Lett. 50 (1983) 1118. (Ga3d)
- KCM96** E.T. Kennedy, J.T. Costello and J.P. Mosnier, J. Electron Spectrosc. 79 (1996) 283. (Li1s, Ba4d, La4d, Mg2p, Al2p, Si2p)
- KCN82** H.P. Kelly, S.L. Carter and B.E. Norum, Phys. Rev. A 25 (1982) 2052. (Ba, Ba<sup>2+</sup>, 4d)
- KC&96** M.O. Krause, C.D. Caldwell, A. Menzel, S. Benzaud and J. Jiminez-Mier, J. Electron Spectrosc. 79 (1996) 241. (O1s)
- KC&97a** L.M. Kiernan, J.T. Costello, E.T. Kennedy, J.P. Mosnier and B.F. Sonntag, J. Phys. B 30 (1997) 4801. (Zn3p)
- KC&97b** N. Kosugi, R.G. Cavell and A.P. Hitchcock, Chem. Phys. Lett. 265 (1997) 490. (PF<sub>3</sub> - P2p)
- KC&92** G. Kuper, R. Chauvistre, J. Hormes, F. Frick, M. Jansen, B. Luer and E. Hartmann, Chem. Phys. 165 (1992) 405. [P<sub>4</sub>O<sub>6</sub>, P<sub>4</sub>O<sub>10</sub>, P(CH<sub>3</sub>H<sub>5</sub>O)<sub>3</sub>, PO(CH<sub>3</sub>H<sub>5</sub>O)<sub>3</sub> - P1s]
- KC&95** W. Köble, J.T. Costello, J.P. Mosnier, E.T. Kennedy and M. Martins, J. Phys. B 28 (1995) 181. (Au5p, Au4f)
- KC&99** E.T. Kennedy, J.T. Costello, A. Gray, C. McGuiness, J.P. Mosnier and P. van Kampen, J. El. Spec. 101-103 (1999) 161. (Cr3p, Na2s, Mg2s, Si2p)
- KC&06** A. Kivimaki, M. Coreno, R. Richter, J. Alvarez Ruiz, E. Melero Garcia, M. de Simone, G. Vall-llosera and K.C. Prince, J. Phys. B: At. Mol. Opt. Phys. 39 (2006) 1101. (H<sub>2</sub>O-O1s)
- KC&16** A. Kivimäki, M. Coreno, P. Miotti, F. Frassetto, L. Poletti, C. Stråhlman, M. de Simone, R. Richter, J. El. Spec. 209 (2016) 26. (SF<sub>6</sub> – S2p)
- KDC79** F. Kaspar, W. Domcke and L.S. Cederbaum, Chem. Phys. Lett. 44 (1979) 33. (CO-C1s, N<sub>2</sub>-N1s)
- KD&92** G. Kaindl, M. Domke, C. Laubshat, E. Meschke and C. Xue, Rev. Sci. Inst. 63 (1992) 1234 (Ar2p, CO - C1s, N<sub>2</sub> - N1s)
- KD&99** E. Kukk, J.D. Bozek, et al., J. Chem. Phys. 111 (1999) 9642. (CO – C 1s)
- KE75** B.M. Kincaid and P. Eisenberger, Phys. Rev. Lett. 34 (1975) 1361. (GeCl<sub>4</sub> - Ge1s; Kr1s; Br<sub>2</sub> - Br1s)
- KE&83** F.W. Kutzler, D.E. Ellis, T.I. Morrison, G.K. Shenoy, P.J. Viccaro, P.A. Montano, E.H. Appelman, L. Stein, M.J. Peleu and D.M. Gruen, Sol. St. Comm. 46 (1983) 803. (Kr1s; KrF<sub>2</sub>-Kr1s)
- KE&98** A. Karakajzyk, P. Erman, P. Hatherly, E. Raclew, M. Stankiewicz and K.Y. Franzen, Phys. Rev. A 58 (1998) 314. (CS<sub>2</sub> – C1s, S2p)
- KF&98** L.V. Ky, P. Faucher, H.L. Zhou, A. Hibbert, Y.Z. Qu, J.M. Li and F. Bely-Dubau, Phys. Rev. A 58 (1998) 3688. (Li 1s)
- KF&20** L Kaiser, K Fehre et al., J. Phys. B: At. Mol. Opt. Phys. 53 (2020) 194002. (CH<sub>3</sub>OH – O1s)
- KGM77** A.A. Krasnoperova, E.S. Gluskin and L.N. Mazalov, J. Struct. 18 (1977) 206 [Zh. Struk. Khim. 18 (1977) 255]. (COS,CS<sub>2</sub> - S2p)
- KG&76** A.A. Krasnoperova, E.S. Gluskin, L.N. Mazalov and V.A. Kochubei, J. Struct. Chem. 17 (1976) 947 [Zh.

- Struk. Khim. 17 (1976) 1113]. (SO<sub>2</sub> - S2p)
- KG&97** H. Köppel, F.X. Gadea, G. Klatt, J. Schirmer and L.S. Cederbaum, J. Chem. Phys. 106 (1997) 4415. (C<sub>2</sub>H<sub>4</sub>, C<sub>2</sub>H<sub>2</sub>D<sub>2</sub> - C1s)
- KG&00** P. van Kampen, Ch. Gerth, M. Martins, P.K. Carroll, J. Hirsch, E.T. Kennedy, O. Meighan, J.P. Moisner, P. Zimmermann and J.T. Costello, Phys. Rev. A 61 (2000) 062706. (U5d)
- KG&18** S. Klumpp, A. A. Guda, et al., Photoabsorption of the molecular IH cation at the iodine 3d absorption edge, Physical Review A 97, 033401 (2018). (IH<sup>+</sup>-I3d)
- KH90** U. Kuetgans and J. Hormes, SIF Conf. Proc. 25 (1990) 59. (TiCl<sub>4</sub> - Ti1s)
- KH91** U. Kuetgans and J. Hormes, Phys. Rev A 44 (1991) 264. (Ar1s)
- KHS05** T. Kaneyasu, Y. Hikosaka and E. Shigemasa, UVSOR Annual Report 2005, 50. (Ar2p)
- KHS07** T. Kaneyasu, Y. Hikosaka and E. Shigemasa, J. El. Spec. 156-158 (2007) 279. (N<sub>2</sub>-N1s)
- KH&87** T. Koizumi, T. Hayaishi, Y. Itikawa, T. Nagata, Y. Sato and A. Yagashita, J. Phys. B 20 (1987) 5393. (Rb3d, Sr3d)
- KH&89** T. Koizumi, T. Hayaishi, T. Matsuo, K. Shima, H. Tawara, T. Tonuma and A. Yagashita, J. Phys. Soc. Jpn. 58 (1989) 13. (Xe2p)
- KH&90** T. Koizumi, T. Hayaishi, Y. Itikawa, Y. Itoh, T. Matsuo, T. Nagata, Y. Sato, E. Shigemasa, A. Yagashita and M. Yoshino, J. Phys. B 23 (1990) 403. (Rb3d, Sr3d)
- KH&92** B. Kammerling, A. Hausmann, J. Lauger and V. Schmitt, J. Phys. B 25 (1992) 4773. (Mg2p)
- KH&00** A. Kivimaki, U. Hergenhahn, B. Kempgens, R. Hentges, M.N. Piancastelli, K. Maier, A. Rudel, J.J. Tulkki and A.M. Bradshaw, Phys. Rev. A 63 (2000) 012716. (Xe3d)
- KH&01a** M. Kitajima, M. Hoshino, M. Okamoto, T. Suzuki, H. Tanaka, Y. Shimizu, Y. Muramatsu, H. Chiba, K. Ueda, T. Hayaishi, M. Simon and M. Kimura Phys. Rev. A 63, (2001) 050703 (SF6 – S2p)
- KH&01b** N. Kosugi, T. Hatsui, M. Nagasano, T. Gejo and E. Shigemasa, UVSOR Ann. Report 2001, 125. (SO<sub>2</sub> - S2p)
- KI00** N. Kosugi and T. Ishida, Chem. Phys. Lett. 329 (2000) 138. (SO<sub>2</sub>, COS – S2p, PF<sub>3</sub> – P2p)
- KI&84** H. Kanamori, S. Iwata, A. Mikuni, and T. Sasaki, J. Phys. B 17 (1984) 3887. (BF<sub>3</sub>-B1s)
- KI&95a** T. Koizumi, Y. Itoh, M. Sano, M. Kimura, T.M. Kojima, S. Kravis, A. Matsumoto, M. Oura, T. Sekioka and Y. Awaya, J. Phys. B 28 (1995) 609. (Ba 4d)
- KI&95b** B. Kemgens, B.S. Itchkawitz, K.J. Randall, J. Feldhaus, A.M. Bradshaw, H. Koppel, F.X. Gadea, D. Nordfors, J. Schirmer and L.S. Cederbaum, Chem. Phys. Lett. 246 (1995) 347. (C<sub>2</sub>H<sub>4</sub>, 1,1-C<sub>2</sub>H<sub>2</sub>D<sub>2</sub>, C<sub>2</sub>H<sub>2</sub>D<sub>2</sub>, C<sub>2</sub>D<sub>4</sub> - C1s)
- KI&96** H.M. Köppe, B.S. Itchkawitz, A.L.D. Kilcoyne, J. Feldhaus, B. Kempgens, A. Kivimaki, M. Neeb and A.M. Bradshaw, Phys. Rev. A 53 (1996) 4120. (CH<sub>4</sub> - C1s)
- KI&97** B. Kempgens, B.S. Itchkawitz, J. Feldhaus, A.M. Bradshaw, H.M. Köppel, M. Doscher, F.X. Gadea and L.S.

Cederbaum, Chem. Phys. Lett. 277 (1997) 436. ( $\text{C}_2\text{H}_2$  - C1s)

- KJ&94** A. Knop, H.W. Jochims, A.L.D. Kilcoyne, A.P. Hitchcock and E. Rühl, Chem. Phys. Lett. 223 (1994) 553. ( $\text{Ar}$ ,  $\text{Ar}_n$  - Ar2p)
- KJ&95** B. Krassig, M. Jung, D.S. Gemmell, E.P. Kanter, T. LeBrun, S.H. Southworth and L. Young, Phys. Rev. Lett. 75 (1995) 4736. (Ar1s)
- KK83** N. Kosugi and H. Kuroda, Chem. Phys. Lett. 94 (1983) 377. ( $\text{N}_2$ -N1s; CO,  $\text{CO}_2$  - C1s, O1s)
- KKS89** B. Kammerling, H. Kossman and V. Schmidt, J. Phys. B 22 (1989) 841. (Xe4d)
- KK&92** M. Kanno, G. Kutluk, T. Takaku, T. Nagata, E. Shigemasa, A. Yagashita and F. Kolka, Photon Factory Ann. Rep. (1992) 42. (K2p, Ca2p, Mn2p, Fe2p)
- KK&95a** U. Koble, L.M. Kiernan, J.T. Costello, J.P. Mosnier, E.J. Kennedy, V.K. Ivanov, V.A. Kupchenko and M.S. Shendick, Phys. Rev. Lett. 74 (1995) 2188. (La4d)
- KK&95b** H.M. Koppe, A.L.D. Kilcoyne, J. Feldhaus and A.M. Bradshaw, J. Electron Spectrosc. 75 (1995) 97. (CO - C1s)
- KK&96a** B. Kempgens, A. Kivimaki, M. Neeb, H.M. Köppe, A.M. Bradshaw and J. Feldhaus, J. Phys. B 29 (1996) 5389. ( $\text{N}_2$  -N1s)
- KK&96b** H.M. Köppe, B. Kempgens, A.L.D. Kilcoyne, J. Feldhaus and A.M. Bradshaw, Chem. Phys. Lett. 260 (1996) 223. (CO -C1s)
- KK&97a** B. Kempgens, H.M. Köppe, A. Kivimaki, M. Neeb, K. Maier, U. Hergenhahn and A.M. Bradshaw, Phys. Rev. Lett. 79 (1997) 35. ( $\text{C}_2\text{H}_x$ ,  $x=2,4,6$  - C1s)
- KK&97b** B. Kempgens, A. Kivimaki, H.M. Köppe, M. Neeb, A.M. Bradshaw and J. Feldhaus, J. Chem. Phys. 107 (1997) 4219. ( $\text{C}_2\text{H}_2$  - C1s)
- KK&97c** B. Kempgens, H.M. Köppe, A. Kivimaki, M. Neeb, L.S. Cederbaum and A.M. Bradshaw, Phys. Rev. Lett. 79 (1997) 3617. ( $\text{C}_2\text{H}_2$  - C1s)
- KK&98a** A. Kivimaki, B. Kempgens, M.N. Piancastelli, M. Neeb, K. Maier, A. Rudel, U. Hergerhahn, and A.M. Bradshaw, J. Electron Spectrosc. 93 (1998) 81. ( $\text{O}_2$  - O1s)
- KK&98b** A. Kivimaki, E. Kukk, J. Karvonen, J. Mursu, E. Nommiste, H. Aksela and S. Aksela, Phys. Rev. A 57 (1998) 2724. (HCl - Cl2p)
- KK&98c** B. Kempgens, A. Kivimaki, B.S. Itchikawitz, H.M. Köppe, M. Schmidbauer, M. Neeb, K. Maier, J. Felhaus, and A.M. Bradshaw, J. El. Spec. 93 (1998) 39. ( $\text{C}_2\text{H}_4$  - C1s)
- KK&99** B. Kempgens, H.M. Köppe, A. Kivimaki, M. Neeb, K. Maier, U. Hergenhahn, and A.M. Bradshaw, Surf. Sci. 425 (1999) L376. ( $\text{C}_2\text{H}_2$ ,  $\text{C}_2\text{H}_4$ ,  $\text{C}_2\text{H}_6$ ,  $\text{C}_6\text{H}_6$  - C1s)
- KK&02** H. Kjeldsen, B. Kristensen, F. Folkmann and T. Andersen, Phys. Rev. B 35 (2002) 3655. (Fe3p)
- KL86** F. Keller and H Levebvre-Brion, Z. Phys. D 4 (1986) 15. (HBr-Br3d; HI-I4d)

- KLW77a** R.B. Kay, Ph.E. van der Leeuw and M.J. Van der Wiel, J. Phys. B 10 (1977) 2513. (CO - C1s; N<sub>2</sub> - N1s)
- KLW77b** R.B. Kay, Ph.E. van der Leeuw and M.J. Van der Wiel, J. Phys. B 10 (1977) 2521. (CO - C1s)
- KL&92** D.Y. Kim, K.Lee, C.I. Ma, M. Mahalingam, D.M. Hanson and S.L. Hubert, J. Chem. Phys. 97 (1992) 5915. (H<sub>2</sub>O - O1s)
- KL&96** L.M. Kiernan, M.K. Lee, B.F. Sonntag, P. Zimmermann, J.T. Costello, E.J. Kennedy, A. Gray and L.V. Ky, J. Phys. B 29 (1996) L181. (Li1s)
- KM83** A.V. Kondratenko, and L.N. Mazalov, Theor. Chim. Acta 62 (1983) 537. (HCl-Cl2p, H<sub>2</sub>S-S2p, PH<sub>3</sub>-P2p, SiH<sub>4</sub>-Si2p)
- KMK79** A.V. Kondratenko, L.N. Mazalov and B.A. Kornev, J. Struct. Chem. 20 (1979) 833 [Zh. Struk. Khim. 20 (1979) 963]. (NO-N1s; O<sub>2</sub>-O1s)
- KML01** T Kroin, S E Michelin and M-T Lee, J. Phys. B 34 (2001) 1829. (CO – C1s)
- KMN79** A.V. Kondratenko, L.N. Mazalov and K.M. Neiman, J. Struct. Chem. 20 (1979) 170, 785 [Zh. Struk. Khim. 20 (1979) 203, 919]. (N<sub>2</sub>-N1s; CO-C1s,O1s)
- KMN80a** A.V. Kondratenko, L.N. Mazalov and K.M. Nieman, Opt. Spectrosc. 49 (1980) 266 [Opt. Spektrosk. 49 (1980) 488]. (SO<sub>2</sub>-S2p,S1s)
- KMN80b** A.V. Kondratenko, L.N. Mazalov and K.M. Nieman, Theor. Chim. Acta 54 (1980) 179. (Cl<sub>2</sub> - Cl 2p)
- KMR77** G.C. King, J.W. McConkey and F.H. Read, J. Phys. B 10 (1977) L541. (N<sub>2</sub>-N1s, CO-C1s)
- KM&77** A.V. Kondratenko, L.N. Mazalov F. Kh. Gel'mukhanov, V.I. Avdeev and E. A. Saprykina, J. Struct. Chem. 18 (1977) 437 [Zh. Struk. Khim. 18 (1977) 546]. (CO -C1s, O1s; N<sub>2</sub>- N1s)
- KM&80** G.C. King, J.W. McConkey, F.H. Read and B. Dobson, J. Phys. B 13 (1980) 4315. (N<sub>2</sub>, NO, N<sub>2</sub>O -N1s; CO, CO<sub>2</sub> - C1s)
- KM&84** O. Keski-Rahkonen, G. Materlick, B. Sonntag and J. Tulkki, J. Phys. B 17 (1984) L121. (Ba2s,2p; Hg2s,2p)
- KM&98** A. Kivimaki, K. Maier, U. Hergerhahn, M.N. Piancastelli, B. Kempgens, A. Rudel, and A.M. Bradshaw, Phys. Rev. Lett. 81 (1998) 301. (N<sub>2</sub> - N1s)
- KM&02a** A. Kivimaki, E. Melero Garcia, J. Alvarez Riuz, P. Erman, E. Rachlew, J. Rius I Riu and M. Stankiewicz, Max Lab annual report 2002 (N<sub>2</sub>-N1s)
- KM&02b** M. Kutzner, V. Maycock, J. Thorarinson, E. Pannwitz, and J. A. Robertson, Phys. Rev. A 66 (2002) 042715. (Ca2p,Mg2p, Sr2p)
- KM&03** T. Kroin, S. E. Michelin, A. S. Falck, F. Arretche, M.-T. Lee, and I. Iga, Phys. Rev. A 68 (2003) 012071. (CO<sub>2</sub>, COS, CS<sub>2</sub> – C1s)
- KM&07** M. Kato, Y. Morishita, M. Oura, H. Yamaoka, Y. Tamenori, K. Okada, T. Matsudo, T. Gejo, I.H. Suzuki and N. Saito, J. El. Spec. 160 (2007) 39. (Ar2p, Kr2p, Xe3d, N<sub>2</sub>-N1s)
- KNP92** A. Koch, B.M. Nestmann and S.D. Peyerimhoff, Chem. Phys. 161 (1992) 169 (CH<sub>4</sub> - C1s; SiH<sub>4</sub> - Si1s, NH<sub>4</sub><sup>-</sup>

- N1s, PH<sub>4</sub>-P1s)
- KNS90** A.G. Kochur, A.M. Nadolinskii and V. Sukhorukov, Opt. Spectrosc USSR 69 (1990) 278 [Opt. i Spek. 69 (1990) 464]. (F1s)
- KNY93** A.N. Khoperskii, A.M. Nadolinskii and V.A. Yanna, Opt. Spectrosc. 74 (1993) 493. (Kr2p, Xe3p)
- KN&96** A. Kivimaki, M. Neeb, B. Kempgens, H.M. Köppe, A.M. Bradshaw, Phys. Rev. A 54 (1996) 2137. (N<sub>2</sub> - N1s)
- KN&97a** J. Karvonen, E. Nommiste, H. Aksela and S. Aksela, J. Chem. Phys. 106 (1997) 3466. (C<sub>60</sub> - C1s)
- KN&97b** A. Kivimaki, M. Neeb, B. Kempgens, H.M. Köppe, K. Maier and A.M. Bradshaw, J. Phys. B 30 (1997) 4279. (N<sub>2</sub> - N1s)
- KN&13** A. Kivimäki, P. Norman, M. Coreno, M. de Simone, C. Grazioli, R. Totani, B. Ressel, H. Ottosson, and C. Puglia, Phys. Rev. A 88 (2013) 062502. (C<sub>4</sub>GeH<sub>12</sub> – Ge 3p)
- KO&98** T.M. Kojima, M. Oura, Y. Itoh, T. Koizumi, M Sano, T. Sekioka, N. Watanabe, H. Yomaska and Y. Awaya, J. Phys. B 31 (1998) 1463. (Eu4d)
- KP92a** A. Koch and S.D. Peyerimhoff, Chem. Phys. Lett. 195 (1992) 104. (CH<sub>4</sub>-C1s)
- KP92b** A. Koch and S.D. Peyerimhoff, Z. Phys. D 23 (1992) 239. (SiH<sub>4</sub>, SiH<sub>3</sub>F - Si1s)
- KP93** A. Koch and S.D. Peyerimhoff, Chem. Phys. 172 (1993) 21. (SiF<sub>2</sub>H<sub>2</sub> - Si 1s)
- KP94a** A. Koch and S.D. Peyerimhoff, Mol. Phys. 83 (1994) 471. (SiH<sub>4</sub> - Si1s)
- KP94b** A. Koch and S.D. Peyerimhoff, Chem. Phys. 189 (1994) 67. (H<sub>2</sub>O, D<sub>2</sub>O - O1s)
- KPR81** Y.S. Kim, R.H. Pratt and A. Ron, Phys. Rev. A 24 (1981) 1626. (U 4f, Sn 3d)
- KP&01** C. Kolczewski, R. Puttner, O. Plashkevych, H. Agren, V. Staemmler, M. Martins, G. Snell, A.S. Schlachter, M. Sant'Anna, G. Kaindl and L.G.M. Pettersson, J. Chem. Phys. 115 (2001) 6426. (C<sub>5</sub>H<sub>5</sub>N – C1s, N1s)
- KP&06** C. Kolczewski, R. Püttner, M. Martins, A. S. Schlachter, G. Snell, M. M. Sant'Anna, K. Hermann, and G. Kaindl, J. Chem. Phys. 124 (2006) 034302. (C<sub>6</sub>H<sub>6</sub>, C<sub>6</sub>H<sub>8</sub>, C<sub>6</sub>H<sub>10</sub>, C<sub>6</sub>H<sub>12</sub>, C<sub>8</sub>H<sub>8</sub>, C<sub>8</sub>H<sub>10</sub> – C1s)
- KRT77** G.C. King, F.H. Read and M. Tronc, Chem. Phys. Lett. 52 (1977) 50. (N<sub>2</sub> - N1s)
- KR&90** M. Kutzner, V. Rdojevic, H.P. Kelly and Z. Altun, Phys. Scripta 41 (1990) 823 (Ba4d)
- KR&02a** E. Kukk, R. Ruus, R. Sankari, J. Rius i Riu, J. Nikkinen, A. Penttila, S. Ohmekhin, H. Aksela and S. Aksela, Max Lab annual report 2002, 176. (CsBr-Cs4d; CaBr<sub>2</sub> – Ca 2p)
- KR&02b** E. Kukk, J. Rius i Riu, M. Stankiewicz, P. A. Hatherly, P. Erman, E. Rachlew, P. Winiarczyk, M. Huttula and S. Aksela, Phys. Rev. A 66 (2002) 012704. (CD<sub>4</sub> – C1s)
- KS79** E.E. Koch and B.F. Sonntag in, Topics in Current Physics 10 *Synchrotron Radiation*. (Springer, Heidelberg, 1979) 269. (review)
- KS98** P. Van Kempen and G. O'Sullivan, J. Phys. B 31 (1998) L135. (Sc3p, Ti3p)

- KS01** T Kerkau and V Schmidt, J. Phys. B 34 (2001) 839. (CO – C1s, O1s)
- KSP96** A.G. Kochur, V.L. Sukhorukov and I.D. Petrov, J. Phys. B 29 (1996) 4565. (Eu4d)
- KSY92** N. Kosugi, K. Shigesma and A. Yagashita, Chem. Phys. Lett. 190 (1992) 481 (O<sub>2</sub> - O1s).
- KS&84** P.H. Kibrin, S. Southworth, C.M. Truesdale, D.W. Lindle, U. Becker and D.A. Shirley, Phys. Rev. A 29 (1984) 194. (Ne1s)
- KS&86** I. Kojima, A.K. Srivastava, E. Miyazaki and H. Adachi, J. Chem. Phys. 84 (1986) 4455. (CO-C1s,O1s)
- KS&93** A.L.D. Kilcoyne, M. Schmidbauer, A. Koch, K.J. Randall and J. Feldhaus, J. Chem. Phys. 98 (1993) 6735. (H<sub>2</sub>CO, C<sub>2</sub>H<sub>4</sub> - C1s)
- KS&05** A. Kivimäki, S. L. Sorensen, M. Tchaplyguine, M. Gisselbrecht, R. R. T. Marinho, R. Feifel, G. Öhrwall, S. Svensson, and O. Björneholm, Phys. Rev. A 71 (2005) 033204. (Ar, Ar<sub>n</sub> - Ar2p)
- KS&06** E. Kukk, R. Sankari, M. Huttula, A. Sankari, H. Aksela and S. Aksela, 2005-06 Max Lab Annual Report (2006) 232. (C<sub>2</sub>H<sub>3</sub>N – N1s)
- KS&07** E. Kukk, R. Sankari, M. Huttula, A. Sankari, H. Aksela and S. Aksela, J. El. Spec. 155 (2007) 141. (C<sub>2</sub>H<sub>3</sub>N – N1s)
- KT&77** G.C. King, M. Tronc, F.H. Read and R.C. Bradford, J. Phys. B 10 (1977) 2479. (Ar2p, Kr3d, Xe4d)
- KT&96** H. Kjeldsen, T.D. Thomas, P. Lablanquie, M. Lavollée, F. Penent, M. Hochlaf and R.I. Hall, J. Phys. B 29 (1996) 1689. (Ar2p)
- KU&95** N. Kosugi, K. Ueda, Y. Shimizu, H. Chiba, M. Okunishi, K. Ohnori, Y. Sato and E. Shigemasa, Chem. Phys. Lett. 246 (1995) 475. (CH<sub>3</sub>F - C1s)
- KU&99** N.M. Kaachnik, K. Ueda, Y. Muaramtsu and Y. Sato, J. Phys. B 31 (1998) L1791. (HCl – Cl2p)
- KW81** A.B. Kunz and T.O. Woodruff, Sol. St. Comm. 38 (1981) 629. (LiH-Li1s)
- KWM93** M. Kutzner, D. Winn and S. Mattingly, Phys. Rev. A 48 (1993) 404. (Be1s, Mg2p, Ca3p, Sr3d, Ba3d, Ba4d)
- KWR98** A. Knop, B. Wassermann and E. Rühl, Phys. Rev. Lett. 80 (1998) 2302. (Kr<sub>n</sub> - Kr3d)
- KW&98** E. Kukk, A. Wills, N. Berrah, B. Langer, J.D. Bozek, O. Nayadin, M. Alsherhi, A. Farhat and D. Cubaynes, Phys. Rev. A 57 (1998) R1485. (HCl - Cl2p)
- KY90** A.N. Khoperskii and V.A. Yavna, Opt. Spec. (USSR) 69 (1990) 314. (Opt. i Spekt. 69 (1990) 523). (Ar2p)
- KY91** A.N. Khoperskii and V.A. Yavna, Opt. Spec. (USSR) 70 (1991) 154. (Opt. i Spekt. 70 (1990) 258) (Mn3p)
- KY95** A.N. Khoperskii and V.A. Yavna, J.E.T.P. 81 (1995) 671. (ZETP(R) 108 (1995) 1223). (Ar1s)
- KY97** A.N. Khoperskii and V.A. Yavna, Opt. Spectosk (USSR) 82 (1997) 1. (Opt. Spec. 82 (1997) 5). (Ar2s)
- KYK86** N. Kosugi, T. Yokoyama and H. Kuroda, Chem. Phys. 104 (1986) 449. (BF<sub>3</sub>-B1s)

- KYN09a** N. Kosugi, H Yamane and M. Nagasaka, UVSOR Ann Rep 2009, 32. ( $C_{10}H_{10}Fe$ ,  $C_{20}H_{30}Fe$ - $Fe2p$ )
- KYN09a** N. Kosugi, H Yamane and M. Nagasaka, UVSOR Ann Rep 2009, 33. ( $O_2$  - O1s)
- KY&87** A.N. Khoperskii, V.A. Yavna and I.D. Petrov, Opt. Spec. (USSR) 63 (1987) 119. (Opt. i Spekt. 63 (1987) 204). (Ar2p)
- KY&02** K Kawatsura, H Yamaoka, M Oura, T Hayaishi, T Sekioka, A Agui, A Yoshigoe and F Koike, J. Phys. B 35 (2000) 4147. (O1s, Ne1s)
- L65** R.J. Liefeld, Appl. Phys. Lett. 7 (1965) 276. (Ne1s)
- L72** R.E. LaVilla, J. Chem.Phys. 57 (1972) 899. ( $SF_6$  - S1s, S2p, F1s)
- L73** R.E. LaVilla, J. Chem. Phys. 58 (1973) 3841. ( $CH_xF_{4-x}$  ( $x=1-4$ ) - F1s)
- L75a** R.E. LaVilla, J. Chem. Phys. 62 (1975) 2209. ( $H_2S$  - S1s)
- L75b** R.E. LaVilla, J. Chem. Phys. 63 (1975) 2733. ( $O_2$ ,  $CO_2$  - O1s)
- L79** R.E. LaVilla, Phys. Rev. A 19 (1979) 1999. (Na1s)
- L86** E. Lindholm, J. Chem. Phys. 85 (1986) 1484. ( $C_4H_6$ ,  $C_6H_6$ -C1s)
- L89** D.W. Lindle, Nucl. Inst. Meth. A 280 (1989) 161. ( $CH_3Cl$  - Cl1s)
- L91** D.L. Lynch, Phys. Rev. A 43 (1991) 5176. ( $N_2$ -N1s; CO-C1s)
- L92** A. Lisini, AIP Conf. Proc. (Grenoble SR Dynamics) 258 (1992) 149. (Li1s)
- L94** F.P. Larkins, Nucl. Inst. Meth. B 87 (1994) 215. ( $CO_2$  - C1s;  $N_2O$  - N1s)
- L95** P. Lablanquie, J. Electron Spectrosc. 76 (1995) 63. ( $Fe(CO)_2(NO)_2$  - C1s)
- L96a** B. Lahmann, Aust. J. Phys. 49 (1996) 365. (Ar2p)
- L96b** F.P. Larkins, Aust. J. Phys. 49 (1996) 457. (CO -C1s;  $O_2$  - O1s)
- L98a** Z.H. Levine, J. Phys. B 31 (1998) 3155. (Fe3p, Mn3p)
- L98b** R. Lakanen, J. El. Spec. 87 (1998) 253. (Rb3d)
- L99a** M. Lavollée, Rev. Sci. Inst. 70 (1999) 2968. ( $CS_2$  – S2p)
- L99b** K.T. Leung, Valence and inner shell non-dipole excitation spectroscopy of polyatomic molecules by angle-resolved inelastic electron scattering at high energy, J. El. Spectrosc. Rel. Phen. 100 (1999) 23. (REVIEW,  $CF_{4-n}Cl_n$  ( $n=0-4$ ),  $CHF_{3-m}Cl_m$  ( $m=1-3$ ) – C1s)
- LA93** C. Liegener and H. Agren, Phys. Rev. B 48 (1993) 789. ( $C_2H_4$ ,  $C_4H_6$ ,  $C_6H_8$  - C1s)
- LAG96** Y. Luo, H. Agren and F. Gel'mukhanov, Phys. Rev. A 53 (1996) 1340. ( $C_6H_7N$  -C1s;  $CF_2Cl_2$ ,  $CF_3Cl$  -Cl 1s)

- LAL91** E. Lindholm, L. Asbrink and S. Ljunggren, J. Phys. Chem. 95 (1991) 3923. ( $\text{CH}_4$ ,  $\text{C}_2\text{H}_n$ ,  $n=2,4,6$ ;  $\text{C}_3\text{H}_4$ ,  $\text{C}_3\text{H}_8$ ,  $\text{C}_4\text{H}_8$ , c- $\text{C}_3\text{H}_6$ ,  $\text{C}_6\text{H}_6$ ,  $\text{C}_6\text{H}_{12}$ ,  $\text{C}_{10}\text{H}_8$  - C1s; CO,  $\text{CO}_2$ ,  $\text{H}_2\text{CO}$ ,  $\text{H}_2\text{CO}_2$ ,  $\text{CH}_3\text{OH}$ ,  $\text{CH}_3\text{OCH}_3$  - C1s, O1s; HCN,  $\text{CH}_3\text{NH}_2$ ,  $\text{NMe}_3$  - C1s, N1s;  $\text{N}_2$ ,  $\text{N}_2\text{O}$ ,  $\text{NH}_3$ ,  $\text{NF}_3$  - N1s;  $\text{F}_2$ , HF,  $\text{NF}_3$  - F1s;  $\text{CF}_4$ ,  $\text{CH}_3\text{F}$ ,  $\text{C}_2\text{F}_4$  - C1s, F1s)
- LA&95** Y. Luo, H. Agren, J. Guo, P. Skytt, N. Wassdahl and J. Nordgren, Phys. Rev. A 52 (1995) 3730. ( $\text{C}_6\text{H}_5\text{NH}_2$  - C1s)
- LBB92** G. Li, F. Bridges and G.S. Brown, Phys. Rev. Lett. 68 (1992) 1609 (Kr1s).
- LBH90** A. Lisini, P.G. Burke and A. Hibbert, J. Phys. B 23 (1990) 3767. (Li1s)
- LBZ64** A.P. Lukirskii, I.A. Brytov and T.M. Zimkina, Opt. Spectrosc. 17 (1964) 234 [Opt. Spektrosk. 17 (1964) 438]. ( $\text{Kr}3\text{d}$ ; Xe4d;  $\text{CH}_4$ ,  $\text{CH}_2(\text{OCH}_3)_2$  - C1s)
- LB&90** J.C. Levin, C. Biedermann, N. Keller, L. Liljeby, C.S. O, R.T. Short, I.A. Sellin and D.W. Lindle, Phys. Rev. Lett. 65 (1990) 988. (Ar1s)
- LB&91** J.C. Levin, C. Biedermann, N. Keller, L. Liljeby, R.T. Short, I.A. Sellin and D.W. Lindle, Nucl. Inst. Meth. B 56/57 (1991) 124. (Ar1s)
- LB&93** Z.F. Liu, G.M. Bancroft, K.H. Tan and M. Schachter, Phys. Rev. A 48 (1993) R4019. (HBr - Br3d)
- LB&94a** Z.F. Liu, G.M. Bancroft, K.H. Tan and M. Schachter, Phys. Rev. Lett. 72 (1994) 621. (HBr - Br3d)
- LB&94b** C.U. Larsson, A. Beutler, O. Björneholm, F. Federmann, U. Hahn, A. Rieck, S. Verbin and T. Möller, Nucl. Inst. Meth. A 337 (1994) 603. ( $\text{N}_2$  - N1s; Ne1s;  $\text{H}_2\text{O}$  - O1s)
- LB&94c** Z.F. Liu, G.M. Bancroft, K.H. Tan and M. Schachter, J. El. Spec. 67 (1994) 299. (HHBr - Br 3d)
- LB&95** Z.F. Liu, G.M. Bancroft, J.S. Tse and Z.Z. Yang, Chem. Phys. 192 (1995) 255. ( $\text{H}_2\text{S}$  - S2p,  $\text{HCl}, \text{Cl}_2$  - Cl2p;  $\text{PH}_3$  - P2p;  $\text{SiH}_4$  - Si 2p)
- LB&96** B. Langer, N. Berrah, A. Farhat, O. Hemmers and J.D. Bozek, Phys. Rev. A 53 (1996) R1946. (Xe4d)
- LB&97** B. Langer, N. Berrah, A. Farhat, M. Humphrey, D. Cubaynes, A. Menzel and U. Becker, J. Phys. B 30 (1997) 42551. (Xe4d)
- LCH03** J.F. Lehmann, J. Cuny, A.P. Hitchcock, (2003) unpublished. ( $\text{C}_4\text{H}_6\text{O}_5$  - C1s, O1s)
- LCS87** P. Letardi, R. Camilloni and G. Stefani, J. Phys. (Paris) 48 C-9 (1987) 1125 (CF4 - C1s EXELFS)
- LCS89** P. Letardi, R. Camilloni and G. Stefani, Phys. Rev. B 49 (1989) 3311. ( $\text{CO}_2$  - O1s)
- LC&87** D.W. Lindle, P.L. Cowan, R.E. LaVilla, T.E. Jach, R.D. Deslattes, R.C.C. Perera and B. Karlin, J. Phys. (Paris) 48 C-9 (1987) 761. (CF<sub>3</sub>Cl - Cl1s)
- LC&88a** D.W. Lindle, P.L. Cowan, R.E. LaVilla, T.E. Jach, R.D. Deslattes, B. Karlin, J.A. Sheehey, T.J. Gil and P.W. Langhoff, Phys. Rev. Lett. 60 (1988) 1010. ( $\text{CH}_3\text{Cl}$ -Cl1s)
- LC&88b** D.W. Lindle, P.L. Cowan, R.E. LaVilla, T.E. Jach, R.D. Deslattes, R.C.C. Perera and B. Karlin, SPIE 911 (1988) 54. ( $\text{CH}_3\text{Cl}$ -Cl1s)

