

BIBLIOGRAPHY OF ATOMIC AND MOLECULAR INNER-SHELL EXCITATION STUDIES

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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
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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)

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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 ⁺ ; relative, laser generated and probed; MC-SCF calc.
	KMC96	80-100	P	laser plasma study of Al ⁺ ; comp. to Mg, Si ⁺⁺
	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 ⁺ , Al ⁺⁺ cross-sections
Ar 2p	P34	200-300	P	FIRST ATOMIC CORE EXCITATION MEASUREMENT
	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 (248.62,250.77), 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 ⁻¹
	SB84	244.37(2)	E	calibration standard(2p _{3/2} >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 (CSR)
	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_2^+ 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_n 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.
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_n ; 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 $2\pi^*$ 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	$\text{L}^3\text{M}^{23}\text{M}^{23}$ 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 ($E/dE \sim 4000$); 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^{2+} , Ar^{3+} ; PCI at L_2 edge
L96a	250-450	E,R	Auger-scattered electron coincidence; angular distribution
RK&96	240-265	P	comp to clusters, TIY, AEW
SK&96	243-253	P	high res.; $\Gamma(4s)=114(2)$ eV up to $\Gamma(6d)=139(10)$ 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 lifetime 111(3) meV, comp. to others (113 -121 meV)
VP&99	244	P	GOS; comp to theory (MB93); 4s structured; areas used; no geom. overlap correction; 1.5 to 9.5° scattering angle
Ar 2p ..	FL00	240-255	E

	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 ₂ matrices.
	K04	243-253	P,T	Ar(g) comp to Xe, Kr, N ₂ 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 _n
	FN&06	246	P	(3p,2p) interference at $2p_{1/2} \rightarrow 4s$; relative PES, β -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)
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
	US&91	3.19-3.22	P	total and partial ion yields, Ar ⁺ to Ar ⁶⁺ ; threshold effects
	DMD92	3.20-3.60	P,T	absolute; KM, KL double excit.; HF & DF calc.
Ar 1s ...	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 ² mixes with (1s,2p) ⁻¹ 4p ² - 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
Au 5p	KC&95	40-120	P,T	dual lasers; ground & ($5d^96s^2$)-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 & ($5d^96s^2$)-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,4f ^l 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 ⁺ Ba ²⁺ series, absolute
	C82a	90-140	T	collapse of 4d->4f continuum res. in Ba, Ba ⁺ , Ba ²⁺ series
	CM82	90-140	T	ab initio, potential barrier, relativistic effects, (Ba, Ba ⁺ , Ba ²⁺)
	KCN82	90-140	T	absolute X-section, Ba and Ba ²⁺ , compared to expt (HL81)
	NSZ82	80-180	T	absolute cross-section, Ba, Ba ⁺ Ba ²⁺ , density functional method
	C83	90-155	T	quantum defect theory calc., compared to expt (LM&81)
	CF83	60-220	T	4d->f (Xe, Cs ⁺ , Ba ²⁺ etc), comp. to (LM81), cent. barr.; 4f collapse
	C84	60-220	T	res. width/energy relation
	BC&86	40-140	P,T	absolute, excitation of Ba*(6s6p ¹ P), compared to LDRA theory
	BC&89	116-180	P	absolute, partial PI, comp. to theory
	HB&89	100-150	P	laser plasma, Ba ²⁺ , 4f res., 4f partially collapsed
Ba4d . . .	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^+ , 2^+); 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 ₆₀ - inside cage; EXAFS
	KWM93	40-1000	T	RPA(E) cacl. of σ , BR and β for all alkaline earths
	BC94	80-160	R	collapse of giant resonances in Ba, Ba $^+$, Ba $^{2+}$ 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 $^{2+}$, Ba $^{3+}$ yields
	R95	80-160	P,R	comp. of Ba, Ba $^+$, Ba $^{++}$; 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 $^+$, Ba $^{++}$; 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 $^+$, Ba $^{++}$ PIY; 4f collapse mapped; isonuclear identical; $\Sigma(OOS)$ ~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 σ , BR and β 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 (<u>1s</u> ,2p), comp. to Ne-like series
	CF&90	106	P	AI decay of (<u>1s</u> ,2p); spectator dominates
	VS&92	120-145	T	absolute, R-matrix, comp. to expt. (KC87a,b)
	KWM93	40-1000	T	RPA(E) cacl. of σ , BR and β for all alkaline earths
	BPQ97	20-125	T	Be $^+$; 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 ₂ , 50 meV fwhm
	CS96	50-800	P,T	Br, Br $^+$, Br $^{++}$; 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 $^{4+}$, soft X-ray plasma source and sample generator
	JNT90	260-480	P	C I , C II , C III , C V , soft X-ray source & sample; strong Ryd.&cont.; like CH ₄
	GJ91	297.4	T	IP;; f calc of common interstellar elements; KL structure
	HK&92	275-500	P	laser-ionized; laser continuum source; C $^{2+}$, C $^{3+}$, C $^{4+}$ spectra identified
	TG&93	300-500	P,T	C $^{2+}$ (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 III , C IV , C V lines; C IV PI X-sect; comp. to RM79
	MBH97	300-500	T	absolute PI for C(IV); comp to JN&95
	W01	280-480	P,R	review of atom and ion photoionization
C 2s	CM&04	40	T	GOS
Ca 3p	SH&85	30-35	P	Ca $^+$, Ca $^{2+}$ 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 ⁺ , partial cross-section
	KWM93	40-1000	T	RPA(E) cacl. of σ , BR and β for all alkaline earths
	GA&97	30-400	T	partial PI for 3p resonances in 3d-excited Ca ⁺
	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 ⁺ , Ca ²⁺ , Ca ³⁺ yields; cascade Auger from shake-up/off
	OH&02	345-360	P	TIY, PIY, resonant PES, configuration mixing
	AL&93	4.03-4.06	P,T	absolute; strong 1s 3p white line; LSD-HF-CI calc.
Ca 1s	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
Cd 4d	C84	400-700	T	res. width/energy relation
	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)
Ce 4d . . .	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.
Ce 3d	HZ96	90-150	P,R	relative, partial & total ion yields; review ion yield spect. of atoms
	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-CI; intermediate coupling; 21 meV fwhm; Γ = 16 meV – much less than expected (85 meV from KO79 – empirical)
Cl 1s	M01	202-212	T	relativistic CI; absolute, Rydberg excitations
	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 ⁺⁺ , Co ⁺) 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
	DF76	30-80	T	interference lineshape, multiplet effects, compared to solid
	M77	30-70	P	photographic
Cr 3p	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
	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 ⁺
Cr 3p . . .	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⁻ ... La ³⁺
	KA&02a	40-160	P	absolute, Cs ⁺ PIY; 4f collapse mapped; isonuclear identical; Σ(OOS) ~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.
Eu 4d ..	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.; (Eu^{2+} - 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	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	Eu^0 , 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 ($1s$, $2p^6$) S 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 Fe^{n+} , n=0 to 13; evolution of 3p6d res.
	SZ92	30-80	R	comp. of 3p edges of 3d-transition metal atoms
	FF&96	50-70	P,T	absolute; total and partial (Fe^{++} , 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; Fe^+ , Fe^{++} ionization/absorption; R-matrix
	KK&02	30-180	P	absolute; 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 Fe^-
Fe 2p	KK&92	701-725	P	relative, oven, photoion yield, comp. of (Ca,K,Mn