- LC&90** Z.F. Liu, J.N. Cutler, G.M. Bancroft, K.H. Tan, R.G. Cavell and J.S. Tse, Chem. Phys. Lett. 172 (1990) 421. (PX<sub>3</sub>, X=H, CH<sub>3</sub>, CF<sub>3</sub> - P2p)
- LC&91** D.W. Lindle, P.L. Cowan, T. Jach, R.E. LaVilla, R.D. Deslattes and R.C.C. Perera, Phys. Rev. A 43 (1991) 2353. (CH<sub>3</sub>Cl, CF<sub>x</sub>Cl<sub>4-x</sub>, x=1,2,3 - Cl1s)
- LC&92a** Z.F. Liu, J.N. Cutler, G.M. Bancroft, K.H. Tan, R.G. Cavell and J.S. Tse, Chem. Phys. 168 (1992) 133. (POCl<sub>3</sub>, POF<sub>3</sub>, PF<sub>5</sub> - P2p).
- LC&92b** W.G. Lyman, P.K. Carroll, J.T. Costello, D. Evans and G. O'Sullivan, J. Phys. B 25 (1992) 3963 (B1s).
- LC&07** R. Lessard, J. Cuny, G. Cooper and A.P. Hitchcock, , Chemical Physics 331 (2007) 289. (C<sub>2</sub>H<sub>5</sub>N<sub>3</sub>O<sub>2</sub>, C<sub>3</sub>H<sub>6</sub>O<sub>3</sub>, C<sub>3</sub>H<sub>6</sub>N<sub>2</sub>O<sub>2</sub>, C<sub>4</sub>H<sub>6</sub>O<sub>3</sub>, C<sub>4</sub>H<sub>6</sub>O<sub>5</sub>, C<sub>4</sub>H<sub>7</sub>NO<sub>2</sub>, C<sub>5</sub>H<sub>8</sub>O<sub>2</sub>, C<sub>5</sub>H<sub>8</sub>O<sub>4</sub>, C<sub>7</sub>H<sub>12</sub>O<sub>4</sub>, C<sub>10</sub>H<sub>19</sub>NO<sub>4</sub>, C<sub>13</sub>H<sub>10</sub>O<sub>3</sub> - Cl1s, N1s, O1s)
- LC&11** K.T. Lu, J.M. Chen, J.M. Lee, S.C. Haw, S.A. Chen, Y.C. Liang, J. El. Spec. 184 (2011) 140. (SiCl<sub>4</sub>-Cl2p)
- LC&25** Juliette Leroux,] Jean-Yves Chesnel, et al., Structures of Gas-Phase Hydrated Phosphotyrosine Revealed by Soft X-ray Action Spectroscopy Chem. Eur. J. 31 (2025) e202403665 (C<sub>9</sub>H<sub>11</sub>NO<sub>5</sub>P – O1s)
- LD66** R.E. LaVilla and R.D. Deslattes, J. Chem. Phys. 44 (1966) 4399. (SF<sub>6</sub>, H<sub>2</sub>S - S1s)
- LD72** R.E. LaVilla and R.D. Deslattes, spectra shown in D72. (CF<sub>3</sub>SF<sub>5</sub>, SF<sub>2</sub>O<sub>2</sub>, SF<sub>2</sub>O - S1s)
- LDN07** A.F. Lago, J.Z. Dávalos and A. Naves de Brito, J. El. Spec. 156-158 (2007) 241. (C<sub>3</sub>ClH<sub>5</sub>O- C1s, O1s, Cl 1s)
- LDR83** A. Lahmam-Bennani, A. Duguet and M. Roualt, J. Chem. Phys. 78 (1983) 1838. (Ne1s - compton profile)
- LD&92a** S. Lee, P.A. Dowben, A.T. Wen, A.P. Hitchcock, J.A. Glass and J.T. Spencer, J. Vac. Sci. Tech. A 10 (1992) 881. (B<sub>5</sub>H<sub>9</sub>, B<sub>10</sub>H<sub>14</sub>, C<sub>2</sub>B<sub>10</sub>H<sub>12</sub> - B1s)
- LD&92b** R. Locht, W. Denzer, E. Ruhl and H Baumgartel, Chem. Phys. 160 (1992) 477 (N<sub>2</sub> - N1s)
- LD&06** A.F. Lago, J.Z. Davalos, U. Kerdpin and A.S. Schlachter, J. Phys. Chem. A 110 (2006) 13717. (CH<sub>2</sub>Cl<sub>2</sub> – Cl1s)
- LE&88** F.P. Larkins, W. Eberhardt, I.W. Lyo, R. Murphy and E.W. Plummer, J. Chem. Phys. 88 (1988) 2948. (N<sub>2</sub>O - N1s,O1s)
- LF&88** D.W. Lindle, T.A. Ferrett, P.A. Heiman and D.A. Shirley, Phys. Rev. A 37 (1988) 3808. (Xe4d)
- LG&86** F.W. Lytle, R.B. Gregor, G.H. Via, J.M. Brown and G. Meitzner, J. Phys. (Paris) 47 C-8 (1986) 149. (Ar1s; CCl<sub>4</sub>, C<sub>2</sub>H<sub>4</sub>Cl<sub>2</sub> - Cl1s); Stanford prop #944 (1987) (Cl<sub>2</sub>, CCl<sub>4</sub> - Cl1s)
- LG&96** T. Luhmann, Ch. Gerth, M. Martins, M. Richter and P. Zimmermann, Phys. Rev. Lett. 76 (1996) 4320. (Eu4d, Sm4d)
- LG&98** T. Luhmann, Ch. Gerth,et al.,, Phys. Rev. A 57 (1998) 282. (Xe4d)
- LG&05** A. Lindgren, M. Gisselbrecht, F. Burmeister, A. Kivimäki and S.L. Sorensen, J. Chem. Phys. 122 (2005)

114306. ( $\text{NH}_3$ -N1s)
- LG&09** R. Lewinski, C. Graf, B. Langer, R. Flesch, H. Bresch, B. Wassermann and E. Rühl, Eur. Phys. J. Spec. Top. 169 (2009) 67. ( $\text{C}_5\text{H}_5\text{N}$  – C1s, N 1s)
- LHC02** H.Lin, C. S. Hsue, and K.T. Chung, Phys. Rev A 65 (2002) 032706. (Be1s)
- LH&87** D.W. Lindle, P.A. Heiman, T.A. Ferrett, M.N. Piancastelli and D.A. Shirley, Phys. Rev. A 35 (1987) 4605. (Kr3d)
- LH&94** K. Lee, S.L. Hulbert, P. Kuiper, D. Ji and D.M. Hanson, Nucl. Inst. Meth. A 347 (1994) 446. (Ar2p;  $\text{N}_2\text{O}$  - N1s)
- LH&12** Li H, Hua W, Lin Z, Luo Y., First-principles study on core-level spectroscopy of arginine in gas and solid phases. J Phys Chem B 116 (2012) 12641. (arginine,  $\text{C}_6\text{H}_{14}\text{N}_4\text{O}_2$  – C1s, N1s, O1s)
- LKC16** I. Ljubic', A. Kivimaki and M. Corenec, Phys. Chem. Chem. Phys. 18 (2016) 10207 ( $\text{C}_9\text{H}_{12}\text{NO}$ ,  $\text{C}_{10}\text{H}_{13}\text{N}_2\text{O}_2$ ,  $\text{C}_{10}\text{H}_{11}\text{N}_2\text{O}_2$  – C 1s, N1s, O1s)
- LK&84** D.W. Lindle, P.H. Kobrin, C.M. Truesdale, T.A. Ferrett, P.A. Heiman, H.G. Kerkoff, U. Becker and D.A. Shirley, Phys. Rev. A 30 (1984) 239. ( $\text{CH}_3\text{I}$ -I4d)
- LK&90** K. Lee, D.Y. Kim, C.I. Ma, D.A. Lapiano-Smith and D.M. Hanson, J. Chem. Phys. 93 (1990) 7936. ( $\text{N}_2$  - N1s;  $\text{O}_2$  - O1s)
- LK&94** K. Lee, D.Y. Kim, C.I. Ma, and D.M. Hanson, J. Chem. Phys. 100 (1994) 8550. ( $\text{N}_2$  - N1s)
- LK&20a** M.A. Leutenegger, S. Kühn et al., High-Precision Determination of Oxygen K  $\alpha$  Transition Energy Excludes Incongruent Motion of Interstellar Oxygen, Phy. Rev. Lett. 125 (2020) 243001. (O<sub>2</sub>-O1s)
- LK&20b** Juliette Leroux, Amir Kotobi, et al., Mapping the electronic transitions of protonation sites in peptides using soft X-ray action spectroscopy, Phys. Chem. Chem. Phys. 25 2023, 25603. ( $\text{C}_{10}\text{H}_{18}\text{N}_5\text{O}_5$  (G<sub>5</sub>), G<sub>4</sub>H, G<sub>4</sub>K, G<sub>4</sub>R, PG<sub>4</sub> – N1s)
- LL00** P. Lin and R.R. Lucchese, J. Chem. Phys. 113 (2000) 1843. ( $\text{C}_2\text{H}_2$  – C1s)
- LLM90c** T. LeBrun, M. Lavallee and P. Morin, AIP Conf. Proc. 215 (1990) 846. ( $\text{N}_2\text{O}$  - N1s; HBr - Br3d)
- LL&90a** D. Lapiano-Smith, K. Lee, C.I. Ma, K. Wu and D.M. Hanson, J. Electron Spectrosc. 51 (1990) 221. ( $\text{O}_2$  - O1s)
- LL&90b** D. Lapiano-Smith, K. Lee, C.I. Ma, K. Wu and D.M. Hanson, J. Chem. Phys. 93 (1990) 2169. ( $\text{O}_2$  - O1s)
- LL&93** T. LeBrun, M. Lavallee, M. Simon and P. Morin, J. Chem. Phys. 98 (1993) 2534. ( $\text{N}_2\text{O}$ -N1s)
- LL&14a** Lin Y-S, Lu K-T, Lee YT, Tseng C-M, Ni C-K, Liu C-L Near-edge X-ray absorption fine structure spectra and site-selective dissociation of phenol. J Phys Chem A 118 (2014) 1601. ( $\text{C}_6\text{H}_6\text{O}$  – C1s, 1s)
- LL&14b** Yi-Shiue Lin, Shu-Yu Lin, Yuan T. Lee, Chien-Ming Tseng, Chi-Kung Ni, Chen-Lin Liu, Cheng-Cheng Tsai, Jien-Lian Chenand Wei-Ping Hu, J. Phys. Chem. A 118 (2014) 7803. ( $\text{C}_{12}\text{H}_{10}\text{O}$ ,  $\text{C}_{18}\text{H}_{14}\text{O}_2$  – C1s, 1s)
- LM82a** R.R. Lucchese and V. McKoy, Phys. Rev. A 25 (1982) 2572. (CO<sub>2</sub>-O1s)

- LM82b** R.R. Lucchese and V. McKoy, Phys. Rev. A 26 (1982) 1406. (CO<sub>2</sub>-C1s,O1s)
- LM84** D.L. Lynch and V. McKoy, Phys. Rev. A 30 (1984) 1561. (N<sub>2</sub>-N1s)
- LM91** P. Lablanquie and P. Morin, J. Phys. B 24 (1991) 4349. (Kr3d)
- LMS81** R.E. LaVilla, G. Mehlman and E.B. Saloman, J. Phys. B 14 (1981) L1. (Na2s)
- LM&81** T.B. Lucarto, T.J. McIlrath, J. Sugar, S.M. Younger, Phys. Rev. Lett. 47 (1981) 1124. (Ba, Ba<sup>+</sup>, Ba<sup>2+</sup> - Ba 4d)
- LM&89** D.A. Lapiano-Smith, C.I. Ma, K.T. Wu and D.M. Hanson, J. Chem. Phys. 90 (1989) 2162. (CF<sub>4</sub> - C1s,F1s; SiF<sub>4</sub> - F1s)
- LM&94** D.W. Lindle, W.L. Manner, L. Steinbeck, E. Villalobos, J.C. Levin and I.A. Sellin, J. El. Spec. 67 (1994) 375. (Ar1s; Xe2p; H<sub>2</sub>S-S1s; CH<sub>3</sub>Cl, CF<sub>3</sub>Cl, HCl - Cl 1s)
- LN43** A.E. Lindh and A. Nilsson, Arkiv. Mat. Astron. Fysik, 29A (1943) 1. (HCl,Cl<sub>2</sub> - Cl1s)
- LOL84** G. Leveque, C.G. Olson and D.W. Lynch, Sol. St. Comm 51 (1984) 377 (In 4d)
- LPL85** X. Liang, X. Pan and J. Li, Chin. Phys. Lett. 2 (1985) 545. (NO-N1s)
- LP&95** T. Liebsch, O. Plotzke, F. Heisen, U. Heigenhahn, Oltemmers, R. Wehlitz, J. Viefhaus, B. Langer, S.B. Whitfield and U. Becker, Phys. Rev. A 52 (1995) 457. (C<sub>60</sub> - C1s)
- LP&00** P. Lablanquie, F. Pennent, R.I. Hall, H. Kjeldsen, J.H. D. Eland, A. Muehleisen, P. Pelican, Z. Smit, M. Zitnik and F. Koike, Phys. Rev. Lett. 84 (2000) 47. (Ar2s)
- LP&12** P. Lablanquie, F. Penent, H. Iwayama, K. Soejima and E. Shigemasa, UVSOR Annual report 2012, 64. (HCl - Cl2p)
- LS&87** S.V. Lavrentev, V.L. Suhkorukov, A.N. Khoperskii and I.D. Petrov, Opt. Spectrosc. (USSR) 62 (1987) 278 [Opt. i Spek. 62 (1987) 466] (Ar2s).
- LS&89** P. Lablanquie, A.C.A. de Souza, G.G.B. de Souza, P. Morin and I. Nenner, J. Phys. Chem. 90 (1989) 7078. (SiF<sub>4</sub> - Si2p)
- LS&02** P. Lablanquie, S. Sheinerman, F. Penent, R.I. Hall, M. Ahmad, T. Aoto, Y. Hikosaka and K. Ito, J. Phys. B 35 (2002) 3265. (Xe4d)
- LS&04** A. Lindgren, S.L. Sorensen, M. Gisselbrecht, A. Kivimaki, F. burmeister nad A. Naves de Brito, Max Lab annual report 2004, 192. SO<sub>2</sub> – O1s.
- LS&05** A.F. Lago, A.C.F. Santos, W.C. Stolte, A.S. Schlachter, G.G.B. de Souza, J. El. Spec. 144-147 (2005) 161. CHCl<sub>3</sub> – Cl1s)
- LS&12** P. Lablanquie, S. Sheinerman, L. Andric, J. Palaudoux, Y. Hikosaka, K. Ito, F. Penen, J. El. Spec. 185 (2012) 198. Ar2s)
- LT&84** D.W. Lindle, C.M. Truesdale, P.H. Kobrin, T.A. Ferrett, P.A. Heimann, U. Becker, H.G. Kerkhoff and D.A. Shirley, J. Chem. Phys. 81 (1984) 5375. (N<sub>2</sub>, NO - N1s)

- LUH97** J.F. Lehmann, S.G. Urquhart and A.P. Hitchcock, unpublished. ( $C_7H_{12}O_2$ ,  $C_9H_8O_2$ ,  $C_{14}H_{10}O_3$ ,  $C_{15}H_{24}O$  - C1s, O1s)
- LUH99** R. Lessard, S.G. Urquhart and A.P. Hitchcock, (1999) unpublished. ( $C_8H_6$ ,  $C_{29}H_{20}O$  - C1s)
- LU&99** J.F. Lehmann, L. Ennis, A.P. Hitchcock, S.G. Urquhart, K. Hatano, S. Gupta and M.K. Denk, Organometallics **18** (1999) 1862. ( $C_{10}GeH_{20}N_2$ ,  $C_{10}GeH_{22}N_2$ ,  $C_{10}GeH_{24}N_2$  – C1s, Ge3p, N1s;  $C_{10}H_{20}N_2Si$ ,  $C_{10}H_{22}N_2Si$ ,  $C_{10}H_{24}N_2Si$  – C1s, N1s, Si1s;  $C_{10}H_{20}N_2$ ,  $C_{10}H_{22}N_2$ ,  $C_{11}H_{22}N_2$ ,  $C_{11}H_{24}N_2$ ,  $C_{11}H_{24}N_2$  – C1s, N1s)
- LU&11** B. Langer, K. Ueda, O.M. Al-Dossary and U. Becker, J. El. Spec. **184** (2011) 154. (O<sub>2</sub>-O1s)
- LV&91** B.Langer, J. Viefhaus, O. Hemmers, A. Menzel, R. Wehlitz and U. Becker, Phys. Rev. A **43** (1993) 1652 (Li1s).
- LW74** S. Lundqvist and G. Wendum, J. El. Spectrosc. **5** (1974) 513. (Ba4d)
- LWP89** J.M. Li, Y.J. Wu and R.H. Pratt, Phys. Rev. A **40** (1989) 3036. (Ne1s)
- LWW09** D Lukic, S B Whitfield and R Wehlitz, Lithium inner-shell resonances in the 70–77 eV photon energy region, J. Phys. B: At. Mol. Opt. Phys. **42** (2009) 085004. \*(Li – Li1s)
- LZ63** A.P. Lukirskii and T.M. Zimkina, Bull. Acad. Sci USSR Phys. Ser. **27** (1963) 333, 808 [Izv. Akad. Nauk. SSSR Fiz. Ser. **27** (1963) 324, 817]. (Ar2p)
- LZB64** A.P. Lukirskii, T.M. Zimkina and I.A. Brytov, Bull. Acad. Sci USSR Phys. Ser. **28** (1964) 681 [Izv. Akad. Nauk. SSSR Fiz. Ser. **28** (1964) 772]. (Kr3d, Xe4d)
- M38** T. Magnusson, Nova Acta Reg. Soc. Sci. Upsal. **11** (1938) No. 3. (N<sub>2</sub> -N1s)
- M66** D.L. Mott, Phys. Rev. **144** (1966) 94. (GeCl<sub>4</sub> - Ge2p,2s; SiCl<sub>4</sub> - Si1s)
- M70** E.J. McGuire, Sandia Lab Report SC-RR-721 (1970). (Na2p)
- M71** L.N. Mazalov, Theor. Exp. Chem. **7** (1971) 37 [Teor. i Eksp. Khim. **7** (1971) 46]. (H<sub>2</sub>S - S1s)
- M75** M.W.D.Mansfield, Proc. Roy. Soc. London A **346** (1975) 554. (K2p)
- M76a** M.W.D. Mansfield, Proc. Roy. Soc. London A **348** (1976) 143. (Ca2p)
- M76b** Yu. F. Migal, J. Struct. Chem. **17** (1976) 350 [Zh. Struk. Khim. **17** (1976) 404] (SF<sub>6</sub>-S2p)
- M77** M.W.D. Mansfield, Proc. Roy. Soc. London A **358** (1977) 253. (Cr3p)
- M85** P. Morin, Photophysics and Photochemistry above 6 eV, F. Lahmani, ed., (Elsevier, Amsterdam, 1985) 1. (Si(CH<sub>3</sub>)<sub>4</sub>-Si2p)
- M90** D. Menzel, Appl. Phys. A **51** (1990) 163. (Ar2p)
- M93** T. Möller, Synchrotron Radiation News, **6** (1993) 4-16. (N<sub>2</sub>-N1s; H<sub>2</sub>O-O1s)
- M99** N. Murphy, J. Phys. B **32** (1999) L525. (Te4d)

- M01** M. Martins, J.Phys. B 34 (2001) 1321, (Cl2p)
- M02** M. Martins, J.Phys. B 35 (2002) L223. (Sc3p)
- MA&98** K.E. Miyano, U. Arp, S.H. Southworth, T.E. Meehan, T.R. Walsh and F.P. Larkins, Phys. Rev. A 57 (1998) 2430. (COS - S1s)
- MA&00** S. Motoki, J Adachi, Y. Hikosaka, K. Ito, M. Sano, K. Soejima, A. Yagashita, G. Raseev and N. Cherepkov, J. Phys. B 33 (100) 4193. (CO – C1s, O1s)
- MA&03** E. Melero Garcia, J. Alvarez Ruis, P. Erman, A. Kivimaki, S. Menmuir and E. Raclew, MaxLab Ann. Re. 2003. 196. (SF<sub>6</sub>, COS - S2p)
- MB84** H. Morawitz and P.S. Bagus, Chem. Phys. Lett. 107 (1984) 59. (AsF<sub>x</sub>, x=3,5,6 - As1s)
- MB87** D. Mathur and C. Badrinathan, Phys. Lett. A 123 (1987) 345. (I<sub>2</sub> - I4d)
- MB93** M.P. de Miranda and C.E. Bielschowsky, J. Mol. Struct. (Theochem) 282 (1993) 71. (Ar2p, CO<sub>2</sub> - C1s, O1s)
- MB97** L.M.M.A. Martins and C.E. Bielschowsky, Phys. Rev. A 56 (1997) 2720. (Mg2p, Mg2s, Mg1s)
- MBH97** C. McGuiness, K.L. Bell and A. Hibert, J. Phys. B 30 (1997) 59. (C 1s)
- MBN95** M.P. de Miranda, C.E. Bielschowsky and M.A.C. Nascimento, J. Phys. B 28 (1995) L15. (C<sub>2</sub>H<sub>2</sub>-C1s; N<sub>2</sub>-N1s; CO<sub>2</sub> - O1s)
- MBS95** D.V. Morgan, R.J. Burtlett and M. Sagurton, Phys. Rev. A 51 (1995) 2939. (Ar1s)
- MB&72** L.N. Mazalov, V.M. Bertenev, A.P. Sadovskii and T.I. Guzhavina, J.Struct. Chem. 13 (1972) 799 [Zh. Struk. Khim. 13 (1972) 855]. (SO<sub>2</sub> - S1s)
- MB&79** H. Morawitz, P. Bagus, T.C. Clarke, W.D. Gill, P.M. Grant, G.B. Street and D.E. Sayers, Synth. Meth. 1 (1979) 267. (AsF<sub>3</sub>, AsF<sub>5</sub> - As1s)
- MB&93** M.P. de Miranda, C.E. Bielschowsky, Optical and generalized oscillator strengths for inner-shell excitations in Ar and CO<sub>2</sub> J Molecular Structure: THEOCHEM, 282, (1993) 71. (Ar2p, CO<sub>2</sub>-C1s, O1s)
- MB&94a** M.P. de Miranda, C.E. Bielschowsky, H.M. Boechat Roberty and G.G.B. de Souza, Phys. Rev. A 49 (1994) 2399. (C<sub>2</sub>H<sub>2</sub> - C1s)
- MB&94b** M.P. de Miranda, J.A. Beswick, P. Parent, C. Laffon, G. Tourillon, A. Cassut, G. Nicolas and E.X. Gadea, J. Chem. Phys. 101 (1994) 5500. (C<sub>2</sub>H<sub>4</sub>, C<sub>4</sub>H<sub>6</sub>, C<sub>4</sub>H<sub>8</sub> - C1s; C<sub>2</sub>H<sub>3</sub>CN - C1s,N1s)
- MB&96** A. Menzel, S. Benzaid, M.O. Krause, C.D. Caldwell, U. Hergenhahn and M. Bissen, Phys. Rev. A 54 (1996) R991. (O1s)
- MB&98** C. Miron, M. Bassler et al., MaxLab report (1998) 192. (COS – C1s, S2p)
- MB&01** R.R.T. Marinho, O. Björneholm, S.L. Sorensen, I. Hjelte, S. Sundin, M. Bässler, S. Svensson, and A. Naves de Brito, Phys. Rev. A 63(2001) 032514. (Ar2p)
- MB&17** A.Müller, Dietrich Bernhardt, et al., Photoionization of Ne Atoms and Ne + Ions Near the K Edge: Precision Spectroscopy and Absolute Cross-sections, The Astrophysical Journal, 836 (2017) 166

- MB&23** A. Müller, A. Borovik, et al., Near-K-edge single and double photoionization of C<sup>2+</sup> ions, Physical Review A 107, 032806 (2023) C<sup>2+</sup> - C1s
- MC68** S.T. Manson and J.W. Cooper, Phys. Rev. 165 (1968) 126. (theory of centrifugal barriers; Xe4d, Kr3d)
- MC75a** M.W.D. Mansfield and J.P. Connerade, Proc. Roy. Soc. London A 342 (1975) 421. (Rb3d, Rb3p)
- MC75b** M.W.D. Mansfield and J.P. Connerade, Proc. Roy. Soc. London A 344 (1975) 303. (Sr3d, Sr3p)
- MC76** M.W.D. Mansfield and J.P. Connerade, Proc. Roy. Soc. London A 352 (1976) 125. (Eu4d)
- MC82** M.W.D. Mansfield and J.P. Connerade, J. Phys. B 15 (1982) 503. (Rb3d, Sr3d)
- MC2014** B.K. Miller and P.A. Crozier, Microsc. Microanalysis 30 (2014) 815-824
- MCS82** G. Mehlman, J.W. Cooper and E.B. Saloman, Phys. Rev. A 25 (1982) 2113. (Li1s)
- MC&87** R. McLaren, S.A. Clark, I. Ishii and A.P. Hitchcock, Phys. Rev. A 36 (1987) 1683. (C<sub>2</sub>F<sub>x</sub>H<sub>4-x</sub>, x=0-4; C<sub>4</sub>H<sub>6</sub>-C1s; C<sub>4</sub>F<sub>6</sub> - C1s,F1s)
- MC&91** Y. Ma, C.T. Chen, G. Meigs, K. Randall and F. Sette, Proc. X-90, AIP Conf. Proc.(1991); Phys. Rev. A 44 (1991) 1848. (CO,CO<sub>2</sub>, C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>D<sub>2</sub>, C<sub>2</sub>H<sub>6</sub>, C<sub>2</sub>D<sub>6</sub> - C1s; N<sub>2</sub>, NO, N<sub>2</sub>O - N1s; O<sub>2</sub> - O1s)
- MC&99** T. Möller, A.R.B. de Castro, K. von Haeften, A. Kolmakov, T. Laarmann, O. Löfken, C. Nowak, F. Picucci, M. Riedler, C. Rienerer, A. Wark and M. Wolff, J. El. Spec. 101-103 (1999) 185. ((NaCl)<sub>n</sub> – Cl2p)
- MC&00** J.P. Mosnier, J. Costello, E. Kennedy and W. Whity, J. Phys. B 33 (2000) 5203. (Li1s)
- MC&02** C. Miron, D. Ceolin, et al. , MAXLab Annual report 2001/02 (2002) 192. (CO<sub>2</sub>-C1s)
- MC&03** S. E. Michelin, A. de Campos, L. S. S. da Silva, A. S. Falck, E. A y Castro, O. Pessoa, H. L. Oliveira and M. -T. Lee, Chem. Phys. 293 (2003) 365. (N<sub>2</sub> – N1s)
- MC&12** A.R. Milosavljević, F. Canon et al., Gas-Phase **Protein** Inner-Shell Spectroscopy by Coupling an Ion Trap with a Soft X-ray Beamline J. Phys. Chem. Lett. 3 (2012) 1191. (cytochrome c (12 kDa, C<sub>42</sub>H<sub>52</sub>FeN<sub>8</sub>O<sub>6</sub>S<sub>2</sub>) – C1s, N1s, O1s)
- MD89** F. Muller-Plathe and G.R. Diercksen, Phys. Rev. A 40 (1989) 696. (H<sub>2</sub>O -O1s)
- ME74** G. Mehlman and J.M. Esteva, Astrophys. J. 188 (1974) 191 (Be1s)
- ME88** R. Murphy and W. Eberhardt, J. Chem. Phys. 89 (1988) 4054. (N<sub>2</sub>O - O1s)
- ME&78** G. Mehlman, D.L. Ederer, E.B. Saloman and J.W. Cooper, J. Phys. B 11 (1978) L689. (Li 1s)
- ME&84** L.N. Mazalov, S.B. Erenburg, A.A. Voityuk, Yu.A. Dyaden, G.N. Chekhova, V.M. Bertenev and T.M. Polyanskaya, J. Struct. Chem. 25 (1984) 371. (SO<sub>2</sub> - S1s)
- MF&88** L.J. Medhurst, T.A. Ferrett, P.A. Heiman, D.W. Lindle, S.H. Liu and D.A. Shirley, J. Chem. Phys. 89 (1988) 6096. (N<sub>2</sub>-N1s; CO, C<sub>2</sub>H<sub>4</sub>, C<sub>6</sub>H<sub>6</sub> - C1s)

- MF&02** C. Miron, R. Feifel, O. Bjorneholm, S. Svensson, A. Naves de Brito, S.L. Sorensen, M.N. Piancastelli, M. Simon and P. Mori, *Chem. Phys. Lett.* 359 (2002) 48. ( $\text{BF}_3$  - B1s)
- MGK03** S. Masuda, T. Gejo and N. Kosugi, *UVSOR Ann. Rep.* (2003) 105.  $\text{N}_2\text{-N1s}$ ,  $\text{C}_2\text{H}_2$  - C1s)
- MGN16** A.R. Milosavljević, A. Giuliani and C. Nicolas, “Gas-Phase Near-Edge X-Ray Absorption Fine Structure (NEXAFS) Spectroscopy of Nanoparticles, Biopolymers, and Ionic Species” in X-ray and Neutron Techniques for Nanomaterials Characterization, Springer (2016) 451-505. (REVIEW:  $\text{C}_2\text{H}_4\text{NO}_2$  – Gly,  $\text{C}_4\text{H}_8\text{N}_2\text{O}_2$  - Gly-gly – C1s, N1s, O1s;  $\text{Ti}^{+}_n$ , n=1-5,7,10 –  $\text{Ti}2\text{p}$ ;  $(\text{NH}_4)_2\text{SO}_4$  – S2p;  $(\text{Na}_2\text{SO}_4)_n$  – O1s, S2p;  $\text{C}_{42}\text{H}_{52}\text{FeN}_8\text{O}_6\text{S}_2$  = cytochrome-c – C1s, N1s, O1s)
- MG&98** C. Miron, R. Guillemin, N. Leclercq, P. Morin and M. Simon, *J. Electron Spectrosc.* 93 (1998) 95. ( $\text{SiF}_4$ ,  $\text{SiCl}_4$  - Si2p)
- MG&99** M. Magnusson, J. Guo, G. Sathe, J.E. Rubensson, J. Nordgren, P. Glans, L. Yang, P. Satek and H. Agren, *Phys. Rev. A* 59 (1999) 4281. (COS – C1s, O1s, S2p)
- MG&04** I. Minkov, F. Gel'mukhanov, R. Friedlein, W. Osikowicz, C. Suess, G. Öhrwall, S. L. Sorensen, S. Braun, R. Murdey, W. R. Salaneck and H. Ågren, *J. Chem. Phys.* 121 (2004) 5733. ( $\text{C}_{10}\text{H}_8$  - C 1s)
- MG&05** S. Masuda, T. Gejo, M. Hiyama and N. Kosugi, *J. El. Spec.* 144-147 (2005) 215. ( $\text{C}_2\text{H}_2$  – C1s)
- MH92** M. Mahalingham and D.M. Hanson, *J. Chem. Phys.* 97 (1992) 2183. ( $\text{O}_2$  - O1s)
- MH&89** P. Millie, A.P. Hitchcock, S. Bodeur and I. Nenner, unpublished. ( $\text{CO}_2$ , COS,  $\text{CS}_2$  - C1s, S2p, S1s, O1s)
- MH&90** J. Murakami, T. Hayaishi, A. Yagashita and Y. Morioka, *Phys. Scripta* 41 (1990) 408. (Kr3d)
- MH&92a** T. Matsuo, T. Hayaishi, Y. Itoh, T. Koizumi, T. Nagata, Y. Sato, E. Shigemasa, A. Yagashita, M. Yoshino and Y. Itikawa, *J. Phys. B* 25 (1992) 121 (K2p, Ca2p).
- MH&92b** L.J. Medhurst, P.A. Heimann, M.R.F. Siggle, D.A. Shirley, C.T. Chen, Y. Ma, S. Modesti and F. Sette, *Chem. Phys. Lett.* 193 (1992) 493 (CO-C1s,  $\text{N}_2\text{-N1s}$ )
- MH&95** C.I. Ma, D.M. Hanson, K. Lee and R.G. Hayes, *J. Electron Spectrosc.* 75 (1995) 83. ( $\text{NH}_3$  -N1s)
- MH&99** E. Murakami, T. Hayaishi, Y. Lu, Y. Morioka, F. Koike, E. Shigemasa and A. Yagashita, *J. El. Spec.* 101-103 (1999) 167. (Xe2s)
- MI80** S.T. Manson and M. Inokuti, *J. Phys. B* 13 (1980) L323. (Cl 1s, Cu 1s, etc.)
- MJ81** N. Martensson and B. Johansson, *J. Phys. B* 14 (1981) L37. (Rb3d, Sr3d)
- MK80** L.N. Mazalov and A.V. Kondratenko, Proc. 6th Int. Conf. on Vac. UV Rad. Phys. II-71 (Charlottesville, 1980) ( $\text{CS}_2$ -S2p;  $\text{PCl}_3$ -P2p, Cl2p)
- MK98** B.M. McLaughlin and K.P. Kirby, *J. Phys. B* 31 (1998) 4991. (O1s)
- MK&76** L.N. Mazalov, A.V. Kondratenko, V.V. Murakhtanov and T.I. Guzhavina, *J. Struct. Chem.* 17 (1976) 149. [Zh. Struk. Khim. 17 (1976) 174] (Ne-Nels, Ar-Ar1s, HF-F1s, HCl-Cl1s)
- MK&98a** J. Mursu, A. Kivimaki, H. Aksela and S. Aksela, *Phys. Rev. A* 38 (1998) R1645. (HCl – Cl2p)

- MK&98b** K. Maier, A. Kivimaki, B. Kempgens, U. Hergenhahn, M. Neeb, A. Rüdel, M.N. Piancastelli and A.M. Bradshaw, Phys. Rev. A 58 (1998) 3654. ( $\text{CO}_2 - \text{O}1\text{s}$ )
- ML77** J.J. McIlrath and T.B. Lucarto, Phys. Rev. Lett. 38 (1977) 1390. ( $\text{Li}^* - \text{Li}1\text{s}$ )
- ML01** L.B. Madsen and P. Lambropoulos , J. Phys. B 34 (2001) 1855. ( $\text{Li}1\text{s}$ )
- MLE88** R. Murphy, I.W. Lyo and W. Eberhardt, J. Chem. Phys. 88 (1988) 6078. ( $\text{N}_2 - \text{N}1\text{s}$ )
- MLH93** M. Mahalingham, K. Lee and D.M. Hanson, J. Chem. Phys. 98 (1993) 5239. ( $\text{NO} - \text{N}1\text{s}$ )
- MLL89** P. Morin, T. LeBrun and P. Lablanquie, Bull. Roy. Soc. Science Liege 58 (1989) 135. ( $\text{Kr}3\text{d}, \text{C}_2\text{H}_3\text{Br}, \text{C}_2\text{H}_5\text{Br} - \text{Br}3\text{d}$ )
- ML&82** L.E. Machado, E.P. Leal, G. Csanak, B.V. McKoy and P.W. Langhoff, J. Electron Spectrosc. 25 (1982) 1. ( $\text{C}_2\text{H}_2 - \text{C}1\text{s}$ )
- ML&91** R. Meyer, D.W. Lindle, S.H. Southworth and P.L. Cowan, Phys. Rev. A 43 (1991) 235. ( $\text{H}_2\text{S} - \text{S}1\text{s}$ )
- ML&93** P. Morin, M. Lavollée, M. Meyer and M. Simon, AIP Conf. Proc. 295 (1993) 139. ( $\text{N}_2\text{O} - \text{N}1\text{s}; \text{CO}_2 - \text{C}1\text{s}; \text{Fe}(\text{CO})_2(\text{NO})_2 - \text{C}1\text{s}, \text{N}1\text{s}$ )
- ML&94a** M. Meyer, J. Lacourrière, M. Simon, P. Morin and M. Larzillière, Chem. Phys. 187 (1994) 143. ( $\text{N}_2, \text{N}_2\text{O} - \text{N}1\text{s}; \text{ICN} - \text{I}4\text{d}$ )
- ML&94b** C.I. Ma, K. Lee, D. Ji, D.Y. Kim and D.M. Hanson, Nucl. Inst. Meth A 347 (1994) 453. ( $\text{N}_2\text{O} - \text{N}1\text{s}$ )
- ML&95** M. Meyer, J. Lacoursière, M. Simon and P. Morin, Rev. Sci. Inst. 66 (1995) 1554. ( $\text{ICN} - \text{I}4\text{d}$ )
- MM12** P. Morin and C. Miron, J. El. Spec. 185 (2012) 259. ( $\text{HBr-Br}3\text{d}; \text{DCl}, \text{HCl-Cl}2\text{p}; \text{H}_2\text{S} - \text{S}2\text{p}, \text{O}_2-\text{O}1\text{s}$ )
- MM&75** L.N. Mazalov, V.V. Murkhanov, T.I. Guzhavina and A.P. Sadovskii, J. Struct. Chem. 16 (1975) 240, 245 [Zh. Struk. Khim. 16 (1975) 262, 267]. ( $\text{HCl} - \text{C}1\text{s}$ )
- MM&87** M. Meyer, B. Muller, A. Nunnemann, Th. Prescher, E. von Raven, M. Richtler, M. Schmidt, B. Sonntag and P. Zimmerman, Phys. Rev. Lett. 59 (1987) 2963. ( $\text{Li}1\text{s}$ )
- MM&99a** C. McGuiness, M.Martins, Ph. Wernet, B.F. Sonntag, P. van Kampen, J. P. Moisner, E.J. Kennedy and J.T. Costello, J. Phys. B 32 (1999) L583. ( $\text{Cr}3\text{p}$ )
- MM&99b** A. Marquette, M. Meyer, F. Sirotti and R.F. Fink, J. Phys. B 32 (1999) L325. ( $\text{N}_2 - \text{N}1\text{s}$ )
- MM&00** C. McGuiness, M.Martins, P. van Kampen, J. Hirsch, J. P. Moisner, W.W. Whity and J.T. Costello, J. Phys. B 33 (2000) 5077. ( $\text{Cr}3\text{p}$ )
- MM&07** A. Mocellin, M.S.P. Mundim, L.H. Coutinho, M.G.P. Homem and A. Naves de Brito, J. El. Spec. 156-158 (2007) 245. ( $\text{O}_3-\text{O}1\text{s}$ )
- MM&09** S.E. Michelin, K.T. Mazon, F. Arretche, W. Tenfen, H.L. Oliveira, A.S. Falck, M.A. Scopel, L.S.S. da Silva, M.M. Fujimoto, I. Iga, M.-T. Lee, J. El. Spectrosc. 171 (2009) 30 ( $\text{C}_2, \text{C}_2\text{N}_2 - \text{C}1\text{s}$ )

- MM&20** A Müller, M Martins, et al, Photoionization and photofragmentation of singly charged positive and negative Sc<sub>3</sub>N@C<sub>80</sub> endohedral fullerene ions, J.Physics: Conf. Series 1412 (2020) 202027 (C<sub>80</sub>NSc<sub>3</sub> – N1s)
- MN86** P. Morin and I. Nenner, Phys. Rev. Lett. 56 (1986) 1913. (HBr-Br3d)
- MN87** P. Morin and I. Nenner, Phys. Scripta T17 (1987) 171. (CH<sub>3</sub>Br, HBr - Br3d; CH<sub>3</sub>I, HI - I4d)
- MNN92** P. Morin, L. Nahon and I. Nenner, AIP Conf. Proc. 258 (1992) 277. (I4d)
- MN&74a** Y. Morioka, M. Nakamura, E. Ishiguro and M. Sasanuma, Proc. 4th Int. Vac. UV Rad. Phys. Conf. (Hamburg, 1974) 92. (N<sub>2</sub>, NO - N1s)
- MN&74b** Y. Morioka, M. Nakamura, E. Ishiguro and M. Sasanuma, J. Chem. Phys. 61 (1974) 1426. (NO - N1s)
- MN&86** J. Murakami, M.C. Nelson, S.L. Anderson and D.M. Hanson, J. Chem. Phys. 85 (1986) 5755. (N<sub>2</sub>O-N1s,O1s)
- MN&15** A.R. Milosavljevic C. Nicolas, M.L. Rankovic, F. Canon,C.Miron and A. Giuliani, J. Phys. Chem. Lett. 6 (2015) 3132–3138. (Ubiquitin – C<sub>660</sub>N MQIFVKTLTGKTITLEVEPSDTIENVKAKIQDKEGIPPD QQRLIFAGKQLEDGRTLSYNIQKESTLHLVLRLRGG, 8.5 kDa protein – C1s, N1s)
- MP81** M. Mazzoni and M. Pettini, Phys. Lett. 85A (1981) 331. (Br3d)
- MP&86** M. Meyer, Th. Prescher, E. Von Raven, M. Richter, E. Schmidt, B. Sonntag and H.E. Wetzel, Z. Phys. D 2 (1986) 347. (Ti3p, Cr3p, Mn3p, Fe3p, Co3p, Ni3p, Ce4d)
- MP&05** S. E. Michelin, O. Pessoa, H. L. Oliveira, E. Veiteinheimer, A. M. S. Santos, M. M. Fujimoto, I. Iga, and M.-T. Lee, Phys. Rev. A 72 (2005) 022730. (C<sub>2</sub>H<sub>2</sub> – C1s)
- MRR84a** D. Mathur, F.A. Rajgara and A. Roy, Chem. Phys. Lett. 104 (1984) 500. (CH<sub>4</sub>-C1s, N<sub>2</sub>-N1s)
- MRR84b** D. Mathur, F.A. Rajgara and A. Roy, Chem. Phys. Lett. 107 (1984) 39. (CH<sub>4</sub>-C1s)
- MR&85** D. Mathur, A. Roy, S.V. Krishna Kumar and F.A. Rajgara, Phys. Rev. A 31 (1985) 2709. (N<sub>2</sub> - N1s)
- MR&89** M. Meyer, E. von Raven, M. Richtor, B. Sonntag, R.D. Cowan and J.E. Hansen, Phys. Rev. A 39 (1989) 4319. (Ca2p)
- MR&90** D. Menzel, G. Rocker, D. Coulman, P. Feulner and W. Wurth, Phys. Scripta 41 (1990) 588. (H<sub>2</sub>O - O1s; NH<sub>3</sub> - N1s; CH<sub>4</sub> - C1s)
- MR&91** M. Meyer, E. von Raven, B. Sonntag and J.E. Hansen, Phys. Rev. A 43 (1991) 177. (Ar2p)
- MR&92** D. Menzel, C. Rocker, H.P. Steinruck, D. Coulman, P.A. Heimann, W. Huber, D. Zebisch and D.R. Lloyd, J. Chem. Phys. 96 (1992) 1724 (C<sub>6</sub>H<sub>6</sub> - C1s)
- MR&02** R. Diez Muino, D. Rolles, F.J. Garcia de Abajo, C.S. Fadley and M.A. Van Hove, J.Phys. B 35 (2002) L359. (CO – C1s; N<sub>2</sub> – N1s)
- MR&21** M. Martins, S. Reinhardt, et al., Disentangling the Photodissociation Dynamics of the HF<sup>+</sup> Molecular Radical via Kinetic-Energy-Release-Resolved F 1s Core Excitation and Ionization, : J. Phys. Chem. Lett. 12 (2021) 1390–1395. (HF<sup>+</sup>-F1s)

- MS71** L.N. Mazalov and A.P. Sadovskii, Theor Exp. Chem. 7 (1971) 37 [Teor i Eksp. Khim. 7 (1971) 46]. (H<sub>2</sub>S - S1s)
- MSB97** D.V. Morgan, M. Sagurton and R.J. Bartlett, Phys. Rev. A 55 (1997) 1113. (Ne1s)
- MSN89** P. Morin, M. Simon and I. Nenner, unpublished. (Fe(CO)<sub>5</sub>, Fe<sub>2</sub>(CO)<sub>9</sub> - C1s, Fe3p, Fe2p, O1s)
- MST83** G. Materlick, B. Sonntag and M. Tausch, Phys. Rev. Lett. 51 (1983) 1300 (Ce, Eu, Gd, Sm - 2s, 2p)
- MSZ96** M. Martins, P. Slodeczek and P. Zimmermann, J. Phys. B 29 (1996) L745. (Au5p)
- MS&73** L.N. Mazalov, A.P. Sadovskii, P.I. Vadash and F.G. Gel'mukhanov, J. Struct. Chem. 14 (1973) 234 [Zh. Struk. Khim. 14 (1973) 262]. (HCl, Cl<sub>2</sub> - Cl1s, H<sub>2</sub>S, SO<sub>2</sub> - S1s)
- MS&84** K. Muller-Dethelfs, M. Sander, L.A. Chewter and E.W. Schag, J. Phys. Chem. 88 (1984) 6098. (CF<sub>3</sub>CH<sub>3</sub>-C1s, F1s)
- MS&86** P. Morin, G.G.B. de Souza, I. Nenner and P. Lablanquie, Phys. Rev. Lett. 56 (1986) 131. (Si(CH<sub>3</sub>)<sub>4</sub> - Si2p)
- MS&89** Y. Ma, F. Sette, G. Meigs, S. Modesti and C.T. Chen, Phys. Rev. Lett. 63 (1989) 2044. (C<sub>2</sub>H<sub>4</sub>, C<sub>2</sub>D<sub>4</sub>, C<sub>6</sub>H<sub>6</sub>, C<sub>6</sub>D<sub>6</sub>)
- MS&90** Y. Ma, F. Sette, G. Meigs, S. Modesti and C.T. Chen, Phys. Scripta 41 (1990) 833. (C<sub>2</sub>H<sub>4</sub>, C<sub>6</sub>H<sub>6</sub> - C1s)
- MS&95a** C. McGuiness, G. O'Sullivan, P.K. Carroll, D. Audley and M.W.D. Mansfield, Phys. Rev. A 51 (1995) 2053. (Sr3d)
- MS&95b** M.A. MacDonald, S.H. Southworth, J.C. Levin, A. Hennis, R.D. Deslattes, T. LeBrun, Y. Azuma, P.L. Cowan and B.A. Karlin, Phys. Rev. A 51 (1995) 3598. (Xe2p)
- MS&97a** M. Martins, P. Slodeczaek, K. Tiedtke and P. Zimmermann, Phys. Rev. A 55 (1997) R8. (Ir5p,4f)
- MS&97b** J.D. Mills, J.A. Sheehey, T.A. Ferrett, S.H. Southworth, R. Meyer, D.W. Lindle and P.W. Langhoff, Phys. Rev. Lett. 79 (1997) 383. (Cl<sub>2</sub> - Cl1s)
- MS&97c** M. Martins, P. Slodeczaek, K. Tiedtke and P. Zimmermann, Phys. Rev. A 56 (1997) 1329. (Ta5p,4f; Rh5p,4f)
- MS&97d** C. Miron, M. Simon, N.Leclerq and P. Morin, Rev. Sci. Inst. 68 (1997) 3728. (N<sub>2</sub>, N<sub>2</sub>O – N1s)
- MS&98a** P. Morin, M. Simon, C. Miron, N. Leclerq and D.L. Hansen, J. Electron Spectrosc. 93 (1998) 49. (N<sub>2</sub>O - N1s; BrCH<sub>2</sub>Cl - Cl2p)
- MS&98b** C. Miron, M. Simon, N.Leclerq, D.L. Hansen and P. Morin, Phys. Rev. Lett. 81 (1998) 4104. (ClCH<sub>2</sub>Br – Br3d, Cl2p)
- MS&00** P. Morin, M. Simon, C. Miron, N.Leclerq, E. Kukk, J.D. Bozek and N. Berrah, Phys. Rev. A 61 (2000) 050701. (CO<sub>2</sub> – C1s)
- MTU04** C. Makochekanwa, H. Tanaka and K. Ueda, Spring8 Ann Rep. (2004) 98. (CO-C1s, O1s); C<sub>2</sub>H<sub>2</sub>-C1s)
- MU&99** Y. Muramatsu, K. Ueda, Y. Shimizu, H. Chiba, K. Amano, Y. Sato and H. Nakamatsu, J. Phys. B 32 (1999) L213. (CF<sub>4</sub> – F1s)

- MW76** G.A. Martin and W.L. Wiese, Phys. Rev. A 13 (1976) 699. (Li1s)
- MYM77** L.N. Mazalov, V.R. Yumatov and V.V. Murakhtanov, *X-ray Spectra of Molecules*, (Russian), Nauka Press, Novosibirsk, 1977.
- MY&02a** T. Matsui, H. Yashii, A. Higurashi, E. Murakami, T. Aoto, T. Onuma, Y. Morioa, A. Yagashita and T. Hayaishi, J.Phys. B 35 (2002) 3069. (Kr3p)
- MY&02b** M. Oura, H. Yamaoka, K. Kawatsura, K.Takahiro, N. Takeshima, Y. Zou, R. Hutton, . Ito, Y. Awaya, M. Terasawa, T. Sekioka and T.Mukoyama, J. Phys. B 35 (2002). 3847. (Ca1s, Ti1s, V1s)
- N70** V. I. Nefedov, J. Struct. Chem. 11 (1970) 273 [Zh. Struk. Khim. 11 (1970) 292]. (SF<sub>6</sub> - S2p, Cr(CO)<sub>6</sub> - Cr1s)
- N71a** V. I. Nefedov, J. Struct. Chem. 12 (1971) 276 [ Zh. Struk. Khim. 12 (1971) 303]. (CCl<sub>4</sub> - Cl2p)
- N71b** G.H. Newsom, Astrophys. J. 166 (1971) 243. (Mg2p)
- N79** K. Nuroh, J. Phys. B 12 (1979) 1125. (Fe3p)
- N87** I. Nenner, NATO ASI on 'Giant Resonances', (1987) 259 (J.P. Connerade, J.M. Esteva and R.C. Karnatak, eds) (SiF<sub>4</sub>,SiH<sub>4</sub>-Si2p)
- N88** I. Nenner, Proc. XV ICPEAC (North-Holland, 1988) 517. (HBr,CH<sub>3</sub>Br - Br3d; SiH<sub>4</sub>, Si(CH<sub>3</sub>)<sub>4</sub> -Si2p)
- N95** H. Nakamatsu. Chem. Phys. 200 (1995) 49. (PCl<sub>3</sub>, PF<sub>3</sub> - P2p)
- N02** K. Nabusada, J. Phys. B 35 (2002) 3055. (CO<sub>2</sub> – C1s)
- NAV88a** S.V. Nekipelov, V.N. Akimov and A.S. Vinogradov, Optics & Spectrosc. 64 (1988) 487 [Opt. Spectrosk. 64 (1988) 817]. (BF<sub>3</sub> - B1s,F1s)
- NAV88b** S.V. Nekipelov, V.N. Akimov and A.S. Vinogradov, Sov. Phys. Sol. St. 30 (1988) 2095 [Fiz. Tverd. Tela (Leningrad) 30 (1988) 3647]. (NO - N1s,O1s; BF<sub>3</sub> - B1s,F1s)
- NAV91** S.V. Nekipelov, V.N. Akimov and A.S. Vinogradov, Sov. Phys. Sol. St. 33 (1991) 378 (Fiz. Tverd. Tela (Len) 33 (1991) 663) (BF<sub>3</sub> - B1s)
- NB71** M.S. Nakhmanson and V.I. Baranovskii, Theor. Exp. Chem. 7 (1971) 11 [Teor. i Eksp. Khim. 7 (1971) 15]. (BF<sub>3</sub>, BCl<sub>3</sub> - B1s)
- NB87** I. Nenner and J.A. Beswick, *Photodissociation and Photoionisation*, Ch. 6 in *Handbook of Synchrotron Radiation*, Vol. 2 (G. Marr, ed) (Elsevier, 1987) (CS<sub>2</sub>-S1s,C1s,S2p; SO<sub>2</sub>-S1s; Si(CH<sub>3</sub>)<sub>4</sub>-Si2p; HBr-Br3d; review)
- NB95** M. Nooijen & R.J. Bartlett, J. Chem. Phys. 102 (1995) 6735. (CO, H<sub>2</sub>CO - C1s, O1s; N<sub>2</sub> - N1s; C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>4</sub> - C1s)
- NBE94** M. Neeb, M. Biermann and W. Eberhardt, J. El. Spec. 69 (1994) 239. (CO<sub>2</sub> - C1s)
- ND&90** L. Nahon, L. Duffy, P. Morin, F. Combet-Farnoux, J. Trembley and M. Larzilliere, Phys. Rev. A 41 (1990) 4879. (I4d)

- NE&88** I. Nenner, J.H.D. Eland, et al., , *Electron-Molecule Scattering and Photoionisation*, (Plenum, 1988), (Proc. XV ICPEAC, Brighton, 1987) p. 15. ( $\text{CH}_3\text{Br}$ -Br3d; CO-C1s,O1s)
- NE&14** S. Nagaoka, H. Endo, K. Nagai, O. Takahashi, Y. Tamenori and I. H. Suzuki, , *J. Electron Spectrosc.* 195 (2014) 18 ( $\text{C}_3\text{Cl}_3\text{H}_9\text{Si}_2$  - Si2p)
- NF&96** S. Nagaoka, T. Fujibuchi, U. Nagashima, S. Kato, K. Takeno and I. Koyano, *J. Electron Spectrosc.* 79 (1996) 499. ( $\text{C}_{11}\text{H}_{21}\text{NOSi}_2$  - Si2p)
- NF&97** S. Nagaoka, T. Fujibuchi, J. Ohshita, M. Ishikawa and I. Koyano, *Int. J. Mass. Spec. Ion Phys.* 171 (1997) 95. ( $\text{C}_5\text{F}_3\text{H}_{13}\text{Si}$  - Si2p)
- NF&02** S. Nagaoka, T. Fujibuchi, J. Ohshita, U. Nagashima I. Koyano, *Chem. Phys.* 276 (2002) 243. ( $\text{CF}_3\text{H}_3\text{Si}$ ,  $\text{C}_5\text{Cl}_3\text{H}_9\text{Si}_2$ ,  $\text{C}_3\text{F}_3\text{H}_9\text{Si}_2$ ,  $\text{C}_4\text{H}_{12}\text{Si}$ ,  $\text{C}_4\text{F}_3\text{H}_{11}\text{Si}_2$ ,  $\text{C}_5\text{F}_3\text{H}_9\text{Si}_2$ ,  $\text{C}_5\text{F}_3\text{H}_{11}\text{Si}_2$ ,  $\text{C}_5\text{Cl}_3\text{H}_9\text{Si}_2$ ,  $\text{C}_6\text{F}_3\text{H}_{15}\text{Si}_2$  Si2p)
- NF&19** Johannes Niskanena,b, Mattis Fondel, Compatibility of quantitative X-ray spectroscopy with continuous distribution models of water at ambient conditions, *Proc. Nat. Acad. Sci.*, 116 (2019) 4058.  $\text{H}_2\text{O}$  – O1s)
- NG99** G. Nicola and F.X. Gadea, *J. Chem. Phys.* 111 (1999) 10537. ( $\text{C}_2\text{H}_4$  – C1s)
- NG&97** J. Nordgren, P. Glans, K. Gunnelin, J. Guo, P. Skytt, C. Sathe and N. Wassdahl, *App. Phys. A* 65 (1997) 97. ( $\text{N}_2$  - N1s; CO,  $\text{CO}_2$ ,  $\text{C}_6\text{H}_5\text{NH}_2$  - C1s; CO,  $\text{CO}_2$ , O<sub>2</sub> - O1s)
- NG&17** G. Nalin, S. Grundmann, et al., Localized or delocalized K-holes in N2: Photoelectron-Auger electron coincidence experiments with high energy resolution, *J. Physics: Conf. Series* 875 (2017) 032009. ( $\text{N}_2$ -N1s)
- NH02** S.A. Navikov and A.N. Hopersky, *J. Phys. B* 35 (2002) L339. (Ne1s)
- NHS74** U. Nielsen, R. Haensel and W.H.E. Schwarz, *J. Chem. Phys.* 58 (1974) 3581. ( $\text{XeF}_6$  -Xe4d)
- NH&88** I. Nenner, M.J. Hubin-Franksin, J. Delwiche, P. Morin and S. Bodeur, *J. Mol. Struct.* 173 (1988) 269. (HBr,  $\text{CH}_3\text{Br}$  - Br3d;  $\text{SiH}_4$ -Si2p; COS,  $\text{CO}_2$ ,  $\text{CS}_2$  -C1s, O1s, S1s, S2p)
- NH&03** J.J. Neville, A..P. Hitchcock, A. Jurgensen and R.G. Cavell, *J. El. Spec.* in preparation. ( $\text{PF}_3$ ,  $\text{PCl}_3$ ,  $\text{PCl}_2\text{CF}_3$  – P2p, Cl2p)
- NH&11** M. Nagasaka, T.i Hatsui, H. Setoyama, E. Rühl and N. Kosugi, *J. El. Spec.* 183 (2011) 29. ( $\text{Kr}_n$ -Kr3d)
- NIH86** D.C. Newbury, I. Ishii and A.P. Hitchcock, *Can. J. Chem.* 64 (1986) 1145. ( $\text{C}_4\text{H}_4\text{O}$ , $\text{C}_4\text{H}_8\text{O}$ , $\text{C}_5\text{H}_8\text{O}$ -C1s,O1s;  $\text{C}_4\text{H}_4\text{NH}$ , $\text{C}_4\text{H}_8\text{NH}$ , $\text{C}_5\text{H}_8\text{NH}$ , $\text{C}_5\text{H}_{10}\text{NH}$ -C1s,N1s)
- NI&81** K. Ninomiya, E. Ishiguro, S. Iwata, A. Mikuni and T. Sasaki, *J. Phys. B* 14 (1981) 1777. (Cl<sub>2</sub>, HCl - Cl2p)
- NI&89** T. Nagata, Y. Itoh, T. Hayaishi, Y. Itikawa, T. Koizumi, T. Matsua, Y. Sato, E. Shigemasa, A. Yagashita and M. Yochimo, *J. Phys. B* 22 (1989) 3865. (Cs4d, Ba4d)
- NI&00** S. Nagaoka, T. Ibuki, et al., *J. Phys. B* 33 (2000) L605. (Kr2p)
- NJ&98** J.J. Neville, A. Jurgensen, R.G. Cavell, N. Kosugi and A.P. Hitchcock, *Chem. Phys.* 238 (1998) 201. ( $\text{PF}_3$ ,

- PCl<sub>3</sub>, PCl<sub>2</sub>CF<sub>3</sub>, OPF<sub>3</sub>, SPF<sub>3</sub> - P2p, P2s; SPF<sub>3</sub> - S2p; PF<sub>3</sub>, PCl<sub>2</sub>CF<sub>3</sub>, OPF<sub>3</sub>, SPF<sub>3</sub> - F1s; PCl<sub>3</sub>, PCl<sub>2</sub>CF<sub>3</sub> - Cl2p)
- NKM90** S. Nagaoka, I. Koyano and T. Masuoka, Phys. Scripta 41 (1990) 472. (Al(CH<sub>3</sub>)<sub>3</sub> - Al2p)
- NK&89** S. Nagaoka, T. Koyano, K. Ueda, E. Shigemasa, Y. Sato, A. Yagashita, T. Nagata and T. Hayaishi, Chem. Phys. Lett. 154 (1989) 363. (Pb(CH<sub>3</sub>)<sub>4</sub> - Pb5p,4f, C1s)
- NK&91** S. Nagaoka, T. Koyano, T. Imamura and T. Masukoka, Appl. Orgmet. Chem. 5 (1991) 269. (Al<sub>2</sub>(CH<sub>3</sub>)<sub>6</sub>, Al(CH<sub>3</sub>)<sub>3</sub>Cl<sub>3</sub> - Al2p)
- NK&96a** M. Neeb, A. Kivimaki, B. Kempgens, H.M. Köppe, J. Feldhaus and A.M. Bradshaw, Phys. Rev. Lett. 76 (1996) 2250. (N<sub>2</sub> - N1s)
- NK&96b** M. Neeb, A. Kivimaki, B. Kempgens, H.M. Köppe and A.M. Bradshaw, J. Electron Spectrosc. 79 (1996) 445. (N<sub>2</sub> - N1s)
- NK&97** M. Neeb, A. Kivimaki, B. Kempgens, H.M. Köppe and A.M. Bradshaw, J. Phys. B 30 (1997) 93. (CF<sub>4</sub> - C1s)
- NK&98** M. Neeb, A. Kivimaki, B. Kempgens, H.M. Köppe, K. Maier, U. Hergenhahn, M.N. Piancastelli, A. Rüdel and A.M. Bradshaw, J. Electron Spectrosc. 88 (1998) 19. (CO<sub>2</sub> - O1s)
- NK&00** M. Neeb, A. Kivimaki, B. Kempgens, H.M. Köppe, K. Maier, A.M. Bradshaw and N. Kosugi, Chem. Phys. Lett. 320 (2000) 217. (N<sub>2</sub> - N1s)
- NL99** A.P.P. Natalense and R.R. Lucchese, J. Chem. Phys. 111 (1999) 5345. (SF<sub>6</sub> - S1s)
- NM92** L. Nahon and P. Morin, Phys. Rev. A 45 (1992) 2887 (I4d,Br3d)
- NM96** I. Nenner and P. Morin, "Electronic and Nuclear Relaxation of Core Excited Molecules" in VUV and Soft X-ray Photoionization, U. Becker and D.A. Shirley, eds. (Plenum, NY, 1996) 291-355 (366 refs). (HBr-Br3d; Br(CH<sub>2</sub>)<sub>n</sub>Cl, n=1,2,3 - Br3d, Cl2p; Cl<sub>2</sub>-Cl1s; N<sub>2</sub>, N<sub>2</sub>O - N1s; CO, N<sub>2</sub>O, O<sub>2</sub> - O1s; H<sub>2</sub>S, SF<sub>6</sub>, SF<sub>5</sub>Cl - S1s; Fe(CO)<sub>2</sub>(NO)<sub>2</sub>, CO-C1s)
- NM12** C. Nicolas and C. Miron, J. El. Spec. 185 (2012) 267. (CO-C1s, review of line-widths)
- NMC92** L. Nahon, P. Morin and F. Combet-Farnoux, Phys. Scripta T41 (1992) 104 (Br3d, I4d)
- NMA90** H. Nakamatsu, T. Mukoyama and H. Adachi, Chem. Phys. 143 (1990) 221. (SF<sub>6</sub> - S2p, F1s, S1s)
- NMA91** H. Nakamatsu, T. Mukoyama and H. Adachi, J. Chem. Phys. 95 (1991) 3167. (SF<sub>6</sub> - S2p, F1s, S1s; H<sub>2</sub>S - S1s, S2p)
- NMK97** S.I. Nagaoka, K. Mase and I. Koyano, Trends in Chem. Phys. 6 (1997) 1. (F<sub>3</sub>Si(CH<sub>2</sub>)<sub>x</sub>SiMe<sub>3</sub>, x=1,2, SiF<sub>3</sub>Me, SiMe<sub>4</sub> - Si2p)
- NML88** I. Nenner, P. Morin and P. Lablanquie, Comm. At. Mol. Phys. 22 (1988) 51. (Xe4d, CH<sub>3</sub>Br-Br3d)
- NM&71** M. Nakamura, Y. Morioka, T. Hayaishi, E. Ishigura and M. Sasanuma, Proc. 3rd Int. VUV Conf. (Tokyo, 1971) 1pA1-6. (CO - C1s,O1s; SF<sub>6</sub> - S2p; O<sub>2</sub> - O1s)
- NM&80** C.R. Natoli, D.K. Misemer, S. Doniach and F.W. Kutzler, Phys. Rev. A 22 (1980) 1104. (GeH<sub>4</sub>, GeCl<sub>4</sub> - Ge1s)

- NM&87b** M.C. Nelson, J. Murakami, S.L. Anderson and D.M. Hanson, *J. Chem. Phys.* 86 (1987) 442. ( $\text{CH}_3)_2\text{CO}$  - O1s)
- NM&88** I. Nenner, P. Morin, M. Simon, P. Lablanquie and G.G.B. da Souza, *Proc. of DIET III, Springer Ser. in Surf. Sci* 13 (1988) 10. (M. Knotek, R.H. Stalen, eds) (HBr,  $\text{CH}_3\text{Br}$  - Br3d;  $\text{SiH}_4$ -Si2p)
- NM&90** I. Nenner, P. Morin, P. Lablanquie, M. Simon, N. Levasseur and P. Millie, *J. Electron Spectrosc.* 52 (1990) 623. ( $\text{CH}_3\text{Br}$  - Br3d;  $\text{C}_2\text{F}_4\text{IBr}$  - I4d, Br3d)
- NM&08** K. Nagaya, H. Murakami, H. Iwayama, M. Yao, *J. El. Spec.* 166-167 (2008) 45. ( $\text{Ar-Kr})_n$ -Kr1s)
- NN&97** A.Naves de Brito, A.Naves de Brito, et al., *MaxLab report* (1997) 146. ( $\text{H}_2\text{S}$  – S2p)
- NO99** S. Nagaoka and J. Ohshita, *UVSOR Report* (1999) 60. ( $\text{C}_5\text{Cl}_3\text{H}_9\text{Si}_2$  – Si2p)
- NO&93** S. Nagaoka, J. Ohshita, M. Ishikawa, T. Masuoka and I. Koyano, *J. Phys. Chem.* 97 (1993) 1488. ( $\text{Cl}_3\text{Si-SiH}_3$  - Si2p)
- NO&95** S. Nagaoka, J. Ohshita, M. Ishikawa, K. Takaro, U. Nogarhima, T. Takeuchi and I. Koyano, *J. Chem. Phys.* 102 (1995) 6078. ( $\text{C}_4\text{F}_3\text{H}_{11}\text{Si}_2$  - Si2p)
- NP&82** J. Nordgren, L. Pettersson, L. Selander, C. Nordling, K. Siegbahn and H. Agren, *J. Phys. B* 15 (1982) L153. ( $\text{CO}_2$  - C1s)
- NP&07** S. Nagaoka, G. Prümper, H. Fukuzawa, M. Hino, M. Takemoto, Y. Tamenori, J. Harries, I. H. Suzuki, O. Takahashi, K. Okada, K. Tabayashi, X.-J. Liu, T. Lischke, and K. Ueda, *Phys. Rev A* 75 (2007) 020502. ( $\text{C}_5\text{F}_3\text{H}_{13}\text{Si}_2$  - Si2p)
- NR&93** M. Neeb, J.E. Rubensson, M. Biermann and W. Eberhardt, *Phys. Rev. Lett.* 71 (1993) 3091. (O<sub>2</sub> - O1s)
- NR&94** M. Neeb, J.E. Rubensson, M. Biermann and W. Eberhardt, *J. El. Spec.* 67 (1994) 261. (CO - C1s; N<sub>2</sub> - N1s; O<sub>2</sub> - O1s)
- NR&99** C. Nowak, C. Rienecker, A. Kolmakov, J.O. Löfken, F. Picucci, M. Riedler, A.V. Soldatov, M. Wolff and T. Möller, *J. El. Spec.* 101-103 (1999) 199. ( $(\text{NaCl})_n$  – Cl2p)
- NSK87** S. Nagaoka, S. Suzuki and I.Koyano, *Phys. Rev. Lett.* 58 (1987) 1524 ( $\text{Pb}(\text{CH}_3)_4$  - Pb5d)
- NSK88** S. Nagaoka, S. Suzuki and I.Koyano, *Nucl. Inst. Meth. A* 266 (1988) 699 ( $\text{M}(\text{CH}_3)_4$  - M = Ge3d, Sn4d, Pb5d)
- NSM91** L. Nahon, A. Svensson and P. Morin, *Phys. Rev. A* 43 (1991) 2328. (I4d)
- NSZ82** K. Nuroh, M.J. Stott and E. Zaremba, *Phys. Rev. Lett.* 49 (1982) 863. (Ba4d)
- NS&68** M. Nakamura, M. Sasanuma, S. Sato, M. Watanabe, H. Yamashita, Y.Iguchi, A. Ejiri, S. Nakai, S. Yamaguchi, T. Sagawa, Y. Nakai and T. Oshio, *Phys. Rev. Lett.* 21 (1968) 1303. (Ar2p)
- NS&69** M. Nakamura, M. Sasanuma, S. Sato, M. Watanabe, H. Yamashita, Y.Iguchi, A. Ejiri, S. Nakai, S. Yamaguchi, T. Sagawa, Y. Nakai and T. Oshio, *Phys. Rev.* 178 (1969) 80. (N<sub>2</sub> - N1s)
- NS&89** S. Nagaoka, S. Suzuki, U. Nagashima, T. Imamura and I.Koyano, *Rev. Sci. Inst.* 60 (1989) 2201 ( $\text{Ga}(\text{CH}_3)_3$  - Ga3d)

- NS&90** S. Nagaoka, S. Suzuki, U. Nagashima, T. Imamura and I.Koyano, J. Phys. Chem. 94 (1990) 2283 (Ga(CH<sub>3</sub>)<sub>3</sub> - Ga3d, BiMe<sub>3</sub> - Bi5d, ZnMe<sub>2</sub> - Zn4d, (M(CH<sub>3</sub>)<sub>4</sub> - M = Ge3d, Sn4d, Pb5d)
- NS&92** A. Naves de Brito, S. Svensson, N. Correia, M.P. Keane and H. Agren, J.Electron Spectrosc 59 (1992) 293. (C<sub>4</sub>H<sub>6</sub>, C<sub>6</sub>H<sub>8</sub> - C1s)
- NS&97** A. Naves de Brito, S. Svensson, S.J. Osborne, A. Ausmees, A. Kivimaki, O.-P. Sairanen, E. Nommiste, H. Aksela, S. Aksela and L.J. Saethre, J. Chem. Phys. 106 (1997) 18. (H<sub>2</sub>S - S2p)
- NS&07** A. Naja, E.M. Staicu-Casagrande, X.G. Ren, F. Catoire, A. Lahmam-Bennani, C. Dal Cappello and C.T. Whelan, J. Phys. B 40 (2007) 2871. (Ar2p)
- NTH99** J.J. Neville, T. Tyliszczak and A.P. Hitchcock, J. Electron Spectrosc. 101-103 (1999) 119. (COS - S1s)
- NT&99a** J.J. Neville, T. Tyliszczak, A.P. Hitchcock, A. Jurgensen and R.G. Cavell, Chem. Phys. Lett. 300 (1999) 451. (SPF<sub>3</sub> - P1s)
- NT&99b** J.J. Neville, T. Tyliszczak, A.P. Hitchcock, A. Jurgensen and R.G. Cavell, unpublished. (PF<sub>3</sub>, OPF<sub>3</sub>, SPF<sub>3</sub> - P1s, S1s)
- NT&08** S. Nagaoka, M. Takemoto, G. Prumper, H. Fukuzawa, Y. Tamenori, I.H. Suzuki and K. Ueda, J. Chem. Phys. 129 (2008) 204309. (C<sub>5</sub>F<sub>3</sub>H<sub>13</sub>Si<sub>2</sub> - Si2p, Si1s)
- NW&86** T. Nagata, J.B. West, T.Hayaishi, Y. Itikawa, Y.Itoh, T. Koizumi, J.Murakami, Y. Sato, H.Shibata, A.Yagashita and M.Yoshino, J.Phys. B 19 (1986) 1281 (Sr4p)
- NY&90** T. Nagata, M. Yoshino, T. Hayaishi, Y. Itikawa, Y. Itoh, T. Koizumi, T. Matsuo, Y. Sato, E. Shigemasa, Y. Takizawa and A. Yagashita, Phys. Scripta 41 (1990) 47. (Xe,Cs,Ba,Eu,Yb - 4d)
- NY&02** K. Nagaya, M. Yao, T. Hayakawa, Y. Ohmasa, Y. Kajihara, M. Ishii, and Y. Katayama Phys. Rev. Lett. 89 (2002) 243401. (Se<sub>n</sub>, n=2-7 – Se1s)
- O96** H. Oyanagi, "X-ray Absorption Fine Structure" in Appl. of Synchrotron Radiation to Materials Analysis, (H. Saisho and Y. Goshi, eds) 207. (Br<sub>2</sub> - Br1s)
- OA&95** S.J. Osborne, A. Ausmee, S. Svensson, A. Kivimachi, O.-P. Sairanen, A. Naves de Brito, H. Aksela and S. Aksela, J. Chem. Phys. 102 (1995) 7317. (CO - C1s)
- OBI95** T.N. Onley, C.E. Brion and T. Ibuki, Chem. Phys. 201 (1995) 505. (BrCN, C1s, N1s, Br3d)
- OCB98** T.N. Onley, G. Cooper and C.E. Brion, Chem. Phys. 232 (1998) 211. (CH<sub>3</sub>I - I4d, 4p, 4s; C1s)
- OCT91** E.M.L. Ohrendorf, L.S. Cederbaum and F. Tarantelli, Phys. Rev. A 44 (1991) 205. (SiH<sub>4</sub>, SiF<sub>4</sub> - Si1s, Si2p)
- OC&97a** T.N. Olney, G. Cooper, W.F. Chan, G.R. Burton, C.E. Brion and K.H. Tan, Chem. Phys. 218 (1997) 127. (CH<sub>3</sub>Br - Br3d, C1s)
- OC&97b** T.N. Olney, N.M. Cann, G. Cooper and C.E. Brion, Chem. Phys. 223 (1997) 59. (SiH<sub>4</sub>, SiF<sub>4</sub> - Si2p; Cl<sub>2</sub> - Cl2p)
- OD93** M. Ohno and P. Decleva, J. Chem. Phys. 99 (1993) 8070. (CO, NiCO - C1s, O1s)

- ODF93** M. Ohno, P. DeCleva and G. Fronzoni, Surf. Sci. 284 (1993) 372. (N<sub>2</sub> - N1s)
- OEK90** K. Okuyama, J.H.D. Eland and K. Kimura, Phys. Rev. A 41 (1990) 4930. (Xe4d)
- OH&02** B. Obst, J. E. Hansen, B. Sonntag, Ph. Wernet, and P. Zimmermann, Phys. Rev. A 65 (2002) 062716. (Ca2p)
- OJ&16** Christian Ozga,Kari Jänkälä, et al. X-ray absorption spectroscopy of the chiral molecules fenchone, a-pinene, limonene and carvone in the C1s excitation region, J. El. Spec. 207 (2016) 34. (C<sub>10</sub>H<sub>13</sub>O, C<sub>10</sub>H<sub>17</sub>, C<sub>10</sub>H<sub>16</sub>, C<sub>10</sub>H<sub>14</sub>O – C1s)
- OK02** H. Oji and N. Kosugi, UVSOR Annual Report 2002, 125. (O<sub>3</sub> - O1s)
- OM03** M. Ono and K. Mitsuke, Chem. Phy. Lett. 366(2003) 595. (SF<sub>6</sub> – S2p)
- OM03** M. Ono and K. Mitsuke, Chem. Phy. Lett. 379(2003) 248. (SF<sub>6</sub> – S2p)
- OM&96** H. Oji, R. Mitsumoto, E. Ito, H. Ishii, Y. Ouchi, K. Seki and N. Kosugi, J. Electron Spectrosc. 78 (1996) 383. (C<sub>18</sub>H<sub>12</sub>, C<sub>20</sub>H<sub>14</sub>, C<sub>24</sub>H<sub>12</sub> - C1s)
- OM&98** H. Oji, R. Mitsumoto, E. Ito, H. Ishii, Y. Ouchi, K. Seki, T. Yokoyama, T. Ohta and N. Kosugi, J. Chem. Phys.109 (1998) 10409. (C<sub>6</sub>H<sub>6</sub>, C<sub>18</sub>H<sub>12</sub>, C<sub>20</sub>H<sub>14</sub>, C<sub>24</sub>H<sub>12</sub> - C1s)
- OR&01** B. Obst, T. Richter, M. Martins and P. Zimmermann, J. Phys. B 34(2001) L657. (Sc2p)
- OS&90** T. Ohta, K. Seki, T. Yokoyama, I. Morisada and K. Edamatsu, Phys. Scripta 41 (1990) 150. (C<sub>6</sub>F<sub>12</sub> - C1s)
- OS&98** S.J. Osborne, S. Sundin, A. Ausmes, S.L. Sorensen, A. Kikas and S. Svensson, J. El. Spec. 95 (1998) 25. (CO – C1s)
- OS&02** G Öhrwall, M M Sant'Anna, W C Stolte, I Dominguez-Lopez, L T N Dang, A S Schlachter and D W Lindle, J. Phys. B 35(2002) 4553. (CO<sub>2</sub> – C1s, O1s)
- OT&86** H. Oyanagi, M. Tokumoto, T. Ishiguro, H. Shirakawa, H. Nemoto, T. Matsushita, H. Kuroda, J. de Physique Colloq. 47 (1986) C8-S12, C8-615. (BrC<sub>6</sub>H<sub>5</sub> – Br 1s)
- OY&02** K. Okada, H. Yoshida, Y. Senba, K. Kaminori, Y. Tamenori, H. Ohashi, K. Ueda and T. Ibuki, Phys. Rev. A 66 (2002) 032503. (CO<sub>2</sub> - O1s)
- OY&05** K. Okada, Y. Yamana, T. Ibuki, A. Fujii, S. Nagaoka, K. Tabayashi, Y. Shimada, Y. Morishita, Y. Tamenori, I.H. Suzuki, K. Ohno, J. El. Spec. 144-147 (2005) 187. (CF<sub>2</sub>CH<sub>2</sub> – C1s)
- P34** J.A. Prins, Physica 1 (1934) 1174. (Ar2p; CCl<sub>4</sub> - Cl2p)
- P39** L.G. Parratt, Phys. Rev. 56 (1939) 295. (Ar1s)
- P99** A.A. Pavylchev, J. Phys. B 32 (1999) 2077. (CO – C1s)
- PA&96** L.G.M. Pettersson, H. Agren, O. Vahtras and V. Caravetta, Surf. Sci. 365 (1996) 581. (CO, Cu<sub>17</sub>CO, Cu<sub>50</sub>CO – C1s, O1s)
- PB90** A.A. Pavlychev and A. Barry, Phys. Scripta 41 (1990) 157. (Ar2p)

- PBV91** A.A. Pavlychev, A. Barry and A.S. Vinogradov, Phys. Scripta 44 (1991) 399. (N<sub>2</sub>O - O1s)
- PB&78** H. Petersen, A. Bianconi, F.C. Brown and R.Z. Bachrach, Chem. Phys. Lett. 58 (1978) 263. (N<sub>2</sub> - N1s)
- PB&99** E. Pahl, J. Brand, L.S. Cederbaum and F. Tarantelli, Phys. Rev. A 60 (1999) 1079. (HF - F1s)
- PB&85** R.C.C. Perera, J. Barth, R.E. LaVilla, R.D. Deslattes and A. Henins, Phys. Rev. A 32 (1985) 1489. (CH<sub>3</sub>Cl - Cl1s)
- PB&07** S. Pilling, H.M. Boechat-Roberty, A.C.F. Santos, G.G.B. de Souza and A. Naves de Brito, J. El. Spec. 156-158 (2007) 139. (C<sub>2</sub>H<sub>4</sub>O<sub>2</sub> - Cl1s)
- PB&08** A.A. Pavlychev, X.O. Brykalova, D.A. Mistrov, R. Flesch, E. Rühl, J. El. Spec. 166-167 (2008) 45. (SF<sub>6</sub>)<sub>n</sub>-S2p
- PB&15** K.C. Prince, P. Bolognesi, V. Feyer, O. Plekan, L. Avaldi, J. El. Spec. 204 (2015) 335. (C<sub>2</sub>H<sub>5</sub>NO<sub>2</sub>, C<sub>4</sub>H<sub>7</sub>N<sub>2</sub>O<sub>3</sub> - N 1s)
- PB&20** A. Perry-Sassmannshausen , T. Buh, et al., Multiple Photodetachment of Carbon Anions via Single and Double Core-Hole Creation, Physical Review Letters 124 (2020) 083203. (C<sup>-</sup> - Cl1s (m=2-5) C-K2)
- PB&21** A. Perry-Sassmannshausen , T. Buh, et al., Multiple photodetachment of silicon anions via K-shell excitation and ionization, Physical Review A 104 (2021) 053107. Si<sup>-</sup> - Si1s (m=2-5) C-K2)
- PC83** M. Pantelouris and J.P. Connerade, J. Phys. B 16 (1983) L23. (U5d)
- PCK87** C. Pan, S.L. Carter and H.P. Kelly, J. Phys. B 20 (1987) L335. (Eu4d)
- PCK91** C. Pan, S.L. Carter and H.P. Kelly, Phys. Rev. A 43 (1991) 1290. (Eu4d)
- PCT99** E. Pahl, L.S. Cederbaum and F. Tarantelli, Phys. Rev. A 60 (1999) 1070. (HF – F1s)
- PC&78** N. Padial, G. Csanak, B.V. McKoy and P.W. Langhoff, J. Chem. Phys. 69 (1978) 2992. (CO-C1s, O1s)
- PC&81a** N. Padial, G. Csanak, B.V. McKoy and P.W. Langhoff, Phys. Rev. A 23 (1981) 218. (CO<sub>2</sub>-C1s, O1s)
- PC&81b** N. Padial, G. Csanak, B.V. McKoy and P.W. Langhoff, J. Chem. Phys. 74 (1981) 4581. (O<sub>3</sub> - O1s)
- PC&87** R.C.C. Perera, P.L. Cowan, D.W. Lindle and R.E. LaVilla, J. Phys. 48 (1987) C9-753. (CF<sub>3</sub>Cl - Cl1s)
- PC&91** R.C. Perera, P.L. Cowan, D.W. Lindle, R.E. LaVilla, T.E. Jach and R.D. Deslattes, Phys. Rev. Lett. 43 (1991) 3609. (CF<sub>2x</sub>Cl<sub>4-x</sub>, x=1-3 - Cl1s)
- PC&98** O. Plashkevych, V. Carravetta, O. Vahtras and H. Agren, Chem. Phys. 232 (1998) 49. (C<sub>2</sub>H<sub>5</sub>O<sub>2</sub>N, C<sub>3</sub>H<sub>7</sub>O<sub>2</sub>N, C<sub>3</sub>H<sub>7</sub>O<sub>3</sub>N, C<sub>3</sub>H<sub>7</sub>O<sub>2</sub>NS, C<sub>5</sub>H<sub>11</sub>O<sub>2</sub>N - Cl1s, N1s, O1s)
- PDK97** R. Püttner, M. Domke and G. Kaindl, Acta Phys. Polonica A 291 (1997) 865. (SiX<sub>4</sub>, X=H,D,F,Cl, Br - Si2p)
- PDK98** R. Püttner, M. Domke and G. Kaindl, Phys. Rev. A 57 (1998) 297. (SiX<sub>4</sub>, X=H,D,F,Cl,Br,Me - Si2p)
- PD&95** R. Püttner, M. Domke, K. Schulz, A. Gutiérrez and G. Kaindl, J. Phys. B 28 (1995) 2425. (HBr - Br3d)

- PD&96** R. Püttner, M. Domcke, K. Shulz and G. Kaindl, Chem. Phys. Lett. 250 (1996) 145. ( $\text{SiF}_4$  - Si2p)
- PD&97** R. Püttner, M. Domke, D. Lentz and G. Kaindl, Phys. Rev. A 56 (1997) 1228. ( $\text{SiH}_4$ ,  $\text{SiD}_4$  - Si2p)
- PD&99** R. Püttner, J. Domingue, T.J. Morgan, C. Cisneros, R.F. Fink, E. Rotenberg, T. Warwick, M. Domke, G. Kaindl and A.S. Schlachter, Phys. Rev. A 59 (1999) 3415. (CO, NO – O1s)
- PF&89** M.N. Piancastelli, T.A. Ferrett, D.W. Lindle, L.J. Medhurst, P.A. Heiman, S.H. Liu and D.A. Shirley, J. Chem. Phys. 90 (1989) 3004. ( $\text{C}_2\text{H}_4$ ,  $\text{C}_6\text{H}_6$ -C1s)
- PF&94** A.W. Potts, H.F. Fadil, J.M. Benson, I.H. Hillier, A.A. McDowell and S. Jones, J. Phys. B 27 (1994) 473. ( $\text{CH}_x\text{Cl}_{4-x}$ , x=0-3;  $\text{CF}_3\text{Cl}$ ,  $\text{CF}_2\text{Cl}_2$ ,  $\text{CFCl}_3$  - Cl 1s)
- PF&98** A.A. Pavlychev, N.G. Faminykh, N. Watanabe, K. Soejima, E. Shigemasa and A. Yagashita, Phys. Rev. Lett. 81 (1998) 3623. ( $\text{N}_2$  – N1s;  $\text{CO}_2$  – O1s)
- PF&00** M.N. Piancastelli, R.F. Fink, R. Feifel, N. Boesch, S.L. Sorensen, C. Miron, H. Wang, I. Hjelte, O. Bjorneholm, A. Ausmees, S. Svensson, P. Salek, F. Kh. Gel'mukhanov and H. Agren, J. Phys. B 33 (2000) 1819. ( $\text{N}_2$  – N1s)
- PF&09** Plekan O, Feyer V, Richter R, Coreno M, Vall-Llosera G, Prince KC et al An experimental and theoretical core-level study of tautomerism in guanine. J Phys Chem A 113 (2009) 9376. ( $\text{C}_5\text{H}_5\text{N}_5\text{O}$  – C1s, N1s, O1s)
- PG&12** M.N. Piancastelli, R. Gillemot, M. Simon, H. Iwayama and E. Shigemasa, UVSOR report 2012, 62. ( $\text{CF}_4$  -C1s)
- PH&95** A.A. Pavlychev, K.H. Hallmeier, C. Hennig, L. Hennig and R. Szargan, Chem. Phys. 201 (1995) 547. ( $\text{C}_4\text{H}_5\text{N}$  - N1s)
- PH&99** M.N. Piancastelli, A. Hempelmann, F. Heiser, O. Gessner, A. Rudel and U. Becker, Phys. Rev. A 59 (1999) 3000. ( $\text{H}_2\text{O}$  – O1s)
- PH&02** R. Püttner, Y.-F. Hu, E. Nõmmiste, G. M. Bancroft, S. Aksela, Phys. Rev. A 65 (2002) 032513. (HBr – Br 3d)
- PK89** C. Pan and H.P. Kelly, Phys. Rev. A 39 (1989) 6232. (Ar2p)
- PK&89** E.D. Poliakoff, L.A. Kelly, L.M. Duffy, B. Space, P. Roy, S.H. Southworth and M.G. White, Chem. Phys. 129 (1989) 65. ( $\text{N}_2$ -N1s)
- PK&93** N. Pargher, H.M. Köppe, J. Feldhaus and J. Haase, Phys. Rev. Lett. 71 (1993) 4385. ( $\text{SO}_2$  - O1s)
- PK&97** M.N. Piancastelli, A. Kivimaki, B. Kempgens, M. Neeb, K. Maier and A.M. Bradshaw, Chem. Phys. Lett. 274 (1997) 13. ( $\text{CO}_2$  – O1s)
- PK&99a** M.N. Piancastelli, A. Kivimaki, B. Kempgens, K. Maier, A. Rudel, U. Hergenhahn and A.M. Bradshaw, J. Phys. B 32 (1999) 2523. ( $\text{N}_2$  – N1s)
- PK&99b** M.N. Piancastelli, A. Kivimaki, B. Kempgens, K. Maier, U. Hergenhahn, A. Rudel and A.M. Bradshaw, J. El. Spec. 98 (1999) 111. ( $\text{N}_2$  – N1s)
- PK&99c** M.N. Piancastelli, B. Kempgens, U. Hergenhahn, A. Kivimaki, K. Maier, A. Rudel and A.M. Bradshaw, Phys. Rev. A 59 (1999) 1336. ( $\text{H}_2\text{O}$  – O1s)

- PK&01** J.P. Gomilsek, A. Kodre, I. Arcon, and R. Preseren, Phys. Rev. A 64 (2002) 022508. (K1s)
- PK&02** M.N. Piancastelli, A. Kivimäki, V. Carravetta, I. Cacelli, R. Cimiraglia, C. Angeli, H. Wang, M. Coreno, M. de Simone, G. Turri, and K. C. Prince, Phys. Rev. Lett. 88 (2002) 243002. (O<sub>2</sub> – O1s)
- PK&04** R. Puttner, C. Kolczewski, M. Martin, A.S. Schlachter, G. Snell, M. Sant'Anna, J. Viehaus, K. Hermann and G. Kaindl, Chemical Physics Letters 393 (2004) 361–366. (C<sub>6</sub>H<sub>6</sub> – C1s)
- PK&17** P. Lablanquie, M.A. Khalal, L. Andric et al, J. El. Spec. 220 (2017) 125. Ar2p, Ar2s
- PL84** R.C.C. Perera & R.E. LaVilla, J. Chem. Phys. 81 (1984) 3375. (CS<sub>2</sub>,COS -S1s)
- PL86** R.C.C. Perera & R.E. LaVilla, J. Chem. Phys. 84 (1986) 4228. (C<sub>4</sub>H<sub>4</sub>S - S1s)
- PL&87** M.N. Piancastelli, D.W. Lindle, T.A. Ferrett and D.A. Shirley, J. Chem. Phys. 86 (1987) 2765; reply to rebuttal, J. Chem. Phys. 87 (1987) 3255. (CO<sub>2</sub> – C1s, O1s; N<sub>2</sub>O – N1s,O1s)
- PL&07** M.N. Piancastelli, T. Lischke, G. Prümper, X.J. Liu, H. Fukuzawa, M. Hoshino, T. Tanaka, H. Tanaka, J. Harries, Y. Tamenori, Z. Bao, O. Travnikova, D. Céolin and K. Ueda, J. El. Spec. 156-158 (2007) 259. (C<sub>3</sub>H<sub>6</sub>O - C1s, O1s)
- PMT81** M. Pettini, M. Mazzoni and U.P. Tozzi, Phys. Lett. A 82 (1981) 168. (I4d)
- PM&93** S.C. Page, L. Mei, D. Palfreyman and F.H. Read, Rev. Sci. Inst. 64 (1993) 2574. (Xe4d)
- PN93** M.J. Puska and R.M. Nieminen, Phys. Rev. A 47 (1993) 1181 (erratum 49 (1994) 629). (Xe, Xe:C<sub>60</sub>-Xe4d; Ba, Ba:C<sub>60</sub>-Ba4d)
- PN&97** M.N. Piancastelli, M. Neeb, A. Kivimaki, B. Kempgens, H.M. Köppe, K. Maier, A.M. Bradshaw and R.F. Fink, J. Phys. B 30 (1997) 5677. (CO - C1s,O1s)
- PN&15** F. Penent, M. Nakano, M. Tashiro, T.P. Grozdanov, M. Žitnik, K. Bučar, S. Carniato, P. Selles, L. Andric, P. Lablanquie, J. Palaudoux, E. Shigemasa, H. Iwayama, Y. Hikosaka, K. Soejima, I.H. Suzuki, N. Berrah, A.H. Wuosmaa, T. Kaneyasu, K. Ito, J. El. Spec. 204 (2015) 303 (C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>2</sub>, CO, C<sub>3</sub>H<sub>6</sub> – C1s; N<sub>2</sub> – N1s)
- PP&00** O. Plashkevych, T. Privalov, H. Agren, V. Carravetta and K. Ruud, Chem. Phys. 260 (2000) 11. (CO, H<sub>2</sub>CO, D<sub>2</sub>CO – C1s, O1s; C<sub>6</sub>FH<sub>5</sub>, C<sub>6</sub>H<sub>6</sub> – C 1s, C<sub>6</sub>H<sub>6</sub>O – C1s, O1s, C<sub>6</sub>H<sub>7</sub>N – C1s, N1s)
- PR00** A.A. Pavlychev and E. Rühl, J. El. Spec. 106 (2000) 207. (N<sub>2</sub> – N1s; CO – Cs, O1s)
- PRW74** H. Petersen, K. Radler and H.W. Wolff, Proc. 4th Int. Vac. UV Rad. Phys. Conf. (Hamburg, 1974) 247. (Ba4d)
- PR&75** H. Petersen, K. Radler, B. Sonntag and R. Haensel, J. Phys. B 8 (1975) 31. (Cs4d, Cs4p)
- PR&86** Th. Prescher, M. Richter, E. Schmidt, B. Sonntag and H.E. Wetzel, J. Phys. B 19 (1986) 1645. (Cs4d,Sm4d)
- PS&01** O. Plashkevych, A. Snis, L. Yang, H. Agren and S.F. Matar, Phys. Scripta 63 (2001) 70. (C<sub>5</sub>H<sub>6</sub>, C<sub>5</sub>H<sub>8</sub>, C<sub>5</sub>H<sub>10</sub>, C<sub>6</sub>H<sub>6</sub>, C<sub>6</sub>H<sub>8</sub>, C<sub>6</sub>H<sub>8</sub>, C<sub>6</sub>H<sub>10</sub>, C<sub>6</sub>H<sub>12</sub> – C1s; C<sub>2</sub>H<sub>3</sub>N, C<sub>3</sub>H<sub>3</sub>N<sub>3</sub>,C<sub>4</sub>H<sub>4</sub>N<sub>2</sub>, C<sub>4</sub>H<sub>4</sub>N<sub>2</sub>, C<sub>4</sub>H<sub>4</sub>N<sub>2</sub>, C<sub>4</sub>H<sub>5</sub>N, C<sub>4</sub>H<sub>5</sub>N, C<sub>4</sub>H<sub>5</sub>N, C<sub>4</sub>H<sub>7</sub>N, C<sub>4</sub>H<sub>7</sub>, C<sub>4</sub>H<sub>7</sub>N, C<sub>4</sub>H<sub>9</sub>N, C<sub>5</sub>H<sub>5</sub>N, C<sub>5</sub>H<sub>7</sub>N, C<sub>5</sub>H<sub>7</sub>N, C<sub>5</sub>H<sub>11</sub>N, C<sub>7</sub>H<sub>5</sub>N – C1s, N1s; C<sub>3</sub>H<sub>9</sub>N, C<sub>5</sub>H<sub>7</sub>N<sub>5</sub>, C<sub>5</sub>H<sub>7</sub>N, C<sub>5</sub>H<sub>9</sub>N, C<sub>5</sub>H<sub>9</sub>N, C<sub>5</sub>H<sub>11</sub>N, C<sub>9</sub>H<sub>7</sub>N, C<sub>9</sub>H<sub>7</sub>N, C<sub>10</sub>H<sub>8</sub>N<sub>4</sub>, C<sub>10</sub>H<sub>27</sub>N, C<sub>12</sub>H<sub>4</sub>N<sub>4</sub>, C<sub>13</sub>H<sub>9</sub>N, C<sub>13</sub>H<sub>9</sub>N – N1s)

- PS&02** M.N. Piancastelli, W.C. Stolte, G. Ohrwall, S.W. Yu, D.Bull, K. Lantz, A.S. Schlachter and D.W. Lindle, J. Chem. Phys. 117 (2002) 8264. ( $C_2H_2$ ,  $C_2H_4$  – C1s)
- PS&05** M. N. Piancastelli, W. C. Stolte, R. Guillemin, A. Wolska, S.-W. Yu, M. M. Sant'Anna, and D. W. Lindle, J. Chem. Phys. 122 (2005) 094312. ( $SF_6$  – S2p, F1s)
- PS&17** R. Puttner, P. Schmid-Wever, T. Kampen, C. Kolczewski, K. Hermann and K. Horn, J. El. Spec. 215 (2017) 16. ( $C_{14}H_{12}$  – C 1s)
- PT&95** M. Perez-Jigato, V. Termath, P. Gardner, N.C. Handy, D.A. King, S. Rassiano and M. Surman, Mol. Phys. 85 (1995) 619. ( $((NO)_2$  - N1s, O1s)
- PT&03** S.Peredkov, M. Tchaplyguine, J. Schulz, A. Kivimaki, S Sorensen, M. Lundwall, G. Ohrwall, T. Rander, A. Lindblad, S. Svensson and O. Bjorneholm. Max Lab report 2003, 206. ( $Kr_n$ )
- PUT04** G. Pruemper, K. Ueda and Y. Tamenori, Spring8 Ann. Rep. (2004) 86. ( $CF_4$ -F1s)
- PU&05** G. Prümper, K. Ueda, U. Hergenhahn, A. De Fanis, Y. Tamenori, M. Kitajima, M. Hoshino, H. Tanaka, J. El. Spec. 144-147 (2005) 227. ( $SF_6$ -F1s)
- PV87** A.A. Pavlychev and A.S. Vinogradov, Opt. Spectrosc. (USSR) 62 (1987) 197; [Opt. Spekt. 62 (1987) 329] ( $N,N_2$ - N1s)
- PV90** A.A. Pavlychev and A.S. Vinogradov, unpublished ( $TeF_6$  - Te4d)
- PVK80** A.A. Pavlychev, A.S. Vinogradov and T.M. Zimkina, Proc. 6th Int. Conf. on Vac. UV Rad. Phys. II-95 (Charlottesville, 1980) ( $SiH_4$ ,  $SiF_4$  - Si2p)
- PVZ82** A.A. Pavlychev, A.S. Vinogradov and T.M. Zimkina, Opt. Spectrosc. 52 (1982) 139. [Opt. Spekt. 52 (1982) 231] ( $Si, SiH_4, SiF_4$ -Si2p)
- PV&79** A.A. Pavlychev, A.S. Vinogradov, T.M. Zimkina, D.E. Onopko and S.A. Titov, Opt. Spect. 47 (1979) 40 [Opt. Spekt. 47 (1979) 73]. ( $SiX_4$  - X=F,Cl,Br - Si2p;  $GeF_4$ ,  $GeCl_4$  - Ge2p)
- PV&80** A.A. Pavlychev, A.S. Vinogradov, T.M. Zimkina, D.E. Onopko and R. Stsargan, Opt. Spect. 48 (1980) 109 [Opt. Spekt. 48 (1980) 192]. ( $SiH_4$  - Si2p)
- PV&82** A.A. Pavlychev, A.S. Vinogradov, T.M. Zimkina, D.E. Onopko and S.A. Titov, Opt. Spect. 52 (1982) 302 [Opt. Spekt. 52 (1982) 506] ( $SiF_4$ -Si2p, F1s)
- PV&85** A.A. Pavlychev, A.S. Vinogradov, I.V. Kondratenko and T.M. Zimkina, Sov. Phys. Sol. St. 27 (1985) 123; [Fiz.Tverd.Tela (Leningrad) 27 (1985) 209] ( $CF_4$ -C1s;  $AF_x$ -A1s)
- PV&86** A.A. Pavlychev, A.S. Vinogradov, I.V. Kondratenko and I.V. Kondzatieveva, Proc. III Conf. Autoionisation Phenomena in Atoms, Moscow St. Univ. 1986, 80. ( $TeF_6$  - Te4d)
- PV&90** A.A. Pavlychev, A.S. Vinogradov, V.N. Akimov and S.V. Nekipelov, Physica Scripta 41 (1990) 160. ( $N_2$ ,  $NH_3$ ,  $NO$  - N1s;  $NO$  -O1s;  $BF_3$  -B1s)
- PV&93** A.A. Pavlychev, A.S. Vinogradov, A.P. Stepanov and S.V. Nekipelov, Opt. Spectrosc. 75 (1993) 327. [Opt. Spek. 75 (1993) 554.] ( $CH_3NO_2$ ,  $NO$ ,  $CF_3NO$ ,  $N_2O$  - O1s)

- PV&97** O. Plashkevych, L. Yang, O. Vahtras, H. Agren and L.G.M. Pettersson, Chem. Phys. 222 (1997) 127. ( $C_6H_xF_{6-x}$  x=1-6 C1s, F1s;  $C_6H_7N$  - C1s,N1s;  $C_6H_6O$  - C1s, O1s)
- PV&99** K.C. Prince, M. Vondráček, J. Karvonen, M. Coreno, R. Camilloni, L. Avaldi, M. de Simone, A critical comparison of selected 1s and 2p core hole widths, J. Elect. Spectrosc. 101-103 (1999) 141-147 (Ar2p, Ne1s; CO-C1s; N<sub>2</sub>, N<sub>2</sub>O-N1s; CO, N<sub>2</sub>O, O<sub>2</sub>-O1s; SF<sub>6</sub>-S2p)
- PV&03** A.B. Preobrajenski, A.S. vingradov, S.L. Sorensen and N. Martensson, Max Lab Ann Rep 2003, 208. ( $B_3N_3H_6$  - B1s)
- PV&04b** G. Prümper, J. Viehaus, S. Cvejanovic, D. Rolles, O. Gessner, T. Lischke, R. Hentges, C. Wienberg, W. Mahler, U. Becker, B. Langer, T. Prosperi, N. Zema, S. Turchini, B. Zada and Fred Senf, Phys. Rev. A 69 (2004) 062717. ( $C_3H_7NO_2$ ,  $C_3H_7NO_3$  - C1s)
- QL89** C.A. Quarles and H.E. Lehithet, Phys. Rev. A 40 (1989) 455. (SF<sub>6</sub> - S1s)
- QO&95** C. Quaresima, C. Ottaviani et. al, Nucl. Inst. Meth. A 364 (1995) 374. (Ar2p, Ne1s, N<sub>2</sub> - N1s, O<sub>2</sub> - O1s)
- R74** K. Radler, Diss. (U. Hamburg) DESY report F41-74/9. (CsI - Cs4p)
- R75** M.B. Robin, Chem. Phys. Lett. 31 (1975) 140. ( $CH_4$  - C1s;  $B_2H_6, BF_3$  - B1s; N<sub>2</sub> - N1s; HCl - Cl2p; H<sub>2</sub>S - S2p; PH<sub>3</sub> - P2p; SiH<sub>4</sub>,SiF<sub>4</sub> - Si2p; SiF<sub>4</sub> - F1s; review)
- R77** E. Radtke, Proc. 5th Int. Vac. UV Rad. Phys. Conf. (Montpellier, 1977) I-23. (La4d, Sm4d)
- R78** F.H. Read, J. de Phys. C1-S5 (1978) 82. (N<sub>2</sub>, Ar, CH<sub>4</sub> - review)
- R79** E.R. Radtke, J. Phys. B 12 (1979) L71. (La4d)
- R83** D.E. Ramaker, Chem. Phys. 80 (1983) 183. (H<sub>2</sub>O-O1s)
- R85** M.B. Robin, *Higher Excited States of Polyatomic Molecules* (Vol. 3, Academic, Florida, 1985) (review).
- R86** R.A. Rosenberg, J. Vac. Sci. Tech. A 4 (1986) 1463. (SiF<sub>4</sub> - Si2p)
- R90** B.F. Rozsnyai, Phys. Rev. A 42 (1990) 286. (Ba4d, Xe4d, Kr3d)
- R92** E. Rühl, Ber. Bunsenges. Phys. Chem. 96 (1992) 1172. ((N<sub>2</sub>)<sub>n</sub>, (N<sub>2</sub>O)<sub>n</sub> - N1s)
- R95** M. Richter, J. Electron Spectrosc. 76 (1995) 21. (Ba4d, Na2p, Eu4d)
- RAZ93** J.J. Rehr, R.C. Alber and S.I. Zabinsky, Phys. Rev. Lett 69 (1993) 3397. (N<sub>2</sub>-N1s, O<sub>2</sub>-O1s)
- RA&92** H. Rabus, D. Arvanitis, M. Domke and K. Baberschke, J. Chem. Phys. 96 (1992) 1560. (C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>4</sub> - C1s)
- RB99** A.B. Rocha and C.E. Bielschowsky, Chem. Phys. 243 (1999) 9. (H<sub>2</sub>O – O1s)
- RB00** A.B. Rocha and C.E. Bielschowsky, J. Chem. Phys. 113 (2000) 7971. (C<sub>2</sub>H<sub>4</sub> – C1s)
- RB02** A.B. Rocha and C.E. Bielschowsky, Phys. Rev. A 66 (2002) 052720. (CO<sub>2</sub> – C1s)

- RB&92** C. Reynaud, S. Bodeur, J.L. Marechal, D.Bazin, P. Millie, I. Nenner, U. Rockland and H. Baumgartel, Chem. Phys. 166 (1992) 411. ( $\text{SF}_5\text{Cl}$ ,  $\text{SF}_6$  - S1s)
- RB&14** Reitsma G, Boschman et al, Deexcitation dynamics of superhydrogenated polycyclic aromatic hydrocarboncations after soft-x-ray absorption. Phys Rev Lett 113 (2014) 053002. ( $\text{C}_{24}\text{H}_{12}$  - C1s)
- RB&15** Reitsma G, Boschman L, Deuzeman MJ, Hoekstra S, Hoekstra R, Schlathölter T, Near edge X-ray absorption mass spectrometry on coronene. J Chem Phys 142 (2015) 024308. ( $\text{C}_{24}\text{H}_{12}$  - C1s)
- RB&23** S. Reinwardt, I. Baev et al. Soft X-Ray-induced Dimerization of Methane, The Astrophysical Journal, 952(2023) 39. ( $\text{CH}_4$  - C1s)
- RC&90** G. Rocker, D. Coulman, P. Feulner, B. Scheurer, Z. Lin and D. Menzel, DIET IV, Springer Ser. Surf. Sci 19 (1990) 261. ( $\text{CH}_4$  - C1s;  $\text{NH}_3$  - N1s;  $\text{H}_2\text{O}$  - O1s)
- RC&01** M. Riedler, A.R.B. de Castro, A. Kolmakov, J.O. Löfken, C. Nowak, A.V. Soldatov, A. Wark, G. Yalovega, and T. Möller, J. Chem. Phys. 115 (2001) 1319. ( $(\text{NaCl})_n$  Na1s)
- RDK93** G. Remmers, M. Domke and G. Kaindl, Phys. Rev. A 47 (1993) 3085. ( $\text{CH}_4$ ,  $\text{CD}_4$ ,  $\text{C}_2\text{H}_6$ ,  $\text{C}_2\text{D}_6$ ,  $\text{C}_3\text{H}_8$ ,  $\text{C}_3\text{D}_8$  - C1s)
- RD&92** G. Remmers, M. Domke, A. Puschmann, T. Mandel, C. Xue, G. Kaindl, E. Hudson and D.A. Shirley, Phys. Rev. A 46 (1992) 3935 ( $\text{H}_2\text{CO}$  - C1s, O1s)
- RD&93** G. Remmers, M. Domke, A. Puschmann, T. Mandel, G. Kaindl, E. Hudson and D.A. Shirley, Chem. Phys. Lett. 214 (1993) 241 (NO - N1s, O1s)
- RE&92** K.J. Randall, W. Eberhardt, J. Feldhaus, W. Erlebach, A.M. Bradshaw, Z. Xu, P.D. Johnson and Y. Ma, Nucl. Inst. Meth. A 319 (1992) 101. (O<sub>2</sub> - O1s)
- RF68** A.P. Rau and U. Fano, Phys. Rev. 167 (1968) 7. (Kr3d)
- RF91** R.A. Rosenberg and S.P. Frigo, Chem. Phys. Lett. 184 (1991) 439. ( $\text{SiCl}_4$  - Si2p)
- RF04** E. Rühl and R. Flesch, J. Chem. Phys. 121 (2004) 5322 ( $\text{CO}_2$  - C1s)
- RF&92** K.J. Randall, J. Feldhaus, W. Erlebach, A.M. Bradshaw, W. Eberhardt, Z. Xu, Y.Ma and P.D. Johnson, Rev. Sci. Inst. 63 (1992) 1367 (CO-C1s; N<sub>2</sub>-N1s; O<sub>2</sub>-O1s)
- RG&96a** C. Reynaud, M.A. Gaveau, P. Millie, S. Bodeur, P. Archirel, B. Levy and I. Nenner, J. Electron Spectrosc. 79 (1996) 357. ( $\text{H}_2\text{S}$ ,  $\text{SO}_2$ ,  $\text{SF}_6$  - S1s)
- RG&96b** C. Reynaud, M.A. Gaveau, K. Bisson, P. Millie, I. Nenner, S. Bodeur, P. Archirel and B. Levy, J. Phys. B 29 (1996) 5403. ( $\text{H}_2\text{S}$ ,  $\text{SO}_2$ ,  $\text{SF}_6$  - S1s)
- RG&02** J. ruis I Riu, E.M. Garcia, J.A. Ruiz, P. Erman, P.A. Hatherly, A. Kivimaki, E. Rachlew and M. Stankiewicz, MAXLab Annual report 2001/02 (2002) 198. (CD<sub>4</sub> – C1s)
- RH89a** E. Rühl and A.P. Hitchcock, J. Am. Chem. Soc. 111 (1989) 2614. ( $\text{Mn}(\text{CO})_5\text{Br}$ ,  $\text{Mn}(\text{CO})_5\text{H}$ ,  $\text{Mn}_2(\text{CO})_{10}$  - C1s, O1s, Mn2p, Mn3p)

- RH89b** E. Rühl and A.P. Hitchcock, J. Am. Chem. Soc. 111 (1989) 5069. (M(Cp)<sub>2</sub>, M=Fe, Cr, Ni; - C1s)
- RH91** E. Rühl and A.P. Hitchcock, Chem .Phys. 154 (1991) 323. H<sub>2</sub>O<sub>2</sub>, H<sub>2</sub>O, CF<sub>3</sub>OOCF<sub>3</sub>, (t-Bu)<sub>2</sub>O<sub>2</sub> - O1s)
- RH&93a** E. Rühl, C. Heinzel, A.P. Hitchcock and H. Baumgartel, J. Chem. Phys. 98 (1993) 2653. (Ar, Ar<sub>n</sub>- Ar2p)
- RH&93b** E. Rühl, C. Heinzel, H. Baumgartel and A.P. Hitchcock, Chem. Phys. 169 (1993) 243. (FeCp<sub>2</sub>, NiCp<sub>2</sub> - C1s, Fe2p, Ni2p)
- RH&93c** E. Rühl, C. Heinzel, A.P. Hitchcock, H. Schmeltz, C. Reynaud, H. Baumgartel, W. Drube and R. Frahm, J. Chem. Phys. 98 (1993) 6820. (Ar, Ar<sub>n</sub>- Ar1s)
- RH&93d** E. Rühl, C. Heinzel, H. Baumgartel, W. Drube and A.P. Hitchcock, Jap. J. Appl. Phys. 32 (Supp.2) (1993) 791. (Ar,Ar<sub>n</sub> - Ar2p, Ar1s)
- RH&93e** E. Rühl, C. Heinzel, A.P. Hitchcock and H. Baumgartel, Proc. VUV-10 (1993). ((C<sub>6</sub>H<sub>6</sub>)<sub>n</sub> - C1s, (N<sub>2</sub>O)<sub>n</sub> - N1s; Ar<sub>n</sub> - Ar2p)
- RH&94** T. Reich, P.A. Heimann, B.L. Petersen, E. Hudson, Z. Hussain and D.A. Shirley, Phys. Rev. A 49 (1994) 4570. (CO - C1s, O1s)
- RH&95** E. Rühl, A.P. Hitchcock, P. Morin and M. Lavollée, J. Chim. Phys. 92 (1995) 521. (Ar<sub>n</sub> - Ar2p)
- RH&97** E.G. Rightor, A.P. Hitchcock, H. Ade, R.D. Leapman, S.G. Urquhart, A.P. Smith, G. Mitchell, D. Fischer, H.J. Shin and T. Warwick, J. Phys. Chem. 101 (1997) 1950. (C<sub>10</sub>H<sub>10</sub>O<sub>4</sub> - C1s, O1s)
- RH&02** E.E. Rennie, U. Hergenhahn, O. Kugeler, A. Rüdel, S. Marburger, and A.M. Bradshaw, J. Chem. Phys. 117 (2002) 6524. (C<sub>4</sub>H<sub>4</sub>O – C1s)
- RH&09** E. Rühl, A.P. Hitchcock, J.D. Bozek, T. Tyliszczak, A.L.D. Kilcoyne, D.N. McIlroy, A. Knop-Gericke and P.A. Dowben, Phys. Stat. Sol. B 246 (2009) 1496. (C<sub>2</sub>B<sub>10</sub>H<sub>10</sub> - B1s, C1s)
- RI&88** M.B. Robin, I. Ishii, R. McLaren and A.P. Hitchcock, J. Electron Spectrosc. 47 (1988) 53. (C<sub>2</sub>H<sub>x</sub>F<sub>4-x</sub>, c-C<sub>5</sub>F<sub>8</sub>, H<sub>x</sub>F<sub>2-x</sub>CO, CF<sub>2</sub>CFCFCF<sub>2</sub>, CH<sub>3</sub>CCCH<sub>3</sub>, CF<sub>3</sub>CCCF<sub>3</sub>, CH<sub>3</sub>COOH, C<sub>3</sub>H<sub>6</sub>O, CF<sub>3</sub>COOH, C<sub>10</sub>H<sub>8</sub>, C<sub>10</sub>F<sub>8</sub>, (CF<sub>3</sub>)<sub>2</sub>CO - C1s, O1s, F1s)
- RJ96** E. Rühl and H.W. Jochims, Z. Phys. Chem Bd 195 (1996) 137. (CO<sub>2</sub> - C1s; N<sub>2</sub>O - N1s)
- RJ&91** E. Rühl, H.W. Jochims, C. Schmale, E. Biller, A.P. Hitchcock and H. Baumgartel, Chem. Phys. Lett. 178 (1991) 558. (Ar2p)
- RK&93** K.J. Randall, A.L.D. Kilcoyne, H.M. Koppa, J. Feldhaus, A.M. Bradshaw, J.E. Rubensson, W. Eberhardt, Z. Xu, P.D. Johnson and Y. Ma, Phys. Rev. Lett. 71 (1993) 1156. (CO - C1s)
- RK&96** E. Rühl, A. Knop, A.P. Hitchcock, P.A. Dowben and D.N. McIlroy, Surface Reviews and Letters 3 (1996) 557. (Ar<sub>n</sub> - Ar2p)
- RK&99** E.E. Rennie, H.M.Koppe, B. Kempgens, U.Hergenhahn, A. Kivimaki, K. Maier, M. Neeb, A. Rudel and A.M. Bradshaw, J.Phys. B 32 (1999) 2691. (C<sub>2</sub>H<sub>6</sub> – C1s)
- RK&00a** E.E. Rennie, B. Kempgens, H.M.Koppe, U.Hergenhahn, J. Feldhaus, B.S. Itchikawitz, A.L.D. Kilcoyne, A. Kivimaki, K. Maier, M.N Piancastelli, M.Polcik, A. Rudel and A.M. Bradshaw, J. Chem. Phys. 113 (2000)

7362. ( $C_6H_6 - C1s$ )

- RK&00b** J. Rius I Riu, E. Kukk, M. Stankiewicz, S. Aksela, J. A. Ruiz, P. Erman, P. Hatherly, M. Huttula, A. Karawajczyk, E. Rachlew and P. Winiarczyk, MaxLab Report (2000) 182. ( $CD_4 - C1s$ )
- RL77** T.N. Rescigno and P.W. Langhoff, Chem. Phys. Lett. 51 (1977) 65. ( $N_2-N1s$ )
- RL&83** R.A. Rosenburg, P.R. LaRoe, V. Rehn, J. Stöhr, R. Jaeger and C.C. Parks, Phys. Rev. B 28 (1983) 3026. ( $H_2O, D_2O(s) - O1s$ )
- RL&85** R.A. Rosenberg, P.J. Love, P.R. LaRoe, V. Rehm and C.C. Parks, Phys. Rev. B 31 (1985) 2634. ( $CO-C1s; N_2, NO, N_2O - N1s; CO, NO - O1s$ )
- RL&95** J.E. Rubensson, J. Lüning, M. Neeb, M. Biermann, B. Küpper and W. Eberhardt, J. Electron Spectrosc. 75 (1995) 47. ( $N_2 - N1s, O_2 - O1s$ )
- RL&96** J.E. Rubensson, J. Lüning, M. Neeb, B. Küpper, S. Eisebitt and W. Eberhardt, Phys. Rev. Lett. 76 (1996) 3919. ( $N_2 - N1s$ )
- RL&97** J.E. Rubensson, J. Lüning, S. Eisebitt and W. Eberhardt, Appl. Phys. A 65 (1997) 91. ( $Ne1s$ )
- RM79** R.F. Reilman and S.T. Manson, Astrophysical J. Suppl. Ser. 40 (1979) 815. (PA X-sections for  $Z < 31$  from 5-5,000 eV)
- RM&89a** M. Richter, M. Meyer, M. Pahler, T. Prescher, E. von Raven, B. Sonntag and H.E. Wetzel, Phys. Rev. A 39 (1989) 5666. ( $Ba4d, La4d, Ce4d$ )
- RM&89b** M. Richter, M. Meyer, M. Pahler, T. Prescher, E. von Raven, B. Sonntag and H.E. Wetzel, Phys. Rev. A 40 (1989) 7007. (Ba to Tb 4d)
- RN&93** J.E. Rubensson, M. Neeb, M. Biermann, Z. Xu and W. Eberhardt, J. Chem. Phys. 99 (1993) 1633. ( $N_2 - N1s$ )
- RN&96** J.E. Rubensson, M. Neeb, A. Bringer, M. Biermann and W. Eberhardt, Chem. Phys. Lett. 257 (1996) 447. ( $Ne1s$ )
- RO79** T.N. Rescigno and A.E. Orel, J. Chem. Phys. 70 (1979) 3390. ( $N_2-N1s$ ).
- RO85** T.N. Rescigno and A.E. Orel, Lect. Notes in Chem. 35 (1985) 215. ( $N_2, NO, N_2O - N1s$ )
- RO&03** T. Richter, B. Obst, M. Martins and P. Zimmermann, J. Phys. B 36 (2003) 155. ( $Sc2p$ )
- RRM84** F.A. Rajgara, A. Roy and D. Mathur, Indian J. Phys. B 57 (1983) 32. ( $N_2-N1s$ )
- RRW74** P. Rabe, K. Radler and H.W. Wolff, Proc. 4th Int. Vac. UV Rad. Phys. Conf. (Hamburg, 1974) 169. ( $Ba4d$ )
- RR&83** R.A. Rosenberg, V. Rehn, A.K. Green, P.R. LaRoe and C.C. Parks, Desorption Induced by Electronic Transitions I (1983). ( $N_2, NH_3 - N1s, D_2O - O1s$ )
- RR&12** N. Rohringer, D. Ryan, R.A. London, M. Purvis, F. Albert, J. Dunn, J.D. Bozek, C. Bostedt, A. Graf, R. Hill, S.P. Hau-Riege and J.J. Rocca, Nature 481 (2012) 488. ( $Ne1s$ )
- RS74** K. Radler and B. Sonntag, Proc. VUV-4 (Hamburg, 1974) 104. ( $LiCl - Li1s$ )

- RS76** K. Radler and B. Sonntag, Chem. Phys. Lett. 39 (1976) 371. (CsCl - Cs4d)
- RSH93** M.L.M. Rocco, G.G.B. de Souza and A.P. Hitchcock, (1993) unpublished. ( $C_{32}H_{16}N_8$ ,  $C_{32}H_{16}N_8Fe$ ,  $C_{32}H_{16}N_8Ni$ ,  $C_{32}H_{16}N_8Zn$  - C1s;  $C_{32}H_{16}N_8Ni$  - N1s)
- RSW76** K. Radler, B. Sonntag and H.W. Wolff, Proc. Int. Conf. on X-ray Spectra (Washington, 1976) 54. (NaCl - Na2p)
- RS&76** K. Radler, B. Sonntag, T.C. Chang and W.H.E. Schwarz, Chem. Phys. 13 (1976) 365. (LiF, LiCl - Li1s)
- RS&86** A. Reimer, J. Schirmer, J. Feldhaus, A.M. Bradshaw, U. Becker, H.G. Kerkhoff, B. Langer, D. Szostak and R. Wehlitz, Phys. Rev. Lett. 57 (1986) 1707 (CO-C1s).
- RS&89** M. Rosi, A. Sgamellotti, F. Tarantelli, M.M. Gofman, V.A. Andreev and V.I. Nefedov, J. Struct. Chem. 30 (1989) 147 [Zh. Struk. Khimii 30 (1989) 171] ( $CH_xF_{4-x}$ , x=0,4 - C1s)
- RS&91** E. Rühl, C. Schmale, H.W. Jochims, E. Biller, M. Simon and H. Baumgartel, J. Chem. Phys. 95 (1991) 6544 (Ar, Ar<sub>n</sub> - Ar2p)
- RS&92a** E. Rühl, C. Schmale, H.W. Jochims, E. Biller, R. Locht, A.P. Hitchcock and H. Baumgartel, AIP Conf. Proc. 258 (1992) 230. (Ar<sub>n</sub> - Ar2p; (CO)<sub>n</sub> - C1s, O1s)
- RS&92b** E. Rühl, C. Schmale, H. Baumgartel and A.P. Hitchcock, (1992) unpublished (( $C_2H_4$ )<sub>n</sub> - C1s; (O<sub>2</sub>)<sub>n</sub> - O1s)
- RUH95** E. Rühl, S.G. Urquhart and A.P. Hitchcock, unpublished. ( $C_6H_{12}N_2$  - C1s, N1s)
- RWH91** E.Rühl, A.T. Wen and A.P. Hitchcock, J. Electron Spectrosc. 57 (1991) 137. (CoCp<sub>2</sub>,  $C_5H_6$ ,  $C_5H_8$ ,  $C_{10}H_{12}$  - C1s; Co<sub>2</sub>(CO)<sub>8</sub>, CpCo(CO)<sub>2</sub> - C1s, O1s)
- RW&90a** R.A. Rosenberg, C.R. Wen, K. Tan and J.M. Chen, J. Chem. Phys. 92 (1990) 5196. (SiF<sub>4</sub> - Si2p)
- RW&90b** R.A. Rosenberg, C.R. Wen, K. Tan and J.M. Chen, Phys. Scripta 41 (1990) 475. (SiCl<sub>4</sub> - Si2p)
- RW&90c** R.A. Rosenberg, C.R. Wen, K. Tan and J.M. Chen, DIET IV, Spring. Ser. Surf. Sci. 19 (1990) 97. (SiF<sub>4</sub>, SiCl<sub>4</sub> - Si2p)
- RW&95** F. Raski, K.R. Wilson, Z. Jiang, A. Ikhlef, C.Y. Coté and J.C. Keiffer, SPIE Vol. 2523 (1995). (SF<sub>6</sub> - S1s)
- RW&96** F. Raski, K.R. Wilson, Z. Jiang, A. Ikhlef, C.Y. Coté and J.C. Keiffer, J. Chem. Phys. 104 (1996) 6066. (SF<sub>6</sub> - S1s)
- RY&92** E.G. Rightor, G.P. Young, S.G. Urquhart, A.T. Wen and A.P. Hitchcock, Microscopy: The Key Research Tool 22 (1992) 67. ( $C_6H_6$  - C1s;  $C_7H_6O$ ,  $C_8H_6O_2$ ,  $C_9H_{10}O_2$  - C1s, O1s; COCl<sub>2</sub>,  $C_8H_{14}O_2Cl_2$  - C1s, O1s, Cl2p)
- S36** S.T. Stephenson, Phys. Rev. 50 (1936) 790. (Br<sub>2</sub>-Br1s)
- S40** C.H. Shaw, Phys. Rev. 57 (1940) 877. (HBr, Br<sub>2</sub> - Br1s)
- S63** H.W. Schnopper, Phys. Rev. 131 (1963) 2559. (Ar1s)
- S66** J.A.R. Samson, Adv. Atom. Mol. Phys. 2 (1966) 178. (review of atomic photoionization cross-sections; Ar2p,

Kr3d, Xe4d)

- S74** W.H.E. Schwarz, Angew. Chem. Int. Ed. Engl. 13 (1974) 454. (theory, review, data summary to 1973; CO-O1s; HCl-Cl2p; XeF<sub>2</sub>-Xe4d)
- S75a** W.H.E. Schwarz, Chem. Phys. 9 (1975) 157. (HCl, H<sub>2</sub>S, PH<sub>3</sub>, SiH<sub>4</sub>)
- S75b** W.H.E. Schwarz, Chem. Phys. 11 (1975) 217. (HCl-Cl2p, H<sub>2</sub>S-S2p, PH<sub>3</sub>-P2p, SiH<sub>4</sub>-Si2p, CH<sub>4</sub>-C1s, H<sub>2</sub>O-O1s, NH<sub>3</sub>-N1s)
- S76a** W.H.E. Schwarz, Chem. Phys. 13 (1976) 153. (HCl-Cl2p, H<sub>2</sub>S-S2p, NH<sub>3</sub>-N1s, SiH<sub>4</sub>-Si2p)
- S76b** M.E. Schwartz, Chem. Phys. Lett. 40 (1976) 1. (NH<sub>3</sub>-N1s)
- S80a** V. Schmidt, Appl. Optics 19 (1980) 4080. (Xe4d, N<sub>2</sub>-N1s)
- S80b** A.F. Starace, Appl. Optics 19 (1980) 4051. (review, Xe4d)
- S82a** G. O'Sullivan, J. Phys. B 15 (1982) L327. (CH<sub>3</sub>I - I4d)
- S82b** G. O'Sullivan, J. Phys. B 15 (1982) 2385. (CCl<sub>4</sub>,CCl<sub>2</sub>F<sub>2</sub>-Cl2p)
- S85** N. Spector, Optica Pura Y Applicada 18 (1985) 183. (Li1s, Na1s, Al2p)
- S86** V. Schmidt, Com. At. Mol. Phys. 17 (1985) 1. (Mn3p,Mn3d)
- S87** B. Sonntag, J. Phys. 48 (1987) C9-439. (U5d, Li1s)
- S90a** H.P. Saha, Phys. Rev. A 42 (1990) 6507. (Ar1s)
- S90b** N. Saito, Research of the Electrotechnical Laboratory, No. 910 (1990) 88 page review. (N<sub>2</sub> - N1s; NO, O<sub>2</sub> - N1s, O1s)
- S91a** B.F. Sonntag, Phys. Scripta T 34 (1991) 93. (Ar2p, Li1s)
- S91b** E. Shigemasa, Photon Factory Ann. Rep. (1991) intro. (SiF<sub>4</sub> - Si2p)
- S92** J. Stöhr, *NEXAFS Spectroscopy*, Spr. Ser. Surf. Sci. (Heidelberg, 1992). (Review; N1s, Ar1s, NH<sub>3</sub>, N<sub>2</sub>H<sub>4</sub> - N1s; O<sub>2</sub>, CO, CO<sub>2</sub>, H<sub>2</sub>CO, CH<sub>3</sub>OH - C1s, O1s; H<sub>2</sub>O - O1s; HF, F<sub>2</sub> - F1s; CH<sub>4</sub>, C<sub>2</sub>H<sub>n</sub>, n=2,4,6; CH<sub>3</sub>NH<sub>2</sub>, CH<sub>3</sub>CN, CH<sub>3</sub>F, C<sub>3</sub>H<sub>4</sub>, C<sub>3</sub>H<sub>6</sub>, c-C<sub>3</sub>H<sub>8</sub>, C<sub>3</sub>H<sub>8</sub>, C<sub>4</sub>H<sub>6</sub>,C<sub>4</sub>H<sub>8</sub>, C<sub>5</sub>H<sub>10</sub>, C<sub>6</sub>H<sub>6</sub>, C<sub>6</sub>H<sub>12</sub> C<sub>2</sub>H<sub>x</sub>F<sub>4-x</sub> - C1s)
- Sc92** V. Schmidt, Rep. Prog. Phys. 55 (1992) 1483. (Ar2p, Ar1s, Kr3d, Kr2p, Kr1s, Xe4d, Xe3d, Xe1s - review)
- S94** S. Sekine, Bull. Electrotech. Lab. 58 (1994) 21. (CO - C1s, O1s; N<sub>2</sub>-N1s)
- S95** E. Shigemasa, Nucl. Inst. Meth. B 99 (1995) 132. (N<sub>2</sub> - N1s)
- S98** E. Shigemasa, J. Electron Spectrosc. 88-91 (1998) 9. (CO - C1s, N<sub>2</sub> - N1s, CO<sub>2</sub> - O1s)
- S09** S.L. Sorensen, Eur. Phys. J. Spec. Top. 169 (2009) 79. (C<sub>2</sub>H<sub>2</sub>-C1s; O<sub>3</sub>, SO<sub>2</sub> – O 1s)
- SA93** S. Svennson and H. Agren, Chem. Phys. Lett. 205 (1993) 387. (SF<sub>6</sub> - F1s)

- SA97** S. Svensson and A. Ausmees, App.Phys. 65 (1997) 107. (Kr3d; HCl-Cl2p; H<sub>2</sub>S-S2p; CO-C1s)
- SAA95** S. Svensson, H. Aksela and S. Aksela, J. Electron Spectrosc. 75 (1995) 67. (CO - C1s)
- SAV87** V.N. Sivkov, V.N. Akimov and A.S. Vinogradov, Opt. Spectr. 63 (1987) 162 [Opt. Spekt. 63 (1987) 275]. (CO<sub>2</sub>-C1s,O1s; CH<sub>4</sub>, CF<sub>4</sub> - C1s)
- SA&84** V.N. Sivkov, V.N. Akimov, A.S. Vinogradov and T.M. Zimkina. Opt. Spectr. 57 (1984) 160 [Opt. Spekt. 57 (1984) 265]. (CO<sub>2</sub>-C1s,O1s)
- SA&86a** G. Stefani, L .Avaldi, A. Lahman-Bennani and A. Duguet, J. Phys. B 19 (1986) 3767. (Ar2p)
- SA&86b** V.N. Sivkov, V.N. Akimov, A.S. Vinogradov and T.M. Zimkina, Opt. Spectrosc. (USSR) 60 (1986) 194; [Opt. Spekt. 60 (1986) 318] (CH<sub>4</sub>-C1s; CF<sub>4</sub> - C1s,F1s)
- SA&95a** S. Svensson, H. Aksela, A. Kivimaki, O.-P. Sairanen, A. Ausmees, S.J. Osborne, A. Naves de Brito, E. Nömmiste, G. Bray and S. Aksela, J. Phys. B 28 (1995) L325. (H<sub>2</sub>S - S2p)
- SA&95b** O.-P. Sairanen, H. Aksela, S. Aksela, J. Mursu, A. Kivimaki, A. Naves de Brito, E. Nömmiste, S.J. Osborne, A. Ausmees, and S. Svensson, J. Phys. B 28 (1995) 4509. (Xe4d)
- SA&95c** E. Shigemasa, J. Adachi, M Oura and A. Yagashita, Phys. Rev. Lett. 74 (1995) 359. (N<sub>2</sub> – N1s)
- SA&97** S. Sundin, A. Ausmees, S.L. Sorensen, O. Bjorneholm, I. Hjelte and S. Svensson, J. Phys. B 30 (1997) L851. (CO - C1s)
- SA&98a** E. Shigemasa, J. Adachi, K. Soejima, N. Watanabe, A. Yagashita and N.S. Cherepkov, Phys. Rev. Lett. 80 (1998) 1622. (CO - C1s)
- SA&98b** S. Sundin, A. Ausmees, O. Bjorneholm, S.L. Sorensen, M. Wiklund, A. Kikas and S. Svensson, Phys. Rev. A 58 (1998) 2037. (CO - C1s)
- SA&98c** S.L. Sorensen, A. Ausmees et al. MaxLab report (1998) 196. (O<sub>2</sub> – O1s)
- SA&99** C.D. Schroter, L. Avaldi, R. Camilloni, G. Stefani, M. Zitnik and M. Stuhek, J. Phys. B 32 (1999) 171. (Ne1s)
- SA&01** R. Sankari, A. Kivimäki, M. Huttula, H. Aksela, S. Aksela, M. Coreno, G. Turri, R. Camilloni, M. de Simone, and K. C. Prince, Phys. Rev. A 63 (2001). (Ar3d)
- SA&05** A. Sankari, S. Alitalo, S. Fritzsche, J. Nikkinen, A. Kivimaki, S. Aksela and H. Aksela, MAX Lab 2005-2006 Annual report. (2006) 250. (Kr3d)
- SB76** W.H.E. Schwarz and R.J. Buenker, Chem. Phys. 13 (1976) 153. (N<sub>2</sub>O, CO<sub>2</sub>)
- SB84** R.N.S. Sodhi and C.E. Brion, J. Electron Spect. 34 (1984) 363. (N<sub>2</sub>-N1s, SF<sub>6</sub>-S2p, F1s, CO-C1s,O1s, Ar2p, Ne1s)
- SB85a** R.N.S Sodhi and C.E. Brion, J. Electron Spect. 37 (1985) 1. (C<sub>3</sub>H<sub>4</sub>, C<sub>4</sub>H<sub>6</sub> - C1s)
- SB85b** R.N.S Sodhi and C.E. Brion, J. Electron Spect. 36 (1985) 187. (CH<sub>3</sub>)<sub>x</sub>NH<sub>3-x</sub>, x=0-3 - C1s,N1s)

- SB85c** R.N.S Sodhi and C.E. Brion, J. Electron Spect. 37 (1985) 97. (PH<sub>3</sub>, P(CH<sub>3</sub>)<sub>3</sub>, PF<sub>3</sub>, PCl<sub>3</sub> - P2p,P2s,F1s,C1s,Cl2p,Cl2s)
- SB85d** R.N.S Sodhi and C.E. Brion, J. Electron Spect. 37 (1985) 125. (PF<sub>5</sub>, POF<sub>3</sub>, OPtCl<sub>3</sub> - P2p,P2s,F1s,O1s,Cl2p,Cl2s)
- SB89** K.H. Sze and C.E. Brion, Chem. Phys. 137 (1989) 353. (ClF<sub>3</sub> - Cl2p,2s, F1s)
- SB90** K.H. Sze and C.E. Brion, Chem. Phys. 140 (1990) 439. (TeF<sub>6</sub> - F1s, Te3p, Te3d, Te4s, Te4p, Te4d; SeF<sub>6</sub> - F1s, Se3s, Se3p, Se3d; SF<sub>6</sub> - S2p, S2s, F1s) (*Erratum* Chem. Phys. 147 (1990) 219)
- SB91a** K.H. Sze and C.E. Brion, J. El. Spect. 57 (1991) 117. (C<sub>3</sub>H<sub>6</sub> - C1s; C<sub>2</sub>H<sub>4</sub>O - C1s, O1s)
- SB91b** J. Stöhr and K. Bauschspeiss, Phys. Rev. Lett. 67 (1991) 3376. (N<sub>2</sub> - N1s, O<sub>2</sub> - O1s)
- SBB68** A.P. Sadovskii, V.M. Bertenev and S.M. Blokhin, Theor. Exp. Chem. 4 (1968) 342 [Teor. i Eksp. Khim. 4 (1968) 533]. (Cl<sub>2</sub>, HCl, CHCl<sub>3</sub>, CCl<sub>4</sub> -Cl1s, Ar1s)
- SBC84** R.N.S. Sodhi, C.E. Brion and R.G. Cavell, J. Electron Spect. 34 (1984) 373. (NF<sub>3</sub>-N1s, F1s)
- SBK89** K.H. Sze, C.E. Brion and A. Katrib, Chem. Phys. 132 (1989) 271. (C<sub>2</sub>FH<sub>3</sub> -C1s,F1s; C<sub>2</sub>ClH<sub>3</sub> - C1s,Cl2p,2s; C<sub>2</sub>BrH<sub>3</sub> - C1s,Br3d,Br3p; C<sub>2</sub>IH<sub>3</sub> - C1s,I4d)
- SBM90** J. Schirmer, M. Braunstein and V. McKoy, Phys. Rev. A 41 (1990) 283. (CO - C1s,O1s)
- SBM91** J. Schirmer, M. Braunstein and V. McKoy, Phys. Rev. A 44 (1991) 5762. (CO - C1s)
- SBS94a** I.H. Suzuki, J.D. Bozek and N. Saito, Chem. Phys. 182 (1994) 81. (CF<sub>2</sub>Cl<sub>2</sub> - C1s, Cl2p, F1s)
- SBS94b** I.H. Suzuki, J.D. Bozek and N. Saito, Chem. Phys. 188 (1994) 367. (CF<sub>4</sub> - C1s, F1s)
- SBS95** N. Sato, J.D. Bozek and I.H. Suzuki, J. Phys. B 28 (1995) 3505. (CF<sub>4</sub> - C1s, F1s)
- SBT88** J. Schirmer, A. Barth and F. Tarantelli, Chem. Phys. 122 (1988) 9. (H<sub>2</sub>CO-C1s, O1s)
- SB&78** W.H.E. Schwarz, W. Butscher, D.L. Ederer, T.B. Lucarto, B. Ziegenbein, W. Mehlhorn and H. Prompeler, J. Phys. B 11 (1978) 591. (Li,Li<sub>2</sub>-Li1s)
- SB&83** S. Southworth, U. Becker, C.M. Truesdale, P.H. Kobrin, D.W. Lindle, S. Owaki and D.A. Shirley, Phys. Rev. A 28 (1983) 261. (Xe4d)
- SB&87** K.H. Sze, C.E. Brion, X.M. Tong and J.M. Li, Chem. Phys. 115 (1987) 433. (SO<sub>2</sub> - S2p,S2s, O1s)
- SB&88** K.H. Sze, C.E. Brion, M. Tronc, S. Bodeur and A.P. Hitchcock, Chem. Phys. 121 (1988) 279. ((CH<sub>3</sub>)<sub>2</sub>S=O - C1s,S2p,O1s,S1s)
- SB&91** B.K. Sorpal, C. Biancard, J.P. Connerade, J.M. Esteva, J. Hormes, R.C. Karnataka and U. Kuettgens, J. Phys. B 24 (1991) 1593. (Sm3d, Tm3d)
- SB&92** D.G.L. Sutherland, G.M. Bancroft, J.D. Bozek and K.H. Tan, Chem. Phys. Lett. 199 (1992) 341. (SiH<sub>4</sub>, SiD<sub>4</sub>, Si<sub>2</sub>H<sub>6</sub>, Si<sub>3</sub>H<sub>8</sub> - Si2p)

- SB&96** J. Schirmer, M.Braunstein, M.T. Lee and V. McKoy, "Core Relaxation Effects in Molecular Photoionization" in VUV and Soft X-ray Photoionization, U. Becker and D.A. Shirley, eds. (Plenum, NY, 1996) 105. (CO, H<sub>2</sub>CO, C<sub>2</sub>H<sub>4</sub> - C1s)
- SB&02** G.G.B. de Souza, H.M. Boechat-Roberty, M.L.M. Rocco and C.A. Lucas, *J. El. Spec.* 123 (2002) 315. (C<sub>10</sub>H<sub>8</sub> – C1s)
- SC76** W.H.E. Schwarz and T.C. Chang, *Int. J. Quant. Chem.* 10 (1976) 91. (LiF,Li<sub>2</sub> - Li1s)
- SC82** E.C. Sewell and A. Crowe, *J. Phys. B* 15 (1982) L357. (Ar2p)
- SC84** E.C. Sewell and A. Crowe, *J. Phys. B* 17 (1984) 2913, L547. (Ar2p)
- SC95** H.D. Schulte and L.S. Cederbaum, *J. Chem. Phys.* 103 (1995) 698. (C<sub>3</sub>H<sub>3</sub><sup>+</sup> - C1s; B<sub>3</sub>N<sub>3</sub>H<sub>6</sub> - B1s, N1s)
- SC02** S. K. Semenov and N. A. Cherepkov, *Phys. Rev. A* 66 (2002) 022708. (N<sub>2</sub> – N1s)
- SCC77** W.H.E. Schwarz, T.C. Chang and J.P. Connerade, *Chem. Phys. Lett.* 49 (1977) 207. (NO<sub>2</sub> - N1s,O1s)
- SCT96** H.D. Schutte, L.S. Cederbaum and F. Tarantelli, *J. Chem. Phys.* 105 (1996) 11106. (N<sub>2</sub> – N1s; CO, H<sub>2</sub>CO – C1s, O1s)
- SC&84** D.A. Shaw, D. Cvejanovic, G.C. King and F.H. Read, *J. Phys. B* 17 (1984) 1173. (HBr,Br<sub>2</sub> - Br3d; HCl - Cl2p)
- SC&87** W.H.E. Schwarz, T.C. Chang, U. Seeger and K.H. Huang, *Chem. Phys.* 117 (1987) 73. (C<sub>6</sub>H<sub>6</sub>, C<sub>6</sub>H<sub>5</sub>F - C1s)
- SC&93** S.J. Schaphorst, C.D. Caldwell, M. O. Krause and J. Jimenez-Mier, *Chem. Phys. Lett.* 213 (1993) 315. (O<sub>2</sub>- O1s)
- SC&02** M de Simone, M Coreno, M Alagia, R Richter and K C Prince, *J. Phys. B* 35 (2002) 61. (CCl<sub>4</sub>,CF<sub>4</sub>,CH<sub>4</sub> – C1s)
- SC&05** S.K. Semenov, N.A. Cherepkov, A. De Fanis, Y. Tamenori, M. Kitajima, H. Tanaka, K. Ueda, *J. el. Spec.* 144-147 (2005) 211. (CO – O1s)
- SD89** N. Shanthi and P.C. Deshmukh, *Phys. Rev. A* 40 (1989) 2400 (Xe4p)
- SDD81** J.R. Swanson, D. Dill and J.L. Dehmer, *J. Chem. Phys.* 75 (1981) 619. (BF<sub>3</sub>-B1s,F1s)
- SDD86** J.A. Stephens, D. Dill and J.L. Dehmer, *J. Chem. Phys.* 84 (1986) 3638. (CF<sub>4</sub>-C1s, F1s)
- SDM88** N. Shanthi, P.C. Deshmukh and S.T. Manson, *Phys. Rev. A* 37 (1988) 1773, 4720. (Kr3p,Kr3d)
- SDT92** A. Sevin, C. Dezarnaud-Dandine and M. Tronc, *Chem. Phys.* 165 (1992) 245 (CH<sub>3</sub>SH - S1s)
- SD&83** V.L. Sukhorukov, V.E. Demekhin, V.A. Yavna, I. Dudenko and V.V. Timoshevskaya, *Opt. Spectrosc.* 55 (1983) 135. [Opt. Spektrosk. 55 (1983) 229] (Ar2p)
- SD&84** R.N.S. Sodhi, S. Davel, C.E. Brion and G.G.B. de Souza, *Ann. Israel. Phys. Soc.* 6 (1984) 200. ((CH<sub>3</sub>)<sub>4</sub>Si-Si2p,C1s)

- SD&85** R.N.S. Sodhi, S. Daviel, C.E. Brion and G.G.B. de Souza, J. Electron Spectr. 35 (1985) 45.  
((CH<sub>3</sub>)<sub>4</sub>Si-Si2p,C1s)
- SD&79** V.L. Sukhorukov, V.F. Demekhin, V.V. Timoshevskaya and S.V. Lavrentev, Opt. Spectrosc USSR 47 (1979) 228 [Opt. i Spek. 47 (1979) 407] (Ne1s, Ar1s)
- SD&12** M Stener, P Decleva, J Adachi, N Miyauchi, M Yamazaki and A Yagishita, j. Phys. B 45 (2012) 194004.  
(H<sub>2</sub>CO – O1s)
- SD&20** Lucas Schwob, Simon Dorner, Kaan Atak, Kaja Schubert, Martin Timm, Christine Bulow, Vicente Zamudio-Bayer, Bernd von Issendorff, J. Tobias Lau, Simone Techert, and Sadia Bari, Site-Selective Dissociation upon Sulfur L-Edge X-ray Absorption in a Gas-Phase Protonated Peptide, J. Phys. Chem. Lett. 11 (2020) 1215.
- SE&13** I. H. Suzuki, H. Endo, K. Nagai, O. Takahashi, Y. Tamenori and S. Nagaoka, J. Chem. Phys. 139 (2013) 174314 (C<sub>3</sub>Cl<sub>3</sub>H<sub>9</sub>Si<sub>2</sub> – Si1s)
- SF&90** D. Sondericker, Z. Fu, J. Bradley and W. Eberhardt, J. Chem. Phys. 92 (1990) 2203. (Ru<sub>3</sub>(CO)<sub>12</sub> - C1s,O1s)
- SF&95** P. Sladeczak, H. Feist, M. Feldt, M. Martins and P. Zimmermann, Phys. Rev. Lett. 75 (1995) 1483. (W5p, W4f)
- SF&99** S.L. Sorensen, R. Fink, A. Naves de Brito, A. Ausmees and S. Svensson, J. El. Spec.c 101-103 (1999) 75.  
(C<sub>2</sub> H<sub>2</sub> – C1s)
- SF&01** S.L. Sorensen, R. Fink, R. Feifel, M.N. Piancastelli, M. Bässler, C. Miron, H. Wang, I. Hjelte, O. Björneholm, and S. Svensson, Phys. Rev. A 64 (2002) 012719. (O<sub>2</sub> – O1s)
- SF&03** N Saito, A De Fanis, K Kubozuka, M Machida, M Takahashi, H Yoshida, I H Suzuki, A Cassimi, A Czasch, L Schmidt, R Dörner, K Wang, B Zimmermann, V McKoy, I Koyano and K Ueda, J. Phys. B 36 (2003) L25.  
(CO<sub>2</sub>- C1s)
- SF&05** N. Saito, A. De Fanis, I. Koyano and K. Ueda, J. El. Spec. 144-147 (2005) 103. (Ar<sub>2</sub>-Ar2p, HCCH-C1s, NO<sub>2</sub>-N1s)
- SG82** A. Shah and S.J. Gurman, X-ray Spectrometry, 11 (1982) 2. (O1s)
- SG&89** J.A. Sheehy, T.J. Gil, C.L. Winstead, R.E. Farren and P.W. Langhoff, J. Chem. Phys. 91 (1989) 1796. (NO, N<sub>2</sub>O, HCN, N<sub>2</sub> - N1s; HCN, H<sub>2</sub>CO, CO, CO<sub>2</sub>, C<sub>2</sub>, C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>4</sub>, C<sub>2</sub>H<sub>6</sub>, C<sub>2</sub>N<sub>2</sub> -C1s; F<sub>2</sub> - F1s; O<sub>2</sub>, H<sub>2</sub>CO, CO, CO<sub>2</sub>, NO, N<sub>2</sub>O - O1s)
- SG&95a** H.C. Schmelz, M.A. Gaveau, C. Reynaud, C. Heinzel, H. Baumgartel and E. Rühl, Physica B 208 (1995) 519. (Kr, Kr<sub>n</sub> - Kr2p)
- SG&95b** P. Skytt, J. Guo, N. Wassdahl, J. Nordgren, Y. Luo and H. Agren, Phys. Rev. A 52 (1995) 3572. (C<sub>6</sub>H<sub>6</sub> - C1s)
- SG&96a** P. Skytt, P. Glans, K. Gunnelin, J.H. Guo, J. Nordgren and H. Agren, Skytt's Ph.D thesis (Uppsala, 1996)  
(CO<sub>2</sub> - O1s)
- SG&96b** P. Skytt, P. Glans, K. Gunnelin, J.H. Guo, C. Sathe, F.Kh. Gel'mukhanov, A. Cesar and H. Agren, Phys. Rev. Lett. 77 (1996) 5035. (CO<sub>2</sub> - O1s)

- SG&97a** P. Skytt, P. Glans, K. Gunnelin, J.H. Guo, J. Nordgren, Y. Luo and H. Agren, Phys. Rev. A 55 (1997) 134. (CO -C1s,O1s)
- SG&97b** P. Skytt, P. Glans, K. Gunnelin, J.H. Guo and J. Nordgren, Phys. Rev. A 55 (1997) 146. (CO -C1s,O1s)
- SG&97c** S. Sundin, F.Kh. Gel'mukhanov, H. Agren, S.J. Osborne, A. Kikas, O. Bjorneholm, A. Ausmees and S. Svensson, Phys. Rev. Lett. 79 (1997) 1451. (CO - C1s)
- SG&97d** S. Sundin, F.Kh. Gel'mukhanov, S.J. Osborne, O. Bjorneholm, A. Ausmees, S.L. Sorensen, A. Naves de Brito, R.R.T. Marinho, S. Svensson and H. Agren, J. Phys. B 30 (1997) 4267. (CO - C1s)
- SG&02** E. Shigemasa, T. Gejo, T. Hatsui and N. Kosugi, UVSOR Ann Rep 2002. 208. (Cl<sub>2</sub> - Cl2p)
- SG&05** Y. Senba, T. Goya, H. Yoshida, A. Hiraya, J. El. Spec. 144-147 (2005) 195. (NH<sub>3</sub>-N1s)
- SG&19** Kaja Schubert, Alexander A. Guda, et al., Absorption spectra at the iodine 3d ionisation threshold following the CH<sub>x</sub>I<sup>+</sup> (x = 0–3) cation sequence, Phys.Chem.Chem.Phys. 21 (2019) 25415. CH<sub>x</sub>I<sup>+</sup> (x = 0–3) I 3d
- SG&20** Kaja Schubert, Meiyuan Guo, et al., The electronic structure and deexcitation pathways of an isolated metalloporphyrin ion resolved by metal L-edge spectroscopy Chem. Sci., 12 (2021) 3966. (C<sub>32</sub>H<sub>28</sub>Co<sup>+</sup> - Co2p)
- SHU11** Shirin Behyan, Yongfeng Hu and Stephen G. Urquhart, Sulfur 1 s near-edge x-ray absorption fine structure (NEXAFS) of thiol and thioether compounds, J. Chem. Phys. 134 (2011) 244304 (CH<sub>3</sub>SH, C<sub>2</sub>H<sub>5</sub>SH, C<sub>2</sub>H<sub>6</sub>S, C<sub>4</sub>H<sub>8</sub>S, C<sub>5</sub>H<sub>11</sub>NOS, C<sub>6</sub>H<sub>5</sub>SH – S1s)
- SH&85** Y. Sato, T. Hayaishi, Y. Itikawa, Y. Itoh, J. Murakami, T. Nagata, T. Sasaki, B. Sonntag, A. Yagashita and M. Yoshino, J.Phys. B 18 (1985) 225 (Ca3p)
- SH&91** A. Svensson, E.A. Hughes, A. Banichevich, S.D. Peyerimhoff and B.A. Hess, J. Phys. B 24 (1991) 2997. (HBr - Br3d)
- SH&93** E. Shigemasa, T. Hayaishi, T. Sasaki and A. Yagashita, Phys. Rev. A 47 (1993) 1824. (CO - C1s, O1s)
- SH&95** N. Saito, F. Heiser, O. Hemmers, A. Hempelmann, K. Wieliczek, J. Viefhais and U. Becker, Phys. Rev. A 51 (1995) R4313. (CO - C1s, O1s)
- SH&96a** E. Shigemasa, T. Hayaishi, K. Okuno, A. Danjo, K. Ueda, Y. Sato and A. Yagashita, J. Electron Spectrosc. 79 (1996) 495. (SiF<sub>4</sub> - Si2p)
- SH&96b** N. Saito, F. Heiser, O. Hemmers, K. Wieliczek, J. Viefhaus and U. Becker, Phys. Rev. A 54 (1996) 2004. (CO - C1s)
- SH&00** N. Saito, A. Hempelmann, F. Heiser, O. Hemmers, K. Wieliczak, J. Viefhaus and U. Becker, Phys. Rev. A 61 (2000) 022709. (N<sub>2</sub> - N1s, CO – C1s)
- SH&01** Stolte W, Hansen D, Piancastelli M, Dominguez Lopez I, Rizvi A, Hemmers O Anionic photofragmentation of CO: a selective probe of core-level resonances. Phys Rev Lett 86(2001) 4504. (CO-C1s)
- SH&22** S. Schippers, A. Hamann, et al., Multiple photodetachment of oxygen anions via K-shell excitation and ionization: Direct double-detachment processes and subsequent deexcitation cascades, Physical Review A 106,

- SH&23** S. Schippers, P.-M. Hillenbrand et al., Vibrationally Resolved Inner-Shell Photoexcitation of the Molecular Anion C<sub>2</sub><sup>-</sup> ChemPhysChem 24 (2023) e202300061. (C<sub>2</sub> C1s)
- SI&92** A.V. Soldatov, T.S. Ivanchenko, I.E. Shtekhin and A. Bianconi, Sov. Phys. Sol. St. 34 (1992) 1047 (Fiz. Tverd. St. Petersburg 34 (1992) 1961). (Ne1s)
- SI&93** A.V. Soldatov, T.S. Ivanchenko, S. Della Longa and A. Bianconi, Phys. Rev. B 47 (1993) 16155. (Ne1s)
- SI&95** T. Sekiguchi, H. Ikeura, K. Tanaka, K. Obi, N. Ueno and K. Honma, J. Chem. Phys. 102 (1995) 422. (H<sub>2</sub>O - O1s)
- SI&96** M. Sano, Y. Itoh, T. Koizumi, T.M. Kojima, S.D. Kravis, M. Oura, T. Sekioka, N. Watanabe, Y. Awaya and F. Koike, J. Phys. B 29 (1996) 5305. (Xe4d)
- SKN51** R. Stephenson, J. Krogstad and F.R. Nelson, Phys. Rev. 84 (1951) 806. (Cl<sub>2</sub> - Cl1s)
- SKR80** D.A. Shaw, G.C. King and F.H. Read, J. Phys. B 13 (1980) L723. (Cl<sub>2</sub> - Cl2p)
- SKR86** D.A. Shaw, G.C. King and F.H. Read, Chem. Phys. Lett. 129 (1986) 17. (CO<sub>2</sub> - C1s, N<sub>2</sub>O-N1s; Kr3d, Xe4d)
- SK&82** D.A. Shaw, G.C. King, F.H. Read and D. Cvejanovic, J. Phys. B 15 (1982) 1785. (Ar2p, N<sub>2</sub>-N1s)
- SK&83** D.A. Shaw, G.C. King, F.H. Read, J. Eichler, W. Fritsel, I.V. Hertel, N. Stolterfoht and U. Wille, Proc. 13th ICPEAC (Berlin, 1983) 278. (Kr3d, Xe4d; CO, CO<sub>2</sub>-C1s, N<sub>2</sub>O-N1s)
- SK&84a** D.A. Shaw, G.C. King, D. Cvejanovic and F.H. Read, J. Phys. B 17 (1984) 2091. (CO-C1s)
- SK&84b** D.A. Shirley, P.H. Kobrin, C.M. Truesdale, D.W. Lindle, T.A. Ferrett, P.A. Heimann, U. Becker, H.G. Kerkoff and S.H. Southworth, S.P.I.E. 447 (1984) 150. (CO, CO<sub>2</sub> - C1s)
- SK&90** S. Svensson, L. Karlsson, N. Martensson, P. Baltzer and B. Wannberg, J. Electron Spectrosc. 50 (1990) C1-7. (F1s)
- SK&91** M. Schmidbauer, A.L.D. Kilcoyne, K.J. Randall, J. Feldhaus, A.M. Bradshaw, M. Braunstein and V. McKoy, J. Chem. Phys. 94 (1991) 5299. (N<sub>2</sub>O - N1s, O1s)
- SK&92a** M. Schmidbauer, A.L.D. Kilcoyne, H.M. Koppe, J. Feldhaus and A.M. Bradshaw, Chem. Phys. Lett. 199 (1992) 119. (CO, CO<sub>2</sub> - C1s, O1s)
- SK&92b** E. Shigemasa, T. Koizumi, Y. Itoh, T. Hayaishi, K. Okuno, A. Danjo, Y. Sato and A. Yagshita., Rev. Sci. Inst. 63 (1992) 1505. (SiF<sub>4</sub> - Si2p)
- SK&93a** S.J. Schaphorst, A.F. Kodre, J. Ruscheinski, B. Crasemann, T. Aberg, J. Tulkki, M.H. Chen, Y. Azuma and G.S. Brown, Phys. Rev. A 47 (1993) 1953. (Kr1s)
- SK&93b** D.G. Sutherland, M. Kasrai, G.M. Bancroft, Z.F. Liu and K.H. Tan, Phys. Rev B 48 (1993) 14989. (Si(OCH<sub>3</sub>)<sub>x</sub>(CH<sub>3</sub>)<sub>4-x</sub>, x=0-4 - Si2p, Si1s)
- SK&94** M. Stuhlec, A. Kodre, M. Hribar, D. Glavic-Cindro, I. Arcon and W. Drube, Phys. Rev. A 49 (1994) 3104. (Ar1s)

- SK&95a** M.H. Sayed, E.T. Kennedy, L. Kiernan, J.-P. Mosnier and J.T. Costello, *J. Phys. B* 28 (1995) 1715. (Si2p)
- SK&95b** M. Schmidbauer, A.L.D. Kilcoyne, H.M. Köppe, J. Feldhaus and A.M. Bradshaw, *Phys. Rev. A* 52 (1995) 2095. (CO<sub>2</sub> - C1s, O1s)
- SK&95c** O.P. Sairanen, A. Kivimaki, E. Nommiste, A. Naves de Brito, H. Aksela and S. Aksela, MAX report (1995) 200. (Ar2p, Kr3d, Xe4d)
- SK&96** O.P. Sairanen, A. Kivimaki, E. Nommiste, H. Aksela and S. Aksela, *Phys. Rev. A* 54 (1996) 2834. (Ar2p, Kr3d, Xe4d)
- SK&02** R. Sankari, A. Kivimäki, M. Huttula, T. Matila, H. Aksela, S. Aksela, M. Coreno, G. Turri, R. Camilloni, M. de Simone, and K.C. Prince, *Phys. Rev. A* 65 (2002) 042702. (Ar2s)
- SK&07** E. Shigemasa, T. Kaneyasu, Y. Tamenori and Y. Hikosaka, *J. El. Spec.* 156-158 (2007) 289. (N<sub>2</sub>-N1s)
- SK&10** I. H. Suzuki, Y. Kono, A. Ieda, T. Ouchi, K. Ueda, O. Takahashi, I. Higuchi, Y. Tamenori and S. Nagaoka, *Phys. Rev. A* 82 (2010) 045401. (SiF<sub>4</sub> – Si1s)
- SK&11** I. H. Suzuki, Y. Kono, A. Ieda, T. Ouchi, K. Ueda, O. Takahashi, I. Higuchi, Y. Tamenori and S. Nagaoka, *J. Chem Phys* 134 (2011) 084312. (Si(CH<sub>3</sub>)<sub>4</sub>, SiF<sub>4</sub> – Si1s)
- SK&13a** I. H. Suzuki, Y. Kono, K. Sakai, M. Kimura, K. Ueda, Y. Tamenori, O. Takahashi and S. Nagaoka, *J. Phys B* 46 (2013) 075101. (SiCl<sub>4</sub> – Si1s)
- SK&13b** I. H. Suzuki, Y. Kono, A. Ikeda, M. Oi, T. Ouchi, K. Ueda, Y. Tamenori, O. Takahashi and S. Nagaoka, *J. Chem Phys* 138 (2013) 02430. (SiF<sub>4</sub> – Si1s)
- SK&22a** J. Stierhof , S. Kühn, et al., A new benchmark of soft X-ray transition energies of Ne, CO<sub>2</sub> , and SF<sub>6</sub> : paving a pathway towards ppm accuracy, *Eur. Phys. J. D* 76 (2022) 38 (Ne1s; CO<sub>2</sub> – O1s; SF<sub>6</sub> – F1s)
- SK&22b** Julius Schwarz, Fridtjof Kielgast, et al., X-Ray absorption spectroscopy of H<sub>3</sub>O<sup>+</sup> *Phys. Chem. Chem. Phys.*, 24 (2022) 23119. (H<sub>3</sub>O<sup>+</sup>-O1s)
- SK&22c** Kiyou Shibata, Kakeru Kikumasa, Shin Kiyohara & Teruyasu Mizoguchi, Simulated carbon K edge spectral database of organic molecules *Scientific Data*, 9 (2022) 214. (calc. of 22,155 molecules, <8 non-H atoms)
- SLD95** M. Stener, A. Lisini and P. Decleva, *Chem. Phys.* 191 (1995) 141. (CO, H<sub>2</sub>CO, HFCO, F<sub>2</sub>CO, Cr(CO)<sub>6</sub>, Mo(CO)<sub>6</sub>, Fe(CO)<sub>5</sub>, Mn(CO)<sub>5</sub>Br, Mn(CO)<sub>5</sub>H, Ni(CO)<sub>4</sub>, NiCO, PdCO, PtCO - C1s, O1s)
- SLS97** J.A.R. Samson, Y. Lu and W.C. Stolte, *Phys. Rev. A* 56 (1997) R2530. (Ar2p)
- SLS01** A.C.F. Santos, C.A. Lucas and G.G.B. de Souza, *J. El. Spec.* 114-116 (2001) 115. (SiF<sub>4</sub> – Si2p)
- SLS02** A.C.F. Santos, C.A. Lucas and G.G.B. de Souza, *Chem. Phys.* 282 (2002) 315. (SiF<sub>4</sub> – Si2p)
- SL&91a** S.H. Southworth, D.W. Lindle, R. Meyer and P.L. Cowan, *Phys. Rev. Lett.* 67 (1991) 1098. (CF<sub>3</sub>Cl - Cl1s)
- SL&91b** M. Simon, T.LeBrun, P. Morin, M. Lavallee and J.L. Marechal, *Nucl. Inst. Meth. B* 62 (1991) 167. (N<sub>2</sub>O - N1s)

- SL&92** M. Simon, M. Lavallee, T.LeBrun, J. Delwiche, M.J. Hubin-Franksin and P. Morin, AIP Conf. Proc. 258 (1992) 323. ( $\text{Fe}(\text{CO})_2(\text{NO})_2$  - C1s, N1s)
- SL&93** M. Simon, T. Lebrun, R. Martins, G.G.B. de Souza, I. Nenner, M.Lavallee and P. Morin, J. Phys. Chem. 97 (1993) 5228. ( $\text{Si}_2(\text{CH}_3)_6$  - Si2p)
- SL&94** D.G.J. Sutherland, Z.F. Liu, G.M. Bancroft and K.H. Tan, Nucl. Inst. Meth. B 87 (1994) 183. ( $\text{SiH}_4$ ,  $\text{SiD}_4$ ,  $\text{Si}_2\text{H}_6$  - Si2p)
- SL&96** M. Simon, M. Lavallee, M.Meyer and P. Morin, J. Electron Spectrosc. 79 (1996) 401. ( $\text{N}_2\text{O}$  - N1s)
- SL&97** W.C. Stolte, Y. Lu, J.A.R. Samson, O. Hemmers, D.L. Hansen, S.B. Whitfield, H. Wang, P. Glans and D.W. Lindle, J. Phys. B 30 (1997) 4489. (O1s)
- SL&99** G. Snell, B. Langer, M. Drescher, N. Müller, B. Zimmermann, U. Hergenhahn, J. Viefhaus, U. Heinzmann and U. Becker, Phys. Rev. Lett. 82 (1999) 2480. (Xe4d)
- SL&07** N. Saito, X.J. Liu, Y. Morishita, I.H. Suzuki and K. Ueda, J. El. Spec. 156-158 (2007) 68. (NO-N1s)
- SL&12** S. Sheinerman, P. Lablanquie, F. Penent, Y. Hikosaka, T. Kenayasu, E. Shigemasa and K. Ito,, J. Phys. B 43 (2010) 115001. (Ar2p)
- SMM79** N.A. Shklyaeva, L.N. Mazalov and V.V. Murakhtanov, J. Struct. Chem. 20 (1979) 621 [Zh. Struk. Khim. 20 (1979) 733]. ( $\text{SO}_2$ -S2p)
- SMN85** G.G.B. de Souza, P. Morin and I. Nenner, J. Chem. Phys. 83 (1985) 492, 2035. ( $\text{Si}(\text{CH}_3)_4$ -Si2p)
- SMN86** G.G.B. de Souza, P. Morin and I. Nenner, Phys. Rev. A 34 (1986) 4770. ( $\text{SiH}_4$ -Si2p)
- SMN89** G.G.B. de Souza, P. Morin and I. Nenner, J. Chem. Phys. 90 (1989) 7071. ( $\text{SiF}_4$ -Si2p)
- SMS91** J.L. Solomon, R.J. Madix and J. Stöhr, J. Chem. Phys. 94 (1991) 4012. ( $\text{C}_4\text{H}_4\text{O}$  - C1s)
- SM&70** A.P. Sadovskii, L.N. Mazalov, V.M. Bertenev and V.V. Murakhantianov, Theor. Exp. Chem. 6 (1970) 409 [Teor. i Eksp. Khim. 6 (1970) 502]. ( $\text{Cl}_2$ ,  $\text{HCl}$  - Cl1s)
- SM&78** R. Szargan, A. Meisel, E. Hartmann and G. Brunner, Proc. Int. Conf. X-ray and XUV Spectrosc., Sendai. Jap. J. Appl. Phys. 17 S-2 (1978) 174. ( $\text{SiF}_4$ -Si2p)
- SM&83** W.H.E. Schwarz, L. Mensching, K.H. Hallmeier and R. Szargan, Chem Phys. 82 (1983) 57. ( $\text{BF}_3$ ,  $\text{BF}_4^-$  -B1s;  $\text{CF}_4$  -C1s)
- SM&94** P. Sladeczek, M. Martin, M. Richter, K.H. Selbmann and P. Zimmermann, J. Phys. B 27 (1994) 4123. (Pt4f,Pt5p)
- SM&95** M. Simon, P. Morin, P. Lablanquie, M. Lavollée, K. Ueda and N. Kosugi, Chem. Phys. Lett. 238 (1995) 42. ( $\text{BF}_3$  - B1s)
- SM&96** G. O'Sullivan, C.M. Grunes, J. Costello, E.T. Kennedy and B. Wienwann, Phys. Rev. A 53 (1996) 3227. (I4d)
- SM&97** M. Simon, C. Miron, N. Leclerc, P. Morin, K. Ueda, Y. Sato, S. Tanaka and Y. Kayanuma, Phys. Rev. Lett. 79 (1997) 3857. ( $\text{BF}_3$  - B1s)

- SM&98** P. Selles, J. Mazeau, P. Lablanquie, L. Malegat and A. Huetz, *J. Phys. B* 31 (1998) L353. (Xe4d)
- SM&02a** S W J Scully, R A Mackie, R Browning, K F Dunn and C J Latimer , *J. Phys. B* 35 (2002) 2703. (SF<sub>6</sub> – S2p)
- SM&02b** S. Schippers, A. Müller, S. Ricz, M.E. Bannister, G.H. Dunn, J. Bozek, A.S. Schlachter, G. Hinojosa, C. Cisneros, A. Aguilar, A.M. Covington, M.F. Gharaibeh, R. A. Phaneuf, *Phys. Rev. Lett.* 89 (2002) 193002. (Sc3p)
- SM&04** N. Saito, Y. Muramatsu, H. Chiba, K. Ueda, K. Kubozuka, I. Koyano, K. Okada, O. Jagutzki, A. Czasch, T. Weber, M. Hattass, H. Schmidt-Böcking, R. Moshammer, M. Lavollée, U. Becker, *J. El. Spec. Rel. Phen.* 141 (2004) 183. (CO<sub>2</sub> - C1s, O1s)
- SM&15** Hiroyuki Shimada, Hirotake Minami, et al., *J. Chem. Phys.* 142, (2015) 175102
- SN&84** B. Sonntag, T. Nagata, Y. Sato, Y. Satow, A. Yagishita and M. Yangihara, *J. Phys. B* 17 (1984) L55. (Xe3d, Cs3d, Ba3d)
- SN&86** S.Suzuki, S.Nagaoka, I.Koyano, K. Tanaka and T. Kato, *Z. Phys. D* 4 (1986) 111. (GeCl<sub>4</sub> - Ge3d; Sn(CH<sub>3</sub>)<sub>4</sub> - Sn4d)
- SN&09** I. H. Suzuki, A. Nitta, H. Fukuzawa, K. Ueda, O. Takahashi, Y. Tamenori and S. Nagaoka, *J. Chem Phys* 131 (2009)164309. (F<sub>3</sub>Si(CH<sub>3</sub>)<sub>s</sub>Si(CH<sub>3</sub>)<sub>3</sub> – Si1s)
- SO&87** J. Stöhr, D.A. Outka, K. Baberschke, D. Arvanitis and J.A. Horsley, *Phys. Rev. B* 36 (1987) 2976. (C<sub>3</sub>H<sub>8</sub> - C1s)
- SO&96** S.L. Sorensen, S.J. Osborne, A. Ausmees, A. Kikas, N. Correia, S. Svensson, A. Naves de Brito, P. Persson and S. Lunell, *J. Chem. Phys.* 105 (1996) 10719. (C<sub>4</sub>H<sub>6</sub> - C1s)
- SO&97** S. Sundin, S.J. Osborne, A. Ausmees, O. Bjorneholm, S.L. Sorensen, A. Kikas and S. Svensson, *Phys. Rev. A* 56 (1997) 480. (CO - C1s)
- SO&01** Y. Shimizu, H. Ohashi, Y. Tamenori, Y. Murumatsu, H. Yoshida, K. Okada, N. Saito, H. Tanaka, I. Koyano, S. Shin and K. Ueda, *J. El. Spec.* 114-116 (2001) 63. (Ne1s, CO<sub>2</sub> – C1s,O1s)
- SO&02** W C Stolte, G Öhrwall, M M Sant'Anna, I Dominguez Lopez, L T N Dang, M N Piancastelli and D W Lindle, *J. Phys. B* 35 (2002) L253. (CH<sub>4</sub>O – C1s, O1s)
- SP66** H.W. Schnopper and L.G. Parratt, *Vort. Int. Symp. Rontgenspektron* (Leipzig, 1966) 314. (Ar1s)
- SP&74** V.P. Sachenko, E.V. Polozhentsev, A.P. Kovtun, Yu. F. Migal, R.V. Vedrinski and V.V. Kolesnikov, *Phys. Lett. A* 48 (1974) 169. (SF<sub>6</sub> - S2p)
- SP&00** F.Sirotti, F.Polack, J.L. Cantin, M. Sacchi, R. Delaunay, M. Meyer and M. Liberati, *J. Synch. Rad.* 7 (2000) 5. (Ar2p, Ne1s, N<sub>2</sub> – N1s)
- SRA02** S. Stranges, R. Richter, and M. Alagia, *J. Chem. Phys.* 116 (2002) 3679. (OD, OH – O1s)
- SR&94** H.C. Schmelz, C. Reynaud, M. Simon and I. Nenner, *J. Chem. Phys.* 101 (1994) 3742. (Br(CH<sub>2</sub>)<sub>n</sub>Cl, n=1-3, Br3d, Cl2p)

- SR&95** I. Song, B. Rickett, P. Janavicus, J.H. Payer and M.R. Antonio, Nucl. Inst. Meth. A 360 (1995) 634. ( $\text{SO}_2$  - S1s)
- SR&00** M. Stankiewicz, J. Ruis I Riu et al, MaxLab (2000) 184. ( $\text{N}_2$  - N1s)
- SR&02** M. Stankiewicz, J. Ruis I Riu, P. Winiarczyk, J. Alvarez Ruiz, P. Erman, P.A. Hatherly, M. Huttula, A. Karawajczyk, E. Kukk and E. Rachlew-Kallne, Surf. Rev. Lett. 9 (2002) 117. ( $\text{CD}_4$ - C1s,  $\text{SF}_6$  - S2p)
- SR&04** M Stankiewicz, J Rius i Riu, J Álvarez Ruiz, P Erman, P Hatherly, A Kivimäki, E Melero García and E Rachlew, J. El. Spec. Rel. Phen. 137-140 (2004) 369. ( $\text{SF}_6$  - S2p)
- SS59** J.A. Soules and C.H. Shaw, Phys. Rev. 113 (1959) 470. (Ar1s)
- SS85** I.H. Suzuki and N. Saito, Bull. Chem. Soc. Japan 58 (1985) 3210. ( $\text{C}_3\text{H}_8$ -C1s)
- SS86a** N. Saito and I.H. Suzuki, Chem. Phys. 108 (1986) 327. ( $\text{CH}_4$ -C1s)
- SS86b** N. Saito and I.H. Suzuki, Chem. Phys. Lett. 129 (1986) 419. ( $\text{N}_2$ -N1s)
- SS87a** N. Saito and I.H. Suzuki, J. Phys. B 20 (1987) L785. ( $\text{N}_2$ -N1s)
- SS87b** I.H. Suzuki and N. Saito, Bull. Chem. Soc. Japan 60 (1987) 2989. ( $\text{C}_2\text{H}_4$ -C1s)
- SS88a** N. Saito and I.H. Suzuki, Int. J. Mass Spec. 82 (1988) 61. ( $\text{N}_2$ -N1s)
- SS88b** N. Saito and I.H. Suzuki, Phys. Rev. Lett. 61 (1988) 2740. ( $\text{N}_2$ -N1s)
- SS89a** N. Saito and I.H. Suzuki, J. Phys. B 22 (1989) L517. ( $\text{O}_2$ -O1s)
- SS89b** N. Saito and I.H. Suzuki, J. Phys. B 22 (1989) 3973. ( $\text{N}_2$ -N1s)
- SS89c** I.H. Suzuki and N. Saito, J. Chem. Phys. 91 (1989) 5324. ( $\text{N}_2$  - N1s)
- SS89d** N. Saito and I.H. Suzuki, J. Chem. Phys. 91 (1989) 5329. ( $\text{O}_2$  - O1s)
- SS90** N. Saito and I.H. Suzuki, J. Chem. Phys. 93 (1990) 4073. ( $\text{O}_2$  - O1s)
- SS91** N. Saito and I.H. Suzuki, Phys. Rev. A 43 (1991) 3662. (NO - N1s,O1s)
- SS92a** N. Saito and I.H. Suzuki, Phys. Scripta 45 (1992) 253. (Ne1s)
- SS92b** N. Saito and I.H. Suzuki, J. Phys. B 25 (1992) 1785. (Xe3p)
- SS92c** A.Schmitt and J. Schirmer, Chem. Phys. 164 (1992) 1. ( $\text{H}_2\text{O}$  - O1s)
- SS92d** I.H. Suzuki and N. Saito, Int. J. Mass. Spec. 115 (1992) 157; I.H. Suzuki and N. Saito, Bull. Electrotech. Lab. 56 (1992) 46. (Ne1s, Ar2p, Kr3d, Xe4d)
- SS94** N. Saito and I.H. Suzuki, Phys. Scripta 49 (1994) 80. (Ne1s, Ar2p, Kr3d, Xe4d)
- SS95** I.H. Suzuki and N. Saito, AIP Conf. Proc. 360 (1995) 105. (CO,  $\text{CO}_2$  - C1s)

- SS97** I.H. Suzuki and N. Saito, Int. J. Mass Spec. Ion Phys. 163 (1997) 229. (CFCl<sub>3</sub> - Cl2p, C1s, F1s)
- SS98a** N. Saito and I.H. Suzuki, J. El. Spec. 88-91 (1998) 65. (Ar2p, Kr3d, Xe4d)
- SS98b** I.H. Suzuki and N. Saito, Chem. Phys. 234 (1998) 255. (CFCl<sub>3</sub> - Cl2p, C1s, F1s)
- SS00** I.H. Suzuki and N. Saito, Chem. Phys. 253 (2000) 351. (C<sub>3</sub>H<sub>6</sub>O – C1s, O1s)
- SS03** I.H. Suzuki and N. Saito, J. El. Spec. 129 (2003) 71. (Xe3p)
- SSB94** I.H. Suzuki, N. Saito and J.D. Bozek, Int. J. Mass Spec. 136 (1994) 55. (CF<sub>2</sub>Cl<sub>2</sub> - Cl2p,C1s,F1s)
- SSB99** I.H. Suzuki, N. Saito and J.D. Bozek, J. El. Spec. 101-103 (1000) 69. (CF<sub>x</sub>Cl<sub>4-x</sub>, x=1-3 - Cl2p, F1s)
- SSE82** M. Simsek, S. Simsek and S. Erkoc, Chem. Phys. Lett. 91 (1982) 456. (Li1s)
- SSH84a** F. Sette, J. Stöhr and A.P. Hitchcock, J. Chem. Phys. 81 (1984) 4906. (24 molecules, sigma-resonance/ bond length correlation)
- SSH84b** F. Sette, J. Stöhr and A.P. Hitchcock, Chem. Phys. Lett. 110 (1984) 517. (F<sub>2</sub>-F1s, C<sub>4</sub>F<sub>8</sub>-C1s)
- SSL91** I. Solomon, J. Silberstein and R.D. Levine, J. Phys. Chem. 95 (1991) 6781. (CH<sub>3</sub>CF<sub>3</sub> - C1s)
- SSS86** W.H.E. Schwarz, U. Seeger and R. Seeger, (unpublished) (CH<sub>3</sub>F - C1s)
- SST96** V.L. Shneerson, D.K. Saldin and W.T. Tysoe, Surf. Sci. 345 (1996) 155. (C<sub>2</sub>H<sub>2</sub>, CO, C<sub>2</sub>H<sub>4</sub> - C1s; N<sub>2</sub>-N1s; O<sub>2</sub>-O1s)
- SST97** V.L. Shneerson, D.K. Saldin and W.T. Tysoe, Surf. Sci. 375 (1997) 340. (N<sub>2</sub>–N1s)
- SS&85** E. Schmidt, H. Schroeder, B. Sonntag, H. Voss and H.E. Wetzel, J. Phys. B 18 (1975) 79. (Mn3p)
- SS&89** N. Saito, I.H. Suzuki, H. Onuki and M. Nishi, Rev. Sci. Inst. 60 (1989) 2190. (Ar2p, N<sub>2</sub> - N1s)
- SS&91** E. Shigemsa, T. Sasaki, A. Yagashita, K. Ueda, Y. Sato and T.Hayaishi, Photon Factory Ann. Rep. (1991) 88-185. (O<sub>2</sub>-O1s)
- SS&95** I.H. Suzuki, N. Saib, M. Koike and J.D. Bozek, Int. J. Mass Spec. Ion Phys. 151 (1995) 45. (CF<sub>3</sub>Cl - Cl2p, C1s, F1s)
- SS&96** J.A.R. Samson, W.C. Stolte, Z.X. He, J.N. Cutler and D.L. Hansen, Phys. Rev. A 54 (1996) 2099. (Ar2p)
- SS&97** B. Santjer, D. Sundermann, M. Wilmer and H. Merz, J. Phys. B 30 (1997) 5501. (Eu4d)
- SS&99** S. Sundin, S.L. Sorensen, A. Ausmees, O. Björneholm, I. Hjelte, A. Kikas and S. Svensson, J. Phys. B32 (1999) 267. (CO – C1s)
- SS&03** W. C. Stolte, M. M. Sant'Anna, G. Ohrwall, I. Dominguez-Lopez, M. N. Piancastelli and D. W. Lindle, Phys. Rev. A 68 (2003) 022701. (H<sub>2</sub>O – O1s)
- SS&05** E. Shigemasa, M. simon, R. guillemin, T. Kaneyasu + Y. Hikosaka, UVSOR Ann. Report 2005. (HCl - Cl2p)

- SS&12** Y. Shibata, K. Soejima, H. Iwayama, E. Shigemasa and Y. Hikosaka, UVSOR Annual Report 2012, 59. ( $\text{CO}_2$  - C1s, O 1s)
- SS&22** Stefan Schippers, Sebastian Stock, et al., Near K-edge Photoionization and Photoabsorption of Singly, Doubly, and Triply Charged Silicon Ions, *The Astrophysical Journal*, 931 (2022) 100. ( $\text{Si}^{m+}$ , m=1-3)
- ST90** W. Sandner and C.E. Theodosiou, *Phys. Rev. A* 42 (1990) 5208. (Ne1s)
- STB83** N. Spector, M.H. Tuilier and C. Bonnelle, *Phys. Rev. A* 27 (1983) 944. (Na1s)
- STS95** V.L. Shneerson, W.T. Tysoe and D.K. Saldin, *Phys. Rev. B* 51 (1995) 13015. ( $\text{C}_2\text{H}_2$  - C1s)
- STS96** V.L. Shneerson, W.T. Tysoe and D.K. Saldin, *Phys. Rev. B* 53 (1996) 10177. ( $\text{N}_2$  - N1s,  $\text{O}_2$  - O1s)
- STZ73** B. Sonntag, T. Tuomi and G. Zimmerer, *Phys. Stat. Sol. B* 58 (1973) 101. ( $\text{Te}_2$  - Te4d)
- ST&93** J. Schirmer, A.B. Trofimov, K.J. Randall, J. Feldhaus, A.M. Bradshaw, Y. Ma, C.T. Chen and F. Sette, *Phys. Rev. A* 47 (1993) 1136. ( $\text{H}_2\text{O}$ -O1s,  $\text{NH}_3$  - N1s,  $\text{CH}_4$ ,  $\text{CD}_4$  - C1s)
- SU&90a** Y. Sato, K. Ueda, A. Yagashita, T. Sasaki, T. Nagata, T. Hayaishi, M. Yoshino, T. Koizumi, Y. Itoh and A.A. MacDowell, *Phys. Scripta* 41 (1990) 55. ( $\text{SiH}_4$  - Si2p)
- SU&90b** E. Shigemasa, K. Ueda, Y. Sato, A. Yagashita, H. Maezawa, T. Sasaki, M. Ukai and T. Hayaishi, *Phys. Scripta* 41 (1990) 67. ( $\text{SiH}_4$  - Si1s)
- SU&90c** E. Shigemasa, K. Ueda, Y. Sato, H. Maezawa, T. Sasaki, A. Yagashita and T. Hayaishi, *Phys. Scripta* 41 (1990) 63. ( $\text{N}_2$  - N1s;  $\text{O}_2$  - O1s)
- SU&92a** E. Shigemasa, K. Ueda, Y. Sato, T. Sasaki and A. Yagashita *Phys. Rev. A* 45 (1992) 2915. ( $\text{N}_2$  - N1s)
- SU&92b** Y. Sato, K. Ueda, H. Chiba, E. Shigemasa, and A. Yagashita *Chem. Phys. Lett.* 196 (1992) 475. ( $\text{SF}_6$  - S2p)
- SU&97** Y. Shimiza, K. Ueda, H. Chiba, M. Okunishi, K. Ohmori, J.B. West, Y. Sato and T. Hayaishi, *J. Chem. Phys.* 107 (1997) 2419. ( $\text{BF}_3$  - F1s)
- SU&00** N. Saito, K. Ueda, M. Simon, K. Okada, Y. Shimizu, H. Chiba, Y. Senba, H. Okumura, H. Ohashi, Y. Tamenori, S. Nagaoka, A. Hiraya, H. Yoshida, E. Ishiguro, T. Ibuki, I. H. Suzuki, and I. Koyano, *Phys. Rev. A* 62 (2000) 042503. ( $\text{CO}_2$  – O1s)
- SU&09** C.P. Schwartz, J.S. Uejio, A.M. Duffin, A.H. England, D. Prendergast, and R. J. Saykally, *J. Chem. Phys.* 131 (2009) 114509. ( $\text{C}_4\text{H}_4\text{N}$  – C1s. N1s)
- SV84** W. Sandner and M. Volkel, *J. Phys. B* 17 (1984) L597. (Ar2p)
- SWD75** R.F. Stewart, D.K. Watson and A. Dalgano, *J. Chem. Phys.* 63 (1975) 3222. (LiH-Li1s)
- SW&98** S.L. Sorensen, M. Wiklund, S. Sundin, A. Ausmees, A. Kikas and A. Svensson, *Phys. Rev. A* 58 (1998) 1879. ( $\text{C}_2\text{H}_4$  – C1s)
- SW&99** I.T. Steinberger, B. Wassermann, C.M. Teodorescu, G. Reichhardt, D. Gravel, C.W. Hutchings, A.P. Hitchcock, P.A. Dowben and E. Rühl, *Phys. Rev. B* 60 (1999) 3995. (Kr3p, Xe4p)

- SW&02** J Schulz, Ph Wernet, K Godehusen, R Müller, P Zimmermann, M Martins and B Sonntag, *J. Phys. B* 35 (2002) 907. (Eu4d)
- SYD82** V.L. Sukhorukov, V.A. Yavna and V.F. Demekhin, *Bull. Acad. Sci. USSR, Phys. Ser.* 46 (1982) 131. (Izv. Akad. Nauk. SSSR Ser. Fiz. 46 (1982) 763] (HF-F1s, H<sub>2</sub>O-O1s; NH<sub>3</sub>-N1s; CH<sub>4</sub>-C1s; HCl-Cl2p, Cl1s; H<sub>2</sub>S-S2p, S1s; PH<sub>3</sub> - P2p, P1s; SiH<sub>4</sub>-Si2p, S1s)
- SY&89** T.K. Sham, B.X. Yang, J. Kirz and J.S. Tse, *Phys. Rev A* 40 (1989) 652. (CO, CO<sub>2</sub>, COS, (CH<sub>3</sub>)<sub>2</sub>CO, C<sub>2</sub>H<sub>5</sub>OH, (C<sub>2</sub>H<sub>5</sub>)<sub>2</sub>O, C<sub>4</sub>H<sub>8</sub>O (THF), C<sub>4</sub>H<sub>8</sub>O<sub>2</sub> (dioxane) - C1s, O1s)
- SY&99** Y. Senba, H. Yoshida, T. Oyata, D. Sakata, A. Hiraya and K. Tanaka, *J. El. Spec.* 101-103 (1999) 131. (CH<sub>3</sub>CN, CD<sub>3</sub>CN – N1s)
- SY&00** Y. Shimizu, H. Yoshida, K. Okada, Y. Murumatsu, N. Saito, H. Ohashi, Y. Tamenori, S. Fritzsche, N.M. Kabachnik, H. Tanaka and K. Ueda, *J. Phys. B* 33 (2000) L685. (Ne1s)
- SZ92** B. Sonntag and P. Zimmermann, *Rep. Prog. Phys.* 55 (1992) 911. (review: Li1s, Ba4d, Cu3p, [Sc,Ti,Cr,Mn,Fe,Co,Ni - 3p]; Mn1s, Cu1s, La4d, Ce4d, Gd4d, Th5d, U5d, W5p, Pt5p, [Ba,La,Ce,Pr, Nd,Sm,Eu,Gd,Tb - 4d])
- SZ&92** G. Stephani, M. Zitnik, L. Avaldi, R. Camilloni, G. Dawbe, G.C. King and M.A. Siggel, *Daresbury Ann. Rep.* (1992) (Xe4p)
- T85** J. Tulkki, *Phys. Rev. A* 32 (1985) 3153. (Xe1s, Rn1s)
- T86** J.A. Tossell, *Am. Minerologist* 71 (1986) 1170. (BF<sub>3</sub>, B(OH)<sub>3</sub> - B1s; H<sub>2</sub>CO<sub>3</sub> - C1s)
- T88** J. Tse, *J. Chem. Phys.* 89 (1988) 920. (XeF<sub>2</sub> - Xe4d)
- T91** J.A. Tossell, *Chem. Phys.* 154 (1991) 211. (SF<sub>4</sub>, SF<sub>6</sub>, S<sub>2</sub>F<sub>10</sub>, SF<sub>2</sub>O, SF<sub>4</sub>O, SF<sub>2</sub>O<sub>2</sub>, SO<sub>2</sub> - S2p, S1s)
- T93** T. Takaynagi, *AIP Conf. Proc.* 295 (1993) 326. (Xe4d)
- T94** J.A. Tossell, *Chem. Phys. Lett.* 219 (1994) 65. (SiH<sub>x</sub>Cl<sub>4-x</sub>, x=0-4, Si2p)
- T98** L.Triguero, Calculations of near-edge x-ray-absorption spectra of gas-phase and chemisorbed molecules by means of density-functional and transition-potential theory, *Physical Review* 58 (1998).8097.
- TA85** J. Tulkki and T. Aberg, *J. Phys. B* 18 (1985) L489. (Ar1s)
- TA&92** J. Tulkki, S. Aksela, H. Aksela, E. Shigemasa, A. Yagashita and Y. Furusawa, *Phys. Rev. A* 45 (1992) 4640. (Kr3d)
- TA&07** T Teramoto, J Adachi, K Hosaka1, M Yamazaki, K Yamanouchi, N A Cherepkov, M Stener, P Decleva and A Yagishita, *J. Phys. B* 40 (2007) F241. (CO<sub>2</sub> – C1s)
- TB&89** T.A. Tyson, M. Benfatto, C.R. Natoli, B. Hedman and K.O. Hodgson, *Physica B* 158 (1989) 425. (SF<sub>6</sub> - S1s)
- TB&99** T.D. Thomas, N. Berrah, J.D. Bozek, T.X. Carroll, J. Halne, T. Karben, E. Kukk and L.J. Saethre, *Phys. Rev. Lett.* 82 (1999) 1120. (C<sub>2</sub>H<sub>2</sub> – C1s)
- TC86** R. Tang and J. Callaway, *J. Chem. Phys.* 84 (1986) 6854. (SF<sub>6</sub>-S2p)

- TC91** T.D. Thomas and T.X. Carroll, Chem. Phys. Lett. 185 (1991) 31. (O<sub>2</sub>-O1s)
- TC&02** D. Tulumello, G. Cooper, E. Halliday and A.P. Hitchcock, (2002) unpublished. (C<sub>5</sub>H<sub>14</sub>OSi, C<sub>8</sub>H<sub>12</sub>O<sub>3</sub>Si, C<sub>8</sub>H<sub>18</sub>O<sub>3</sub>Si - C1s, O1s, Si2p)
- TC&16** Cheng-Cheng Tsai, Jien-Lian Chen, et al., Selectivity of peptide bond dissociation on excitation of a core electron: Effects of a phenyl group Chem. Phys. Letts 660 (2016) 60. (C<sub>8</sub>H<sub>9</sub>NO, C<sub>9</sub>H<sub>11</sub>NO – C1s, N1s, O1s)
- TD84** J.A. Tossel and J.W. Davenport, J. Chem. Phys. 80 (1984) 813. (CH<sub>4</sub>, CF<sub>4</sub>, CCl<sub>4</sub> - C1s; SiH<sub>4</sub>, SiF<sub>4</sub>, SiCl<sub>4</sub> - Si2p)
- TD91** M. Tronc and C. Dezarnaud-Dandine, Chem. Phys. Lett. 184 (1991) 267. (Mo(CO)<sub>6</sub> - Mo2p)
- TD&92a** M. Tronc, C. Dezarnaud, G. Cooper, C.E. Brion and A.P. Hitchcock, (1992) unpublished. (V(CO)<sub>6</sub> - V2p, C1s, O1s; Mo(CO)<sub>6</sub> - Mo3d, Mo2p)
- TD&92b** R. Thissen, J. Delwiche, M.J. Hubin-Franksin, M. Furlan, P. Morin, M. Lavollée and I. Nenner, AIP Conf. Proc. (Grenoble Dynamics) 258 (1992) 341. (CH<sub>3</sub>NH<sub>2</sub> - N1s)
- TE&00** C.M. Teodorescu, J.M. Esteva, M. Womes, A. El Afif, R.C. Karnataka, A.M. Flank and P. Lagarde, J. El. Spec. 106 (2000) 233. (Na, NaF – Na1s)
- TE&01a** C.M. Teodorescu, A. El Afif, J.M. Esteva and R.C. Karnataka, Phys. Rev. B 63 (2001) 233106. (NaBr, NaCl, NaF, NaI - Na1s)
- TE&01b** T. Tyliszczak, I.G. Eustatiu, A.P. Hitchcock, C.C. Turci, A.B. Rocha and C.E. Bielschowsky, J. Electron Spectrosc. 114-116 (2001) 93. (CO<sub>2</sub> – C1s, O1s)
- TF&91** J.C. Tang, X.S. Feng, J.F. Shen, T. Fujikawa and T. Okazawa, Phys. Rev. B 44 (1991) 13018. (C<sub>2</sub>H<sub>4</sub> - C1s)
- TF&95** C.C. Turci, J.T. Francis, T. Tyliszczak, G.G.B. de Souza and A.P. Hitchcock, Phys. Rev. A 52 (1995) 4678. (SF<sub>6</sub> - S2p)
- TF&99** M.K. Thomas, B.O. Fisher, P.A. Hatherly, K. Codling, M. Stankiewicz and M. Roper, J. Phys. B 32 (1999) 2611. (CF<sub>4</sub> – C1s, F1s)
- TF&03** M Tchaplyguine, R Feifel, R.R.T Marinho, M Gisselbrecht, S.L Sorensen, A Naves de Brito, N Mårtensson, S Svensson and O Björneholm, Chem. Phys. 289 (2003) 3. (Ar<sub>n</sub> - 2p)
- TGR98** C.M. Teodorescu, D. Gravel and E. Rühl, J. Chem. Phys. 109 (1998) 9280. (S<sub>n</sub> n=2-8 – S2p)
- TG&99** C.M. Teodorescu, D. Gravel, J. Choi, D. Pugmire, P.A. Dowben, N. Fominykh, A.A. Pavlychev and E. Rühl, J. El. Spec. 101-103 (1999) 193. (S<sub>n</sub> n=3-8 – S2p)
- TG&00** A.B. Trofimov, E.V. Gromov, T.E. Moskovskaya and J. Schirmer, J. Chem. Phys. 113 (2000) 6716. (H<sub>2</sub>CO – C1s)
- TG&18** Toffoli, D.; Guarnaccio, A., et al., Electronic structure characterization of a thiophene benzo-annulated series of common building blocks for donor and acceptor compounds studied by gas phase photoelectron and photoabsorption synchrotron spectroscopies. J. Phys. Chem. A 122 (2018) 8745. (C<sub>4</sub>H<sub>4</sub>S, C<sub>8</sub>H<sub>6</sub>S, C<sub>12</sub>H<sub>8</sub>S –

S2p, C1s)

- THH87** T.A. Tyson, B. Hedman and K.O. Hodgson, SSRL Report (1987) 158. (SF<sub>6</sub>-S1s)
- THY86** K. Tohji, D.M. Hanson and B.X. Yang, J. Chem. Phys. 85 (1986) 7492 (O<sub>2</sub> - O1s)
- TH&92a** T.A. Tyson, K.O. Hodgson, C.R. Natoli and M. Benfatto, Phys. Rev. B 46 (1992) 5997. (Br<sub>2</sub>-Br1s; GeCl<sub>4</sub> - Ge1s; SF<sub>6</sub> - S1s)
- TH&92b** R. Thissen, M.J. Hubin-Franskin, M. Furlar, J.L. Pielle, P. Morin and I. Nenner, Chem. Phys. Lett. 199 (1992) 102. (CH<sub>2</sub>BrCH<sub>2</sub>I - I4d)
- TH&96** T.D. Thomas, R.I. Hall, M. Hochlaf, H. Kjeldsen, F. Penent, P. Lablanquie, M. Lavolleé and P. Morin, J. Phys. B 29 (1996) 3245. (Ar2p)
- TH&98** M.K. Thomas, P.A. Hatherly, K. Codling, M. Stankiewicz, J. Rius I Riu, A. Karawejczyk and M. Roper, J. Phys. B 31(1998) 3407. (C<sub>3</sub>H<sub>8</sub>O - C1s, O1s)
- TJ&99a** D.B. Thompson, De Ji, K. Lee, C.I. Ma and D.M. Hanson, J. Phys. B 32 (1999) 2649. (C<sub>3</sub>H<sub>6</sub>O - C1s,O1s)
- TJ&99b** D.B. Thompson, De Ji, S.Y. Chen and D.M. Hanson, J. Phys. B 32 (1999) 5711. (C<sub>2</sub>H<sub>4</sub>O, C<sub>3</sub>H<sub>6</sub>O, C<sub>3</sub>H<sub>6</sub>O - C1s,O1s)
- TKM81** I.A. Topol, A.V. Kondratenko and L.N. Mazalov, Opt. Spectrosc. 50 (1981) 267. [Opt. Spektrosk. 50 (1981) 494] PCl<sub>3</sub> - P2p, Cl2p)
- TKM82** I.A. Topol, A.V. Kondratenko and L.N. Mazalov, Bull. Acad. Sci. USSR Phys. Ser. 46 (1982) 143. (Izv. Akad. Nauk. SSSR Ser. Fiz. 46 (1982) 776] (PCl<sub>3</sub>,POCl<sub>3</sub>,PSCl<sub>3</sub> - P2p,Cl2p,S2p)
- TKR79** M. Tronc, G.C. King and F.H. Read, J. Phys. B 12 (1979) 137. (CH<sub>4</sub>, CO<sub>2</sub>, C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>4</sub>, CF<sub>4</sub>, COS - C1s)

- TKR80** M. Tronc, G.C. King and F.H. Read, J. Phys. B 13 (1980) 999. (N<sub>2</sub>, NO, N<sub>2</sub>O - N1s)
- TKU98** S. Tanaka, Y. Kayanuma and K. Ueda, Phys. Rev. A 57 (1998) 3437. (BF<sub>3</sub> - B1s)
- TKU15** O. Takahashi, N.V. Kryzhevov and K. Ueda, J. El. Spec. 204 (2015) 290. (XH<sub>m</sub>-YH<sub>n</sub>) X,Y = C,N,O,F; m,n = 0-3 – double core hole IPs) – only CO, C<sub>2</sub>H<sub>6</sub>, N<sub>2</sub> in table
- TK&76** M. Tronc, G.C. King, R.C. Bradford and F.H. Read, J. Phys. B 9 (1976) L555. (CO, CH<sub>4</sub> - C1s)
- TK&92** Y. Takata, Y. Kitajima, H. Aga, S. Yagi, T. Asahi, T. Yokoyama, K. Tanaka and T. Ohta, Photon Factory Ann Rep. (1992) 29. (C<sub>4</sub>H<sub>4</sub>S - S1s)
- TK&93** C.M. Teodorescu, R.C. Karnatak, J.M. Esteva, A. El Afif and J.P. Connerade, J. Phys. B 26 (1993) 4019. (Ar1s, Ne1s)
- TK&00** X.M. Tong, D. Kato, T. Watanabe and S. Ohtani, J. Phys. B 33 (2000) 717. (Eu4d)
- TK&01** X.M. Tong, D. Kato, T. Watanabe and S. Ohtani, Phys. Rev. A 64 (2001) 032716. (Eu4d)
- TK&14** S. Tsuru, M. Kazama, T. Fujikawa, J.-I. Adachi and A. Yagishita, J. Phys. B 47 (2014) 071002. (CO<sub>2</sub> – C1s)
- TL89** X.M. Tong and J.M. Li, J. Phys. B 22 (1989) 1531. (NO<sub>2</sub> - N1s)
- TL91** J.S. Tse and Z.F. Liu, Phys. Rev. A 44 (1991) 7838. (SF<sub>6</sub> - S2p; PF<sub>5</sub> - P2p)
- TLE82** M.H. Tuilier, D. Laporte and J.M. Esteva, Phys. Rev. A 26 (1982) 372. (Na1s)
- TLPI90** X.M. Tang, J.M. Li and R.H. Pratt, Phys. Rev. A 42 (1990) 5348. (Xe3d, Fe3p)
- TL&84** C.M. Truesdale, D.W. Lindle, P.H. Kobrin, U.E. Becker, H.G. Kerkhoff, P.A. Heimann, T.A. Ferrett and D.A. Shirley, J. Chem. Phys. 80 (1984) 2319. (CO,CO<sub>2</sub>-C1s,O1s; CF<sub>4</sub>-C1s; COS-C1s,S2p)
- TL&85** B.T. Thole, G. van der Laan, J.C. Fuggle, G.A. Sawatzky, R.C. Karnatak and J.M. Esteva, Phys. Rev. B 32 (1985) 5107. (La...Yb rare earth 3d)
- TL&89** J.S. Tse, Z.F. Liu, J.D. Bozek and G.M. Bancroft, Phys. Rev. A 39 (1989) 1791. (SiCl<sub>4</sub> - Si2s,2p; Cl2s,2p)
- TL&02** M. Tchaplyguine, M. Lundwall, G. Ohrwall, M. Gisselbrecht, F. Feifel, S. Sorensen, T. Rander, A. Lindblad, S. Svensson and O. Bjorneholm, MAXLab Annual Report 2001/02 (2002) 204. (Kr<sub>n</sub> – Kr3d)
- TMG01** A. B. Trofimov, T. E. Moskovskaya, E. V. Gromov, H. Köppel, and J. Schirmer, Phys. Rev. A 64 (2001) 022504. (H<sub>2</sub>CO – C1s,O1s)
- TMM94** S.S. Tayal, A.Z. Msezene and S.T. Manson, Phys. Rev. A 49 (1994) 956. (Na2p)
- TM&01a** M.Tchaplyguine, R.R.T. Marinho, M. Gisselbrecht, R. Feifel, G. Ohrwall, M. Lundwall, S.L. Sorensen, A. Naves de Brito, N. Martensson, S. Svensson and O. Björneholm, MaxLab Report (2001) 210. ((H<sub>2</sub>O)<sub>n</sub> – O1s)
- TM&01b** A.B. Trofimov, T.E. Moskovskaya, E.V. Gromov, H. Köppel, and J. Schirmer, Phys.Rev. A 64 (2002) 022504. (H<sub>2</sub>CO – C1s, O1s)

- TPA98** L. Triguera, L.G.M. Pettersson and H. Agren, Phys. Rev. B 58 (1998) 8097. (CO, H<sub>2</sub>CO, Me<sub>2</sub>CO – C1s, O1s; C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>4</sub>, C<sub>2</sub>H<sub>6</sub> – C1s)
- TP&24** Bruno Nunes Cabral Tenorio, Jacob Pedersen, Mario Barbatti, Piero Decleva, and Sonia Coriani, Auger-Meitner and X-ray Absorption Spectra of Ethylene Cation: Insight into Conical Intersection Dynamics J. Physical Chemistry A 128 (2024) 107. (C<sub>2</sub>H<sub>4</sub>, C<sub>2</sub>H<sub>4</sub><sup>+</sup> - C1s)
- TR&07** C.C. Turci, A.B. Rocha, M. Barbatti, C.E. Bielschowsky, I.G. Eustatiu, T. Tyliszczak, G. Cooper, A.P. Hitchcock, J. Electron Spectrosc. Rel. Phenom. 155 (2007) 21 (CS<sub>2</sub> - C1s, S2p)
- TSH94** R. Thissen, M. Simon and M.J. Hubin-Franksin, J. Chem. Phys. 101 (1994) 7548. (CH<sub>3</sub>Cl - Cl2p)
- TS&83** C.M. Truesdale, S.H. Southworth, P.H. Kobrin, U. Becker, D.W. Lindle, H.G. Kerlchoff and D.A. Shirley, Phys. Rev. Lett. 50 (1983) 1265. (CO-C1s,O1s)
- TS&05** Os. Takahashi, K. Saito, M. Mitani, H. Yoshida, F. Tahara, T. Sunami, K. Waki, Y. Senba, A. Hiraya and L.G.M. Pettersson, J. El. Spec. Rel. Phen. 142 (2005) 113. (C<sub>3</sub>H<sub>3</sub>O<sub>2</sub>N , C<sub>4</sub>H<sub>5</sub>O<sub>2</sub>N - N1s, O1s)
- TT&05** K. Tabayashi, S. Tada, J. Aoyama, K. Saito, H. Yoshida, S. Wada, A. Hiraya and K. Tanaka, J. El. Spec. 144-147 (2005) 179.((N<sub>2</sub>O)<sub>n</sub> – N1s)
- TUH96** C. Turci, S. Urquhart and A.P. Hitchcock, Can. J. Chem. 74 (1996) 851. (C<sub>6</sub>H<sub>6</sub> - C1s; C<sub>6</sub>H<sub>5</sub>NH<sub>2</sub> - C1s, N1s; C<sub>6</sub>H<sub>5</sub>NO<sub>2</sub>, (1,2)-, (1,3)-, (1,4)-NO<sub>2</sub>C<sub>6</sub>H<sub>4</sub>NH<sub>2</sub> - C1s, N1s, O1s)
- TV93** J.A. Tossell and D.J. Vaughan, J. Col. Int. Sci. 155 (1993) 98. (H<sub>2</sub>CO<sub>3</sub>, NH<sub>3</sub>CS<sub>2</sub>, (OHCS<sub>2</sub>)<sub>2</sub> - C1s; CH<sub>3</sub>SH, H<sub>2</sub>COS<sub>2</sub> - C1s, S1s; H<sub>2</sub>S<sub>2</sub> - S1s; H<sub>2</sub>O<sub>2</sub> - O1s; CuS<sub>2</sub>COH-S1s)
- TWM94** J.A. Tossell, D.C. Winkler and J.H. Moore, Chem. Phys. 185 (1994) 297. (SiMe<sub>2</sub>)<sub>n</sub>, n=3-6 - Si2p)
- TWT92** L.J. Terminello, C.D. Wadwill and J.G. Tobin, Nucl. Inst. Meth. A319 (1993) 271. (N<sub>2</sub>- N1s; CO-C1s)
- TW&99** C.M. Teodorescu, M. Womes, A. El Afif, R.C. Karnataka, J.M. Esteva, A.M. Flank and P.Lagarde, J. El. Spec. 101-103 (1999) 205. (KF, (KF)<sub>n</sub> – K1s)
- TY&91** Y. Takata, T. Yokoyama, S. Yagi, N. Hocco, H. Sato, K. Seki, T. Ohta, Y. Kitajima and H. Kuroda, Surf. Sci. 259 (1991) 266. (C<sub>6</sub>H<sub>5</sub>SH - S1s)
- TY&05** Y. Tamenori, T. Yamaguchi, K. Okada, K. Tabayashi, T. Gejo, K. Honma, J. El. Spec. 144-147 (2005) 235. (C<sub>2</sub>H<sub>5</sub>OH-O1s)
- U91** K. Ueda, Rev. Laser Eng. 19 (1991) 1089. (BF<sub>3</sub> - B1s)
- U93** K. Ueda, AIP Conf. Conf. Proc. 295 (1993) 405. (BF<sub>3</sub> - B1s)
- U98** K. Ueda, J. Electron Spectrosc. 88-91 (1998) 1. (PH<sub>3</sub> - P1s; BF<sub>3</sub> - B1s; SF<sub>6</sub> - F1s)
- UA&99** S.G. Urquhart, H. Ade, A.P. Smith, L.E. Ennis, J.F. Lehmann and A.P. Hitchcock, (1999) unpublished. (C<sub>4</sub>H<sub>7</sub>O<sub>4</sub> - C1s, O1s; C<sub>2</sub>H<sub>5</sub>N<sub>3</sub>O<sub>2</sub>, C<sub>6</sub>H<sub>9</sub>N<sub>3</sub>O<sub>3</sub> , C<sub>21</sub>H<sub>15</sub>N<sub>3</sub>O<sub>3</sub> , C<sub>24</sub>H<sub>21</sub>N<sub>3</sub>O<sub>3</sub> - C1s, O1s, N1s)
- UC&92** K. Ueda, H. Chiba, Y. Sato, T. Hayaishi, E. Shigemasa and A. Yagashita, Phys. Rev. A 46 (1992) R5. (BF<sub>3</sub>- B1s)

- UC&94a** K. Ueda, H. Chiba, Y. Sato, T. Hayaishi, E. Shigemasa and A. Yagashita, J. Chem. Phys. 101 (1994) 3520. (BF<sub>3</sub>-B1s)
- UC&94b** K. Ueda, H. Chiba, Y. Sato, T. Hayaishi, E. Shigemasa and A. Yagashita, J. Chem. Phys. 101 (1994) 7320. (BCl<sub>3</sub>-B1s, Cl2p)
- UF&08** K. Ueda, H. Fukuzawa, X.-J. Liu, K. Sakai, G. Prümper, Y. Morishita, N. Saito, I.H. Suzuki, K. Nagaya, H. Iwayama, M. Yao, K. Kreidi, M. Schöffler, T. Jahnke, S. Schössler, R. Dörner, Th. Weber, J. Harries, Y. Tamenori, J. El. Spec. 166-167 (2008) 3. (Ar<sub>2</sub>, ArKr – Ar2p; ArKr, Kr<sub>2</sub> – Kr3d)
- UG05** S.G. Urquhart and R. Gilles, J. Phys. Chem. A 109 (2005) 2151. (CH<sub>4</sub>, C<sub>2</sub>H<sub>6</sub>, C<sub>3</sub>H<sub>8</sub>, iso- C<sub>4</sub>H<sub>10</sub>, neo-C<sub>5</sub>H<sub>12</sub> – C1s)
- UH96** S.G. Urquhart and A.P. Hitchcock, (1996) unpublished. (C<sub>7</sub>H<sub>9</sub>N - 1s, N1s; C<sub>10</sub>H<sub>6</sub>F<sub>4</sub> - C1s)
- UH98** S.G. Urquhart and A.P. Hitchcock, (1998) unpublished. (C<sub>10</sub>H<sub>12</sub>N – C1s, N1s)
- UHR92** S.G. Urquhart, A.P. Hitchcock and E.G. Rightor, (1994) unpublished. (C<sub>6</sub>H<sub>14</sub>O, C<sub>21</sub>H<sub>15</sub>N<sub>3</sub>O<sub>3</sub> - C1s, N1s, O1s)
- UHR95a** S.G. Urquhart, A.P. Hitchcock and E.G. Rightor, (1992) unpublished. (C<sub>5</sub>H<sub>14</sub>O - C1s, O1s; C<sub>9</sub>H<sub>6</sub>N<sub>2</sub>O<sub>2</sub> , C<sub>13</sub>H<sub>17</sub>N<sub>2</sub>O<sub>4</sub> , C<sub>19</sub>H<sub>22</sub>N<sub>2</sub>O<sub>4</sub> - C1s, N1s, O1s)
- UHR95b** S.G. Urquhart, A.P. Hitchcock, R.D. Priester and E.G. Rightor, Analysis of Polyurethanes using Core Excitation Spectroscopy. Part II. Inner-shell Spectra of Ether, Urea and Carbamate Model Compounds, J. Polymer Science B: Polymer Physics, 33 (1995) 1603-1620.
- UHR97** S.G. Urquhart and A.P. Hitchcock, (1997) unpublished. (C<sub>7</sub>H<sub>8</sub>O – C1s, O1s)
- UHR99** S.G. Urquhart, A.P. Hitchcock and E.G. Rightor, (1999) unpublished. (C<sub>11</sub>H<sub>14</sub>N<sub>2</sub>O<sub>4</sub>, 2,4-C<sub>9</sub>H<sub>6</sub>N<sub>2</sub>O<sub>2</sub> ,2,6-C<sub>9</sub>H<sub>6</sub>N<sub>2</sub>O<sub>2</sub> - C1s, N1s, O1s)
- UH&94a** S.G. Urquhart and A.P. Hitchcock, (1994) unpublished. (C<sub>4</sub>H<sub>9</sub>F<sub>3</sub>O<sub>3</sub>SSi, C<sub>6</sub>H<sub>15</sub>OSi, C<sub>6</sub>H<sub>18</sub>O<sub>3</sub>Si<sub>3</sub>, C<sub>8</sub>H<sub>20</sub>O<sub>4</sub>Si, C<sub>8</sub>H<sub>24</sub>O<sub>4</sub>Si<sub>4</sub> - Si 2p, C1s, O1s, Si1s)
- UH&94b** S.G. Urquhart and A.P. Hitchcock, (1994) unpublished. (C<sub>5</sub>H<sub>15</sub>NSi, C<sub>7</sub>H<sub>18</sub>N<sub>2</sub>Si, C<sub>6</sub>H<sub>18</sub>N<sub>3</sub>Si, C<sub>7</sub>H<sub>21</sub>N<sub>2</sub>Si, C<sub>8</sub>H<sub>24</sub>N<sub>4</sub>Si, C<sub>9</sub>H<sub>21</sub>NSi<sub>3</sub> - Si2p, C1s, N1s, Si1s)
- UH&95a** S.G. Urquhart, A.P. Hitchcock, R.D. Leapman, R.D.Priester and E.G. Rightor, J. Pol. Sci. B. Pol. Phys. 33 (1995) 1593. C<sub>8</sub>H<sub>16</sub>O - C1s, O1s; C<sub>7</sub>H<sub>7</sub>NO<sub>2</sub>, C<sub>7</sub>H<sub>8</sub>N<sub>2</sub>O, C<sub>9</sub>H<sub>11</sub>NO<sub>2</sub>, C<sub>10</sub>H<sub>13</sub>NO<sub>2</sub>, - C1s, N1s, O1s)
- UH&95b** S.G. Urquhart, A.P. Hitchcock, R.D. Leapman, R.D.Priester and E.G. Rightor, J. Pol. Sci. B. Pol. Phys. 33 (1995) 1603. C<sub>4</sub>H<sub>10</sub>O, C<sub>8</sub>H<sub>16</sub>O - C1s, O1s; CH<sub>4</sub>N<sub>2</sub>O, C<sub>3</sub>H<sub>7</sub>NO<sub>2</sub>, C<sub>7</sub>H<sub>7</sub>NO<sub>2</sub>, C<sub>7</sub>H<sub>8</sub>N<sub>2</sub>O, C<sub>8</sub>H<sub>9</sub>NO, C<sub>9</sub>H<sub>11</sub>NO<sub>2</sub>, C<sub>10</sub>H<sub>13</sub>NO<sub>2</sub>, C<sub>13</sub>H<sub>12</sub>N<sub>2</sub>O, C<sub>13</sub>H<sub>13</sub> - C1s, N1s, O1s)
- UH&96** S.G. Urquhart, A.P. Hitchcock, E.G. Rightor and H. Ade, MRS Symp. Proc. 437 (1996) 243. (o-, m-, p-C<sub>10</sub>H<sub>10</sub>O<sub>4</sub> - C1s, O1s)
- UH&97** S.G. Urquhart, A.P. Hitchcock, A.P. Snith, H. Ade and E.G. Rightor, J. Phys. Chem. B 101 (1997) 2267. (C<sub>10</sub>H<sub>10</sub>O<sub>4</sub> - C1s, O1s)
- UH&98** S.G. Urquhart, A.P. Hitchcock, J.F. Lehmann and M. Denk, Organometallics 17 (1998) 2352. (C<sub>10</sub>H<sub>20</sub>N<sub>2</sub>Si, C<sub>10</sub>H<sub>22</sub>N<sub>2</sub>Si, C<sub>10</sub>H<sub>22</sub>N<sub>2</sub>Si, C<sub>10</sub>H<sub>24</sub>N<sub>2</sub>Si - C1s, N1s, Si2p, Si1s)

- UH&99** S.G. Urquhart, A.P. Hitchcock, R. Lessard, E.G. Rightor and G.E. Mitchell, (1999) unpublished ( $C_4H_8N_2O_3$ ,  $C_4H_8N_2O_3$  - C1s, N1s, O1s)
- UM&99** K. Ueda, Y. Muramatsu, Y. Shimizu, H. Chiba, Y. Sato, M. Kitajima, H. Tanaka and N. Nakamatsu, Chem. Phys. Lett. 308 (1999) 45. ( $PF_5$  - P2p)
- UO&95a** K. Ueda, M. Okunishi, H. Chiba, Y. Shimizu, K. Ohmori and Y. Sato, Chem. Phys. Lett. 236 (1995) 311. ( $CH_4$  - C1s)
- UO&95b** K. Ueda, K. Ohmori, M. Okunishi, Y. Shimizu, Y. Sato, T. Hayaishi, E. Shigemasa and A. Yagashita, Phys. Rev. A 52 (1995) R1815. ( $BF_3$  - B1s)
- UO&96** K. Ueda, K. Ohmori, M. Okunishi, H. Chiba, Y. Shimizu, Y. Sato, T. Hayaishi, E. Shigemasa and A. Yagashita, J. Electron Spectrosc. 79 (1996) 411. ( $BF_3$  - B1s)
- US&89a** K. Ueda, E. Shigemasa, Y. Sato, S. Nagaoka, I. Kayano, A. Yagashita, T. Nagata and T. Hayaishi, Chem. Phys. Lett. 154 (1989) 357. ( $Sn(CH_3)_4$  - Sn3d)
- US&89b** K. Ueda, E. Shigemasa, Y. Sato, A. Yagashita, T. Hayaishi and T. Sasaki, Rev. Sci. Inst. 60 (1989) 2193. ( $SiH_4$  - Si1s)
- US&90a** K. Ueda, E. Shigemasa, Y. Sato, S. Nagaoka, I. Kayano, A. Yagashita and T. Hayaishi, Phys. Scripta 41 (1990) 78. ( $Sn(CH_3)_4$  - Sn3d)
- US&90b** K. Ueda, E. Shigemasa, Y. Sato, S. Nagaoka, I. Kayano, A. Yagashita and T. Hayaishi, Chem. Phys. Lett. 166 (1990) 391. ( $Sn(CH_3)_4$  - Sn4p,4s)
- US&90c** K. Ueda, Y. Sato, S. Nagaoka, I. Kayano, A. Yagashita and T. Hayaishi, Chem. Phys. Lett. 170 (1990) 389. ( $Ga(CH_3)_3$  - Ga3p)
- US&91** K. Ueda, E. Shigemasa, Y. Sato, A. Yagashita, M. Ukai, M. Maezawa, T. Hayaishi and T. Sasaki, J. Phys. B 24 (1991) 605. (Ar1s)
- US&96** K. Ueda, Y. Shimizu, H. Chiba, M. Okunishi, K. Ohmori, Y. Sato, E. Shigemasa and N. Kosugi, J. Electron Spectrosc. 79 (1996) 441. ( $CH_4$ ,  $CH_3F$ ,  $CH_2F_2$ ,  $CHF_3$ ,  $CF_4$  - C1s, F1s)
- US&97** K. Ueda, Y. Shimizu, H. Chiba, M. Okunishi, K. Ohmori, J.B. West, Y. Sato, T. Hayaishi, H. Nakamatsu and T. Mukoyama, Phys. Rev. Lett. 79 (1997) 3371. ( $SF_6$  - F1s)
- US&99a** K. Ueda, Y. Shimizu, N.M. Kabachnik, N. Leclerc, I.P. Sazhina, R. Wehlitz, U. Becker, M. Kitajima and H. Tanaka, J. Phys. B 32 (1999) L291. (Ar2p)
- US&99b** K. Ueda, M. Simon, C. Miron, N. Leclerc, R. Guillemin, P. Morin and S. Tanaka, Phys. Rev. Lett. 83 (1999) 3800. ( $CF_4$  - C1s)
- US&01** K. Ueda, Y. Shimizu, H. Chiba, M. Kitajima, H. Tanaka, S. Fritzsche and N.M. Kabachnik, J. Phys. B 34 (2001) 107. (Ar2p)
- UT83** L. Ungier and T.D. Thomas, Chem. Phys. Lett. 96 (1983) 247. ( $N_2$ -N1s; CO- C1s, O1s)

- UT&84** L. Ungier and T.D. Thomas, Phys. Rev. Lett. 53 (1984) 435. (N<sub>2</sub>-N1s, CO-C1s)
- UT&85** L. Ungier & T.D. Thomas, J. Chem. Phys. 82 (1985) 3146 (CO-C1s,O1s; N<sub>2</sub>-N1s)
- UT&97** S.G. Urquhart, C.C. Turci, T. Tylliszcak, M.A. Brook and A.P. Hitchcock, Organometallics 16 (1997) 2080. (C<sub>3</sub>H<sub>10</sub>OSi, C<sub>4</sub>H<sub>12</sub>OSi, C<sub>6</sub>H<sub>16</sub>OSi, C<sub>6</sub>H<sub>18</sub>OSi<sub>2</sub>, C<sub>6</sub>H<sub>18</sub>Si<sub>2</sub>, C<sub>36</sub>H<sub>30</sub>OSi<sub>2</sub>, C<sub>36</sub>H<sub>30</sub>Si<sub>2</sub>, - Si 1s, Si2p, C1s, O1s)
- UT&00** K. Ueda, S. Tanaka, Y. Shimizu, Y. Muramatsu, H. Chiba, T. Hayaishi, M. Kitajima and H. Tanaka, Phys. Rev.Lett. 85 (2000) 3129. (BCl<sub>3</sub> – B1s)
- UX&94** S.G. Urquhart, J.Z. Xiong, A.T. Wen, T.K. Sham, K.M. Baines G.G.B. de Souza, and A.P. Hitchcock, Chem. Phys. 189 (1994) 757. (C<sub>4</sub>H<sub>12</sub>Si, C<sub>6</sub>H<sub>18</sub>Si<sub>2</sub>, C<sub>9</sub>H<sub>28</sub>Si, C<sub>12</sub>H<sub>36</sub>Si<sub>5</sub>, C<sub>12</sub>H<sub>36</sub>Si<sub>6</sub> - Si2p, C1s, Si1s)
- V88** E. Vatai, Phys. Rev. A 38 (1988) 3777. (N<sub>2</sub>-N1s; Ar1s; Ne1s)
- VA&75** A.S. Vinogradov, V.N. Akimov, T.M. Zimkina and E.B. Dobryabova, Izv. Sib. Otd. Akad. Nauk SSSR Ser. Khim. (1975) 88. (C<sub>2</sub>H<sub>5</sub>OH, O<sub>2</sub>, CO<sub>2</sub>-O1s)
- VA&85** A.S. Vinogradov, V.N. Akimov and A.A. Pavylchev, Bull. Acad. Sci. USSR 49 (1985) 1 (Izv. Sib. Otd. Akad. Nauk SSSR Ser. Fiz. 49 (1985) 1458. (N<sub>2</sub>- N1s; BF<sub>3</sub> - B1s, F1s; SF<sub>6</sub> - S2p, F1s, review)
- VA&92** A.S. Vinogradov, V.N. Akimov, S.V. Nekipelov, A.A. Pavylchev, A.A. Boronoev and A. V. Zhadenov, Opt. Spectr. 72 (1992) 599 [Opt. Spek. 72 (1992) 1094]. (CH<sub>3</sub>NO<sub>2</sub> - C1s, N1s, O1s)
- VBA91** R.V. Vedrinskii, L.A. Bugaev and V.M. Airapetyan, Opt. Spectrosc. (USSR) 70 (1991) 715 [Opt. i Spect. 70 (1991) 1223] (CO, CO<sub>2</sub>, COS - O1s)
- VC&06** G. Vall-Ilosera, M. Coreno, A. Kivimäki, K. Jakulowska, M. Stankiewitz and E Rachlew, MAX Lab 2005-2006 Annual report. (2006) 260. (C<sub>4</sub>H<sub>4</sub>N<sub>2</sub> – C1s, N1s)
- VD&98** A. Verwegen, D. Donnelly, A. Hibbert and K.L. Bell, Phys. Rev. A 58 (1998) 3338. (Cu3p)
- VF&96** D.A. Verna, G.J.Ferland, K.T. Korista and D.G. Yakovlev, Astrophys. J. 465 (1996) 487.(Li1s)
- VF&98** P. Vaterlin, R. Fink, E. Umbach and W. Wurth, J. Chem. Phys. 108 (1998) 3313. (C<sub>3</sub>H<sub>8</sub> - C1s)
- VG&08** G. Vall-llosera, B. Gao, A. Kivimäki, M. Coreno, J. Álvarez Ruiz, M. de Simone, H. Ågren and E. Rachlew, J. Chem. Phys. 128 (2008) 044316. (C<sub>3</sub>H<sub>3</sub>N<sub>3</sub>, C<sub>4</sub>H<sub>3</sub>N<sub>2</sub>, C<sub>4</sub>H<sub>4</sub>N<sub>2</sub>, C<sub>4</sub>H<sub>45</sub>N<sub>2</sub>, C<sub>5</sub>H<sub>5</sub>N - C1s, N 1s)
- VK76** R.V. Vedrinskii and V.L. Kraizman, Bull. Acad. Sci. USSR Phys. Ser. 40 (1976) 114 [Izv. Akad. Nauk. SSSR Ser. Fiz. 40 (1976) 2420]. (SF<sub>6</sub> - S2p, S1s)
- VK&74** R.V. Vedrinskii, A.P. Kovtun, V.V. Kolesnikov, Yu. F. Migal, E.V. Polozhentsev and V.P. Sachenko, Bull. Acad. Sci. USSR Phys. Ser. 38 (1974) 8 [Izv. Akad. Nauk. SSSR Ser. Fiz. 38 (1974) 434] (SF<sub>6</sub>-S2p)
- VK&92** I.Y. Vayrynen, T.A. Kaurila, R.G. Cavell and K.H. Tan, J. Electron Spectrosc. 61 (1992) 55. (PF<sub>3</sub> - P2p)
- VK&09** Y. Velkov, V. Kimberg, N. Kosugi, P. Salek & F. Gel'mukhanov, Chem. Phys. Lett. 476 (2009) 147. O<sub>2</sub>-O1s)
- VM&90** E. Von Raven, M. Meyer, M. Pahler and B. Sonntag, J. El. Spect. 52 (1990) 677. (Xe4d, Kr3d, Ar2p)
- VM&06** G. Vall-llosera, E. Melero García, A. Kivimäki, E. Rachlew, M. Coreno, M. de Simone, R. Richter and K. C. Prince, Phys. Chem. Chem. Phys. 8 (2006) 5199. (H<sub>2</sub>S – S2p)

- VM&07** G. Vall-llosera, E. Melero García, A. Kivimäki, E. Rachlew, M. Coreno, M. de Simone, R. Richter and K. C. Prince, Chem. Chem. Phys. 9 (2007) 389. ( $\text{H}_2\text{S}$  – S2p)
- VNP91** A.S. Vinogradov, S.V. Nebipelov and A.A. Pavylchev, Sov. Phys. Sol. St. 33 (1991) 508 (Fiz. Tverd. Tela (Len) 33 (1991) 896) ( $\text{C}_6\text{H}_6$  - C1s;  $\text{B}_3\text{N}_3\text{H}_6$  - B1s)
- VSZ74** A.S. Vinogradov, B. Shlarbaum and T.M. Zimkina, Opt. Spectrosc. 36 (1974) 383 [Opt. Spektrosk. 36 (1974) 658]. ( $\text{N}_2$  - N1s)
- VS&92** L. Volky, H.E. Saraph, W. Eissner, Z.W. Liu and H.P. Kelly, Phys. Rev. A 46 (1992) 3945. (Be1s)
- VW&00** A. Verwegen, Ph. Wernet, P. Glatzel, B. Sonntag, Ch. Gerth, K. Godehusen and P. Zimmermann, J. Phys. B 33 (2000) 1563. (Cu3p)
- VZ71a** A.S. Vinogradov and T.M. Zimkina, Opt. Spectrosc. 31 (1971) 288 [Opt. Spektrosk. 31 (1971) 542 ]. ( $\text{SiF}_4$  - F1s, S2p)
- VZ71b** A.S. Vinogradov and T.M. Zimkina, Opt. Spectrosc. 31 (1971) 364 [Opt. Spektrosk. 31 (1971) 685]. ( $\text{H}_2\text{S}, \text{SO}_2$  - S2p)
- VZ72** A.S. Vinogradov and T.M. Zimkina, Opt. Spectrosc. 32 (1972) 17 [Opt. Spektrosk. 32 (1972) 33]. ( $\text{SF}_6$  - S2p)
- VZF71** A.S. Vinogradov, T.M. Zimkina and V.A. Fomichev, J. Struct. Chem. 12 (1971) 823 [Zh. Struk. Khim. 12 (1971) 899]. ( $\text{SF}_6$  - F1s)
- VZ&74** A.S. Vinogradov, T.M. Zimkina, V.N. Akimov and B. Shlarbaum, Bull. Acad. Sci. USSR Phys. Ser. 38 No. 3 (1974) 69 [Izv. Akad. Nauk. SSSR Fiz. Ser. 38 (1974) 508] ( $\text{N}_2$ ,  $\text{NF}_3$  - N1s;  $\text{NF}_3$  - F1s;  $\text{O}_2$  - O1s)
- W65** F. Wuilleumier, J. de Phys. (Paris) 26 (1965) 776. (Ar1s)
- Wa65** T. Watanabe, Phys. Rev. 139 (1965) 1747. (Ar1s)
- W70** F. Wuilleumier, C.R. Acad. Sci. Paris 270 (1970) 825. (Ne1s)
- W71** F. Wuilleumier, J. de Phys. (Paris) 32 (1971) C4-88.
- W75** G. Wendin, Phys. Lett. A 51 (1975) 291. (Ba4d)
- W76** G. Wendin, J. Phys. B 9 (1976) L297. (Ba4d)
- W80** M.J. Van der Wiel, Proc. XI ICPEAC (Kyoto, 1979) 209. (REVIEW  $\text{SF}_6$ -S1s;  $\text{N}_2$ -N1s; CO-C1s;  $\text{CHCl}_3, \text{CCl}_4$ -Cl2p)
- W84** G. Wendin, Phys. Rev. Lett. 53 (1984) 724. (La3p, Th5d, U5d)
- W92** A.T. Wen, Ph.D. thesis, McMaster University (1992). ( $\text{C}_9\text{H}_7\text{MnO}_3$  - C1s, O1s, Mn3p,2p;  $\text{SiCl}_4$ ,  $\text{Si}_2\text{Cl}_6$  - Si2p, Cl2p;  $\text{SiMe}_4$ ,  $\text{Si}_2\text{Me}_6$ ,  $\text{Si}_6\text{Me}_{12}$ ,  $\text{Si}[\text{Si}(\text{CH}_3)_3]_4$ - C1s, Si2p;  $\text{CpTiCl}_3$ ,  $\text{Cp}_2\text{TiCl}_2$ ,  $\text{TiCl}_4$  -C1s, Cl2p, Ti2p)
- W01** J.B. West, J. Phys. B 34 (2001) R45. (review; Al2p, Ba4d, C1s, Cr2p, I4d, Mg2p, Mn2p, Na2p, Si2p, Xe4d)

- WA&98** N. Watanabe, X. Awaya, A. Fujino, Y. Itoh, M. Kitajima, T.M. Kojima, M.Oura, R.Okuma, M. Sano, T. Sekioka and T. Koizumi, J. Phys. B 31 (1998) 4137.(Xe4d)
- WA&01** J.B. West, T. Andersen, R.L. Brooks, F. Folkmann, H. Kjeldsen, H. Knudsen, Phys. Rev. A 63 (2001) 052719. (Al2p)
- WB72** H.H. Wellenstein and R.A. Bonham, Chem. Phys. Lett. 15 (1972) 530. (Ar2p)
- WB74a** G.R. Wight and C.E. Brion, J. El. Spectrosc. 3 (1974) 191. (CO<sub>2</sub>, N<sub>2</sub>O - C1s, N1s, O1s)
- WB74b** G.R. Wight and C.E. Brion, J. El. Spectrosc. 4 (1974) 25. (CH<sub>4</sub>, NH<sub>3</sub>, H<sub>2</sub>O, CH<sub>3</sub>OH, CH<sub>3</sub>OCH<sub>3</sub>, CH<sub>3</sub>NH<sub>2</sub> - C1s,N1s, O1s)
- WB74c** G.R. Wight and C.E. Brion, J. El. Spectrosc. 4 (1974) 313. (NO, O<sub>2</sub> - N1s, O1s)
- WB74d** G.R. Wight and C.E. Brion, J. El. Spectrosc. 4 (1974) 327. (CF<sub>4</sub> - C1s, F1s)
- WB74e** G.R. Wight and C.E. Brion, J. El. Spectrosc. 4 (1974) 335. (CS<sub>2</sub>, COS - C1s, S2p, O1s)
- WB74f** G.R. Wight and C.E. Brion, J. El. Spectrosc. 4 (1974) 347. [(CH<sub>3</sub>)<sub>2</sub>CO - C1s, O1s]
- WB74g** G.R. Wight and C.E. Brion, Chem. Phys. Lett. 26 (1974) 607. (Z+1 analogy - H<sub>2</sub>O, NH<sub>3</sub>, CH<sub>4</sub>)
- WB74h** G.R. Wight and C.E. Brion, Proc. 4th Int. Vac. UV Rad. Phys. Conf. (Hamburg, 1974) 184. (CH<sub>4</sub>-C1s; NH<sub>3</sub>-N1s; H<sub>2</sub>O-O1s)
- WBW73** G.R. Wight, C.E. Brion and M.J. Van der Wiel, J. El. Spectrosc. 1 (1972/73) 457. (N<sub>2</sub>, CO - C1s, N1s)
- WBW99** K. Weiss, P.S. Bagus and Ch. Woll, J. Chem.Phys. 111 (1999) 6834. (C<sub>3</sub>H<sub>8</sub>,C<sub>4</sub>H<sub>10</sub> – C1s)
- WBW02** R. Wehlitz, J. B. Bluett, and S. B. Whitfield, Phys. Rev. Lett. 89 (2002) 093002. (Li1s)
- WCK91** S.B. Whitfield, C.D. Caldwell and M.O. Krause, Phys. Rev. A 43 (1991) 2338. (Mg2p)
- WC&92** S.B. Whitfield, C.D. Caldwell, D.X. Huang and M.O. Krause, J. Phys. B 25 (1992) 4755. (Xe4d).
- WC&05** J. Wang, G. Cooper, D. Tulumello and A.P. Hitchcock, J. Phys. Chem. A 109 (2005) 10886. (Br<sub>2</sub>C<sub>12</sub>H<sub>8</sub>, C<sub>12</sub>F<sub>10</sub>, C<sub>12</sub>H<sub>10</sub> - C1s)
- WB&76** H.W. Wolff, R. Bruhn, K. Radler, B. Sonntag, Phys. Lett. A 59 (1976) 67. (Ce4d)
- WDD82** S. Wallace, D. Dill and J.L. Dehmer, J. Chem. Phys. 76 (1982) 1217. (NO-N1s,O1s)
- WD&97** F.J. Wuilleumier, S. Diehl, D. Cubaynes, J.M. Bizau and E.T. Kennedy, J. Electron Spectrosc. 88-91 (1997) 41. (Li1s) - ICES-7
- WF&00** H. Wang, R.F. et al. MaxLab Report (2000) 190. (NO – N1s)
- WF&01** H. Wang, R.F. Fink, M N Piancastelli, I Hjelte, K Wiesner, M Bässler, R Feifel, O Björneholm, C Miron, A Giertz, F Burmeister, S L Sorensen and S Svensson, J. Phys. B. 34 (2001) 4417. (NO – N1s)
- WH90** A.T. Wen and A.P. Hitchcock, (1990) unpublished. (C<sub>2</sub>HCl<sub>3</sub> - C1s, Cl2p)

- WH93** A.T. Wen and A.P. Hitchcock, Can. J. Chem. 71 (1993) 1632. ( $\text{CpTiCl}_3$ ,  $\text{Cp}_2\text{TiCl}_2$ ,  $\text{TiCl}_4$  - C1s, Cl2p, Ti2p)
- WHR92** A.T. Wen, A.P. Hitchcock and E. Ruhl, (1992) unpublished. ( $\text{BzCr}(\text{CO})_3$ ,  $\text{CrBz}_2$ ,  $\text{CH}_3\text{-BzCr}(\text{CO})_3$  - C1s,  $\text{Cr}_2\text{p}_3\text{p}$ , O1s;  $\text{C}_9\text{H}_5\text{O}_4\text{V}$  - V2p, C1s, O1s)
- WH&90** A.T. Wen, A.P. Hitchcock, N.H. Werstiuk, N. Nguyen and W.J. Leigh, Can. J. Chem. 68 (1990) 1967. ( $\text{C}_7\text{H}_{10}$ ,  $\text{C}_8\text{H}_{12}$ ,  $\text{C}_8\text{F}_3\text{H}_9$  - C1s)
- WJ&94** F.J. Wuilleumier, L. Journal, B. Roussellow, D. Cubaynes, J.M. Bizeau, Z. Liu, J. Liu, M. Richter, P. Slodeczak, K.H. Selmann and P. Zimmermann, Phys. Rev. Lett. 73 (1994) 3074. (Na2p)
- WJ&01** Th Weber, O Jagutzki, M Hattass, A Staudte, A Nauert, L Schmidt, M H Prior, A L Landers, A Bräuning-Demian, H Bräuning, C L Cocke, T Osipov, I Ali, R Diez Muiño, D Rolles, F J García de Abajo, C S Fadley, M A Van Hove, A Cassimi, H Schmidt-Böcking and R Dörner, J. Phys. B 34 (2001) 3669. (CO – C1s, N<sub>2</sub> – N1s)
- WK74** F. Wuilleumier and M.O. Krause, Phys. Rev. A 10 (1974) 242. (Ne1s)
- WK&94** S.B. Whitfield, M.O. Krause, P. van der Muellen and C.D. Caldwell, Phys. Rev. A 50 (1994) 1269. (Mn3p)
- WK&01** S.B. Whitfield, K. Kehoe, R. Wehlitz, M.O. Krause, C.D. Caldwell, Phys. Rev. A 64 (2002) 022701. (Sc3p)
- WL98** F. Wang and F.P. Larkins, J. Phys. B 31 (1998) 1649. (NO - N1s, O1s)
- WM69** W.S. Watson and F.J. Morgan, J. Phys. B 2 (1969) 277. (Ar2p, Kr3p, Xe4s)
- WM78** J.B. West and R.X. Morton, At. Data Nucl. Data Tables 22 (1978) 106. (total and partial cross-sections)
- WMT89** H.X. Wan, J.H. Moore and J.A. Tossell, J. Chem. Phys. 91 (1989) 7343. ( $\text{SiX}_4\text{H}_{4-x}$ , x=0-3, SiF<sub>4</sub> - Si2p)
- WMT92** H.X. Wan, J.H. Moore and J.A. Tossell, unpublished ( $\text{CCl}_x\text{F}_{4-x}$ , x= 0-4 - C1s)
- WMT94a** D.C. Winkler, J.H. Moore and J.A. Tossell, Chem. Phys. Lett. 219 (1994) 57. ( $\text{SiH}_x\text{Cl}_{4-x}$ , x=0-2 - Si2p)
- WMT94b** D.C. Winkler, J.H. Moore and J.A. Tossell, Chem. Phys. Lett. 222 (1994) 1. ( $\text{SiMe}_x(\text{OMe})_{4-x}$ , x=0-4 - Si2p)
- WPM77** H.T. Wang, W.S. Felps and S.P. McGlynn, J. Chem. Phys. 67 (1977) 2614. (H<sub>2</sub>O - O1s)
- WP&98** H. Wang, M.N. Piancastelli et al. MaxLab Report (1998) 198. (NO – N1s, O1s)
- WRE89a** B. Wastberg, A. Rosen and D.E. Ellis, Z. Phys. D 12 (1989) 377 (Mn<sub>2</sub> - Mn1s; Co<sub>2</sub> - Co1s; Ni<sub>2</sub> - Ni1s)
- WRE89b** B. Wastberg, A. Rosen and D.E. Ellis, Z. Phys. D 13 (1989) 153 (Fe<sub>2</sub> - Fe1s; Ni<sub>2</sub>, Ni<sub>3</sub> - Ni1s)
- WRH89** A.T. Wen, E. Ruhl and A.P. Hitchcock, (1989) unpublished. ( $\text{C}_{13}\text{H}_{20}\text{MnO}$  -C1s, O1s, Mn2p, Mn3p;  $\text{C}_{10}\text{Cl}_2\text{H}_{10}\text{V}$ ,  $\text{C}_{10}\text{H}_{10}\text{Mg}$  – C1s)
- WRH92** A.T. Wen, E. Ruhl and A.P. Hitchcock, Organometallics 11 (1992) 2559. (FeCp<sub>2</sub>,  $\text{Fe}(\text{CO})_5$ ,  $\text{Fe}_2(\text{CO})_9$ ,  $\text{C}_4\text{H}_6\text{Fe}(\text{CO})_3$ , 1,3-C<sub>6</sub>H<sub>8</sub>Fe(CO)<sub>3</sub>, COT-Fe(CO)<sub>3</sub>, Fe(Cp)<sub>2</sub>,  $\text{C}_2\text{H}_3\text{CpFeCp}$ ,  $\text{C}_4\text{H}_9\text{CpFeCp}$  - C1s, O1s, Fe3p, Fe2p)
- WR&82** H.W. Wolff, K. Radler, B. Sonntag and R. Haensel, Z. Phys. 257 (1972) 353. (Na2p,2s)

- WR&98** Xin Wang, Sivasudhan Rathnachalam, et al., Site-selective soft X-ray absorption as a tool to study protonation and electronic structure of gas-phase DNA, *Physical review* 58 (1998) 8097. ( $\text{C}_{14}\text{H}_{14}\text{N}_{12}\text{O}_3$ , 5'-d( $^{\text{F}}$ UAG) - Ns)
- WR&01** K.R. Wilson, B.J. Rude, T. Catalano, R.D. Schaller, J.G. Tobin, D.T. Co and R.J. Saykally, *J. Phys. Chem B* 105 (2001) 3346. ( $\text{H}_2\text{O}$ - O1s)
- WR&21** Xin Wang, Sivasudhan Rathnachalam et al., Site-selective soft X-ray absorption as a tool to study protonation and electronic structure of gas-phase DNA, *Phys. Chem. Chem. Phys.*, 2021, 23, 11900. (5' -d( $^{\text{F}}$ UAG) - N1s)
- WS72** M.J. Van der Wiel and Th.M. El-Sherbini, *Physica* 59 (1972) 453. ( $\text{N}_2$  - N1s; CO - C1s)
- WS76** H.W. Wolff, B.F. Sonntag, 2nd Int. Conf. on Inner Shell Ioniz. Phen., Abstracts, Freiburg (1976) 78. (CsF - Cs4d)
- WS78** G. Wendin and A.F. Starace, *J. Phys. B* 11 (1978) 4119. (Ba4d, La4d)
- WSB70** M.J. Van der Wiel, Th. M. El-Sherbini and C.E. Brion, *Chem. Phys. Lett.* 7 (1970) 161. (CO - C1s, O1s;  $\text{N}_2$  - N1s)
- WS&75** H.F. Wellenstein, H. Schmoranzer, R.A. Bonham, T.C. Wong and J.S. Lee, *Rev. Sci. Inst.* 46 (1975) 92. ( $\text{N}_2$  - N1s)
- WTA91** S.B. Whitfield, J.Tulkki and T. Aberg, *Phys. Rev. A* 44 (1991) R6983. (Mg2p)
- WW71** M.J. Van der Wiel and G. Wiebes, *Physica* 53 (1971) 225. (Ar2p)
- WW77** G.R. Wight and M.J. Van der Wiel, *J. Phys. B* 10 (1977) 601. (Xe4d)
- WW97** D.K. Waterhouse and J.F. Williams, *Phys. Rev. Lett.* 79 (1997) 391. (Ar2p)
- WWT76** M.J. Van der Wiel, G.R. Wight and R.R. Tol, *J. Phys. B* 9 (1976) L5. (Ar2p)
- WW&96** W.B. Weterveld, J. van der Weg, J. van Eck, H.G.M. Heideman and J.B. West, *Chem. Phys. Lett.* 252 (1996) 107. (CO - C1s)
- WW&02** S.B. Whitfield, R. Whelitz, M.O.Krause and C.D. Caldwell, *Surf. Rev. Lett.* 9 (2002) 1229. (Fe3p)
- WZ&97** R.M. Wood, Q. Zheng, A.K. Edwards and M.A. Mangai, *Rev. Sci. Inst.* 68 (1997) 1382. ( $\text{N}_2$  - N1s)
- XJ&95** J.Z. Xiong, D.T. Jiang, Z.F. Liu, K.M. Baines, T.K. Sham, K.H. Tan and X.H. Feng, *Physica B* 208 (1995) 451. ( $\text{C}_{12}\text{H}_{36}\text{Si}_5$  - Si2p, Si1s)
- XJ&96a** J.Z. Xiong, D.T. Jiang, Z.F. Liu, K.M. Baines, T.K. Sham, S.G. Urquhart, A.T. Wen, T. Tyliszczak, A.P. Hitchcock, *Chem. Phys.* 203 (1996) 81. ( $\text{C}_6\text{H}_{18}\text{Si}_2$  - Si2p, Si2s, Si1s)
- XJ&96b** J.T. Zong, D. Jiang, C.E. Dixon, K.M. Baines and T.K. Sham, *Can. J. Chem.* 74 (1996) 2229. ( $\text{SiMe}_4$ ,  $\text{Si}(\text{SiMe}_3)_4$ ,  $\text{Si}(\text{GeMe}_3)_4$ ,  $\text{Ge}(\text{SiMe}_3)_4$  - Si 1s)
- XW&22** Xu, Yuan-Chen, Shu-Xing Wang, Xiao-Jiao Du, Li-Han Wang, and Lin-Fan Zhu. "Probing the Delocalized Core-Hole via Inner-Shell Excitation in  $\text{N}_2$ ." *New Journal of Physics* 24 (2022): 053036.

- XX04** (operators unknown) (2004) unpublished (C<sub>16</sub>H<sub>19</sub>N<sub>4</sub>O<sub>2</sub> – C1s, N1s, O1s)
- Y93** L. Yang, J. Phys.B 26 (1993) 1813. (Na1s)
- YA&86** A. Yagshita, S. Arai, C.E. Brion, T. Hayaishi, J. Murakami, Y. Sato and U. Ukai, Chem. Phys. Lett. 132 (1986) 437. (SiH<sub>4</sub> - Si2p)
- YA96** L. Yang and H. Agren, Phys. Rev. B 54 (1996) 1. (H(C<sub>2</sub>H<sub>2</sub>)<sub>n</sub>H, n=1-5 - C1s)
- YA&96** L. Yang, H. Agren, V. Carravetta and L.G.M. Pettersson, Phys. Scripta 54 (1996) 614. (CO, H<sub>2</sub>CO, CO<sub>2</sub>, (CH<sub>3</sub>)<sub>x</sub>H<sub>2-x</sub>CO, x=0-2, C<sub>3</sub>H<sub>8</sub>CO, C<sub>4</sub>H<sub>10</sub>CO, C<sub>6</sub>H<sub>14</sub>CO - C1s, O1s)
- YA&97** L. Yang, H. Agren, L.G.M. Pettersson and V. Carravetta, J. Electron Spectrosc. 83 (1997) 209. (CO, H<sub>2</sub>CO, CO<sub>2</sub>, H<sub>2</sub>CO, MeHCO, Me<sub>2</sub>CO, EtHCO, Et<sub>2</sub>CO, Pr<sub>2</sub>CO, PrHCO; COCu, COCu<sub>17</sub>, COCu<sub>50</sub> - C1s, O1s)
- YE&99** K. Yoshiki Franzén, P. Erman, A. Karawajczyk, E. Rachlew, P. A. Hatherly and M. Stankiewicz, J. Chem. Phys. 110 (1999) 3621 (CS<sub>2</sub> - C1s)
- YHA05** A. Yagashita, K Hosaka and J.I. Adachi, J. El. Spec. Rel. Phen. 142 (2005) 295. (CO, CO<sub>2</sub> - C1s, O1s, N<sub>2</sub>, NO - N 1s, NO - O1s)
- YHT88** B.X. Yang, D.M. Hanson and K. Tohji, J. Chem. Phys. 89 (1988) 1215. (O<sub>2</sub>-O1s)
- YH&00** B.W. Yates, Y.F. Hu, K.H. Tan, G. Ratzlaff, R.G. Cavell, T.K. Sham and G.M. Bancroft, J. Synchr. Rad. 7 (2000) 296. (N<sub>2</sub>, NO – N1s, CO – C1s)
- YI&17** Zhong Yin, Ludger Inhester, et al., Cationic and Anionic Impact on the Electronic Structure of Liquid Water, J. Phys. Chem. Lett. 8 (2017) 3759. (H<sub>2</sub>O – O1s)
- YK87** B.X. Yang, and J. Kirz, Phys. Rev. B 35 (1987) 6100. (CO<sub>2</sub>-O1s EXAFS)
- YKD90** V.A. Yavan, A.N. Khoperskii and V.F. Demekhin, Opt. Spectrosc. (USSR) 68 (1990) 134. (Opt. i Spekt. 68 (1990) 231). (Kr1s, Xe1s)
- YKS84** B.X. Yang, J. Kirz and T.K. Sham, NSLS Report (1984) 189. (CO<sub>2</sub>-O1s)
- YKS85a** B.X. Yang, J. Kirz and T.K. Sham, Nucl. Inst. Meth. Phys. Res. A 236 (1985) 419. (CO<sub>2</sub> - O1s)
- YKS85b** B.X. Yang, J. Kirz and T.K. Sham, Phys. Lett. A 110 (1985) 301. (O<sub>2</sub>, CO, CO<sub>2</sub>-O1s)
- YKS86** B.X. Yang, J. Kirz and T.K. Sham, J. Phys.(Paris) 47 C-8 (1986) 585. (O<sub>2</sub>, CO, CO<sub>2</sub>, COS - O1s EXAFS)
- YKS87** B.X. Yang, J. Kirz and T.K. Sham, Phys. Rev. A 36 (1987) 4298. (CO, CO<sub>2</sub>, COS, (CH<sub>3</sub>)<sub>2</sub>CO, CH<sub>3</sub>OH, Et<sub>2</sub>O, C<sub>4</sub>H<sub>8</sub>O, C<sub>8</sub>H<sub>8</sub>O<sub>2</sub> - O1s)
- YK&86a** V.A. Yavna, A.N. Khoperskii, I.D. Petrov and V.L. Sukhorukov, Opt. Spect (USSR) 61 (1986) 273; [Opt. Spekt. 61 (1986) 435] (Na1s)
- YK&86b** V.A. Yavna, A.N. Khoperskii, I.D. Petrov and V.L. Sukhorukov, Opt. Spect (USSR) 61 (1986) 577; [Opt. Spekt. 61 (1986) 922] (Ar1s,2p)

- YK&96** T. Yokoyama, K. Kobayashi, T. Ohta and A. Ugawa, Phys. Rev. B 53 (1996) 6111. ( $\text{Br}_2$  -  $\text{Br1s}$ ;  $\text{HgCl}_2$  -  $\text{Hg2p}$ )
- YL94** J.F. Ying and K.T. Leung, J. Chem. Phys. 101 (1994) 7311. ( $\text{CF}_{4-n}\text{Cl}_n$ ,  $n=0-4$  -  $\text{C1s}$ ,  $\text{Cl2p}$ )
- YML93** J.F. Ying, C.P. Mathus and K.T. Leung, Phys. Rev. A 47 (1993) R5. ( $\text{SF}_6$  -  $\text{S2p}$ )
- YM&84** V.D. Yumatov, L.N. Mazalov, A.V. Okotruhl and I.A. Topol, J. Struct. Chem. 25 (1984) 545. ( $\text{POCl}_3$  -  $\text{P2p}$ ,  $\text{Cl2p}$ )
- YM&89** A. Yagashita, H. Maezawa, M. Ukai and E. Shigemasa, Phys. Rev. Lett. 62 (1989) 36. ( $\text{N}_2$  -  $\text{N1s}$ )
- YM&92** A. Yagashita, S. Masui, T. Toyoshima, H. Maezawa and E. Shigemasa, Rev. Sci. Inst. 63 (1992) 1351. ( $\text{CO-C1s}$ ,  $\text{N}_2\text{-N1s}$ ,  $\text{Ne1s}$ )
- YND94** V.A. Yavna, A.M. Nadolinsky and V.F. Demekhina, J. El. Spec. 68 (1994) 267. ( $\text{CO-C1s}$ ;  $\text{CO, O}_2\text{-O1s}$ )
- YNH98** V.A. Yavna, A.M. Nadolinsky and A,N, Hopersky, J. El. Spec. 94 (1998) 49. ( $\text{CO-C1s}$ )
- YN&02** H. Yoshida, K. Nobusada, K. Okada, S. Tanimoto, N. Saito, A. De Fanis, and K. Ueda, Phys. Rev. Lett. 88 (2002) 083001. ( $\text{CO}_2$  -  $\text{C1s}$ )
- YOW01** Yoshinori Iketaki, Kazumasa Ohtsuki and Tsutomu Watanabe , J. Phys. B 34 (2001) 1889. ( $\text{NO-N1s,O1s}$ )
- YO&02** H. Yamaoka, M. Oura, K. Kawatsura, T. Hayaishi, T. Sekioka, A. Agui, A. Yoshigoe, and F. Koike, Phys. Rev. A 65 (2002) 012709. ( $\text{Ne1s}$ )
- YPD91** V.A. Yavna, V.A. Popov and L.A. Demekhina, Opt. Spectrosc. (USSR) 70 (1991) 155 [Opt. i Spek. 70 (1991) 270] ( $\text{HCl-Cl2p}$ )
- YPM85** C.H. Yu, R.M. Pitzer and C.W. McCurdy, Phys. Rev. A 32 (1985) 2134. ( $\text{N}_2\text{-N1s}$ )
- YP&86** V.A. Yavna, I.D. Petrov, L.A. Demekhina, A.N. Khoperskii and V.L. Sukhorukov, Opt. Spect (USSR) 74 (1986) 552; [Opt. Spekt. 74 (1993) 3765] ( $\text{Na1s}$ )
- YP&93** V.A. Yavna, V.A. Popov, S.A. Yavna and L.A. Demekhina, Opt. Spect (USSR) 74 (1993) 413; [Opt. Spekt. 74 (1993) 695] ( $\text{SiH}_4\text{-Si2p}$ )
- YP&97** L.Yang, O. Plachkevytch, H. Agren and L.G.M. Pettersson, J. Phys. C 2 (1997) 227. ( $\text{C}_6\text{H}_7\text{N}$ ,  $\text{C}_6\text{H}_6\text{O}$ ,  $\text{C}_6\text{H}_5\text{F}$ ,  $\text{C}_8\text{H}_6\text{O}_2$  -  $\text{C1s}$ )
- YS92** A. Yagashita and E. Shigemasa, Rev. Sci. Inst. 63 (1992) 1383. ( $\text{CO-C1s}$ ;  $\text{N}_2\text{-N1s}$ ;  $\text{O}_2\text{-O1s}$ )
- YSK94** A. Yagashita, E. Shigemasa and N. Kosugi, Phys. Rev. Lett. 72 (1994) 3961. ( $\text{O}_2$  -  $\text{O1s}$ )
- YS&90** T. Yokoyama, K. Seki, I. Morisada, K. Edamatsu and T. Ohta, Phys. Scripta 41 (1990) 189. ( $\text{C}_6\text{H}_6$  -  $\text{C1s}$ , polyphenylenes, polyacenes)
- YS&02** G. Yalovega, A.V. Soldatov, M. Riedler, M.R. Pederson, A. Kolmakov, C. Nowak and T. Möller, Chem. Phys. Lett. 356 (2002) 23. ( $\text{NaCl}_4$  -  $\text{Cl2p}$ ,  $\text{Na1s}$ )
- YW83** O. Yagci and J.E. Wilson, J. Phys. C 16 (1983) 383. ( $\text{Xe 3d}$ )

- YY&99** H. Yoshida, T. Yangihara et al. UVSOR Report (1999) 66. ( $C_5H_8O_2$  – O1s)
- YZ&02** Z.S. Yuan, L.F. Zhu, X.J. Liu, Z.P. Zhong, W.B. Li, H.D. Cheng, and K.Z. Xu, Phys. Rev A 66(2002) 062701 (Kr3d)
- Z99** O. Zatsarinny, J. Phys. B 32 (1999) L565. (Li1s)
- ZAV87** A.V. Zadenov, V. N Akimov and A.S. Vingradov, Opt. Spectrosc (USSR) 62 (1987) 204; [Opt. Spekt. 62 (1987) 340] ( $N_2N1s$ )
- ZB93** O.I. Zatsarining and L.A. Bandurina, J. Phys. B 26 (1993) 3765. (Na2p)
- ZBS75** P. Ziem, R. Bruch and N. Stolterfoht, J. Phys. B. 8 (1975) L480. (Li1s)
- ZCB90** E.B. Zarate, G. Cooper and C.E. Brion, Chem. Phys. 148 (1990) 289. ( $PH_3$  - P2p,2s)
- ZC&89** W. Zhang, G. Cooper, T. Ibuki and C.E. Brion, Chem. Phys. 137 (1990) 391. ( $CF_4$  - C1s, F1s)
- ZC&09** Zhang W, Carravetta V, Plekan O, Feyer V, Richter R, Coreno M, Prince KC (2009) Electronic structure of aromatic amino acids studied by soft x-ray spectroscopy. J Chem Phys 131 (2009) 035103. ( $C_9H_9N$  Me-indole,  $C_9H_{11}NO_2$  (Ph-Ala),  $C_9H_{11}NO_3$  (tyrosine,  $C_{11}H_{12}N_2O_2$  (Tryp)– C1s, N1, O1s)
- ZF67** T.M. Zimkina and V.A. Fomichev, Sov. Phys. Doklady 11 (1967) 726 [Dokl. Akad. Nauk. SSSR 169 (1966) 1304]. ( $SF_6$  - S2p)
- ZG71** T.M. Zimkina and S.A. Gribovskii, J. de Phys. 32 (1971) C4-282. (review of atomic photoionisation; Kr3d, Xe4d)
- ZIB92** W. Zhang, T. Ibuki and C.E. Brion, Chem. Phys. 160 (1992) 435. ( $CF_xCl_{4-x}$ , x=1-3, F1s, C1s, Cl2p,2s)
- ZKP92** B. Zhan, L. Kissel and R.H. Pratt, Phys. Rev. A 45 (1992) 2983. (Ar2p,Ne1s)
- ZK&15** M. Žitnik, M. Kavčič, R. Bohinc, K. Bučar, A. Mihelič, W. Cao, R. Guillemin, L. Journel, T. Marchenko, S. Carniato, E. Kawerk, M.N. Piancastelli, M. Simon, J. El. Spec. 204 (2015) 356. ( $CCl_2H_2$ ,  $CCl_3H$ ,  $CCl_4$ ,  $C_2ClH_5$ ,  $C_2Cl_2H_2$ ,  $C_2Cl_2H_4$ ,  $C_2Cl_2H_6$ ,  $C_2Cl_3H_3$ ,  $C_6ClH_5$  – Cl 1s)
- ZL84** A. Zangwill and D.A. Liberman, J. Phys. B 17 (1984) L253. (Xe3d)
- ZMP83** A. Zhang, J.F. Morar and R.L. Park, J. Vac. Sci. Tech. A 1 (1983) 461. ( $CO,CO_2$  C1s,O1s;  $N_2N1s$ )
- ZS80** A. Zangwill and P. Soven, Phys. Rev. Lett. 45 (1980) 204. (Ba4d)
- ZS&90** W. Zhang, K.H. Sze, C.E. Brion, X.M. Tong and J.M. Li, Chem. Phys. 140 (1990) 265. ( $NO_2$  - N1s, O1s)
- ZS&91** K. Zhang, E.A. Stern, J.J. Rehr and D.E. Ellis, Phys. Rev. B 44 (1991) 2030. (Xe2p,2s)
- ZTC03** P. Zhu, J. Tang and S. Cao, J. El. Spec. 129 (2003) 27. ( $C_2H_2$ ,  $C_2H_4$ ,  $C_2H_6$  – C1s)
- ZT&79** J.P. Ziesel, D. Teillet-Billy, L. Bouby and R. Paineau, Chem. Phys. Lett. 63 (1979) 47. (CO - K-shell excited negative ion resonances)

- ZV71** T.M. Zimkina and A.S. Vinogradov, J. de.Phys. (Paris) 32 (1971) C4-3. (review; SF<sub>6</sub>,SO<sub>2</sub>,H<sub>2</sub>S-S2p; SiF<sub>4</sub>,SiCl<sub>4</sub>-Si2p; SF<sub>6</sub>,SiF<sub>4</sub>-F1s)
- ZV72** T.M. Zimkina and A.S. Vinogradov, Bull. Acad. Sci. USSR Phys. Ser. 36 (1972) 229 [Izv. Akad. Nauk. SSSR Fiz. Ser. 36 (1972) 248]. (review; SO<sub>2</sub>,CS<sub>2</sub>,H<sub>2</sub>S,SF<sub>6</sub> - S2p; SiF<sub>4</sub> - Si2p; NF<sub>3</sub> - N1s; B<sub>2</sub>H<sub>6</sub>,BF<sub>3</sub> - B1s; SF<sub>6</sub>, SiF<sub>4</sub>,BF<sub>3</sub> - F1s)
- ZY02** J. Zeng and J. Yuan, J. Phys. B 35 (2002) 3041. (O1s)
- ZZ&92** Y. Zhang, Y. Zhou, Z. Luo and D.M. Hanson, J. Phys.Chem. 96 (1992) 2949. (CO-C1s; HCN - C1s,N1s; N<sub>2</sub>O, NO<sub>2</sub> - N1s,O1s; H<sub>2</sub>O, O<sub>3</sub> - O1s)
- ZZL97** Y. Zhang, P.H. Zhang and J.M. Li, Phys. Rev. A 56 (1997) 1819. (N<sub>2</sub> - N1s; CO - C1s, O1s)

---

## REVIEW ARTICLES (time order)

---

- S66** J.A.R. Samson, Adv. Atom. Mol. Phys. 2 (1966) 178.
- FC68** U. Fano and J. W. Cooper, Rev. Mod. Phys. 40 (1968) 441.
- ZG71** T.M. Zimkina and S.A. Gribovskii, J. de Phys. 32 (1971) C4-282.
- ZV71** T.M. Zimkina and A.S. Vinogradov, J. de.Phys. (Paris) 32 (1971) C4-3.
- D72** J.L. Dehmer, J. Chem. Phys. 56 (1972) 4496.
- F72** U. Fano, Comments At. Mol. Phys. 3 (1972) 75.
- C73** K. Codling, Rep. Prog. Phys. 36 (1973) 541.
- AP74** L.V. Azaroff and D.M. Pease, X-ray Absorption Spectroscopy, Ch 6 in *X-ray Spectroscopy* (L.V. Azaroff, ed.) (1974, McGraw-Hill, NY)
- S74** W.H.E. Schwarz, Angew. Chem. Int. Ed. Engl. 13 (1974) 454.
- R75** M.B. Robin, Chem. Phys. Lett. 31 (1975) 140.
- FTD76** U. Fano, C.E. Theodosiou and J.L. Dehmer, Rev. Mod. Phys. 48 (1976) 49.
- C78** J.P. Connerade, Contemp. Phys. 19 (1978) 415.
- R78** F.H. Read, J. Phys. Coll. 1 S5 (1978) 82.
- KS79** E.E. Koch and B.F. Sonntag in, Topics in Current Physics 10 *Synchrotron Radiation*. (Springer, Heidelberg, 1979) 269.
- B80** F.C. Brown, 'Inner-shell Threshold Spectra', Ch. 4 in *Synchrotron Radiation Research*, Winnick and S. Doniach (eds.) (Plenum, NY, 1980).
- S80b** A.F. Starace, Appl. Optics 19 (1980) 4051.
- W80** M.J. Van der Wiel, Proc. XI ICPEAC (Kyoto, 1979) 209.
- B82a** C.E. Brion, Physics of Electronic and Atomic Collisions, (Proc. of XII ICPEAC, Tennessee, 1981), S. Datz, ed. (North-Holland, 1982).
- BD&82** C.E. Brion, S. Daviel, R.N.S. Sodhl and A.P. Hitchcock, Int. Conf. on X-ray and Atomic Inner-Shell Physics, AIP Conf. Proc. 94 (1982) 429.
- DBH83** S. Daviel, C.E. Brion and A.P. Hitchcock, Rev. Sci. Inst. 55 (1984) 182.
- B85** C.E. Brion, Com. At. Mol. Phys. 16 (1985) 249.

- R85** M.B. Robin, *Higher Excited States of Polyatomic Molecules* (Vol. 3, Academic, Florida, 1985).
- VA&85** A.S. Vinogradov, V.N. Akimov and A.A. Pavylchev, Bull. Acad. Sci. USSR 49 (1985) 1 (Izv. Sib. Otd. Akad. Nauk SSSR Ser. Fiz. 49 (1985) 1458).
- NB87** I. Nenner and J.A. Beswick, *Photodissociation and Photoionisation*, Chapter 6 in *Handbook on Synchrotron Radiation*, Vol. 2 (G. Marr, ed) (Elsevier, 1987).
- H89** A.P. Hitchcock, Ultramicroscopy, 28 (1989) 165.
- H90a** A.P. Hitchcock, Phys. Scripta T31 (1990) 159. (**Review:** Ne1s; NH<sub>3</sub>, N<sub>2</sub>H<sub>4</sub>, N<sub>2</sub> - N1s; PCl<sub>3</sub> - Cl2p; C<sub>2</sub>H<sub>6</sub>, C<sub>2</sub>H<sub>3</sub>F<sub>3</sub>, CF<sub>4</sub>, C<sub>2</sub>F<sub>6</sub>, C<sub>2</sub>F<sub>4</sub>, C<sub>6</sub>F<sub>6</sub>, CO, Mn(CO)<sub>5</sub>Br, Fe(CO)<sub>5</sub>, Co<sub>2</sub>(CO)<sub>8</sub>, Ni(CO)<sub>4</sub>, MCp<sub>2</sub> (M = Fe,Co,Ni), C<sub>5</sub>H<sub>6</sub> - C1s; CF<sub>3</sub>O<sub>2</sub>CF<sub>3</sub> - O1s)
- H90b** D.M. Hanson, Adv. Chem. Phys. 77 (1990) 1.
- S90b** N. Saito, Research of the Electrotechnical Laboratory, No. 910 (1990) 88 pages.
- H92b** A.P. Hitchcock, *Collision Processes of Ions, Positrons, Electrons and Photons with Matter*, Proc. ELAF-91 (World Scientific, 1992) 104.
- K92** P. Kitzler, "Directory of Numerical XANES Studies", Phys. Lett. A 172 (1992) 66.
- S92** J. Stöhr, *NEXAFS Spectroscopy*, Spr. Ser. Surf. Sci. Vol. 25 (Heidelberg, 1992).
- Sc92** V. Schmidt, "Photoionisation of Atoms using Synchrotron Radiation", Rep. Prog. Phys. 55 (1992) 1483.
- SZ92** B. Sonntag and P. Zimmermann, *XUV Spectroscopy of Metal Atoms*, Rep. Prog. Phys. 55 (1992) 911-987.
- HM94** A.P. Hitchcock and D.C. Mancini, "Bibliography and Database of Inner-shell Excitation Spectra of Gas Phase Atoms and Molecules", J. Electron Spectrosc. 67 (1994) 1.
- G94** F.M.F. de Groot, "Review of Theory and Experiment for X-ray Absorption Spectra of Transition Metal Compounds", J. Electron Spectrosc. 67 (1994) 529.
- HZ96** T. Hayaishi and P. Zimmermann, *Ion Yield Spectroscopy with Soft X-rays in VUV and Soft X-ray Photoionization*, U. Becker, D.A. Shirley, eds. (Plenum, NY, 1996) 465.
- NM96** I. Nenner and P. Morin, *Electronic and Nuclear Relaxation of Core Excited Molecules in VUV and Soft X-ray Photoionization*, U. Becker and D.A. Shirley, eds. (Plenum, NY, 1996) 291-355 (366 refs).
- O96** H. Oyanagi, *X-ray Absorption Fine Structure in Appl. of Synchrotron Radiation to Materials Analysis*, (H. Saisho and Y. Goshi, eds) 207.
- L99b** K.T. Leung, Valence and inner shell non-dipole excitation spectroscopy of polyatomic molecules by angle-resolved inelastic electron scattering at high energy, J. El. Spectrosc. Rel. Phen. 100 (1999) 23. (REVIEW, CF<sub>4-n</sub>Cl<sub>n</sub> (n=0-4), CHF<sub>3-m</sub>Cl<sub>m</sub> (m=1-3) – C1s)
- H00** A.P. Hitchcock, J. El. Spec. 112 (2000) 9. (inner shell electron impact)
- W01** J.B. West, J. Phys. B 34 (2001) R45. (atomic and ion photoionization)

- HN02** A.P. Hitchcock and J.J. Neville, Chemical Applications of Synchrotron Radiation, Part I: Dynamics and VUV Spectroscopy, Advanced Series in Physical Chemistry Vol 12A, (World Scientific, Singapore, 2002) 154.
- K02** N. Kosugi, Chemical Applications of Synchrotron Radiation, Part I: Dynamics and VUV Spectroscopy, Advanced Series in Physical Chemistry Vol 12A, (World Scientific, Singapore, 2002) 228.
- MG&16** Aleksandar R. Milosavljević, Alexandre Giuliani, and Christophe Nicolas, Gas-Phase Near-Edge X-Ray Absorption Fine Structure (NEXAFS) Spectroscopy of Nanoparticles, Biopolymers, and Ionic Species, Chapter xx in C.S.S.R. Kumar (ed.), X-ray and Neutron Techniques for Nanomaterials Characterization, DOI 10.1007/978-3-662-48606-1\_8. (REVIEW:  $\text{C}_2\text{H}_4\text{NO}_2$  – Gly,  $\text{C}_4\text{H}_8\text{N}_2\text{O}_2$  - Gly-gly – C1s, N1s, O1s;  $\text{Ti}^{+}_n$ , n=1-5,7,10 – Ti2p;  $(\text{NH}_4)_2\text{SO}_4$  – S2p;  $(\text{Na}_2\text{SO}_4)_n$  – O1s, S2p;  $\text{C}_{42}\text{H}_{52}\text{FeN}_8\text{O}_6\text{S}_2$  = cytochrome-c – C1s, N1s, O1s)
- PS&01** Lashkevych, A. Snis, et al. NEXAFS of Carbon-Nitride molecules, *Physica Scripta* **63** (2001) 70. (REVIEW, many CN molecules, C1s, N1s )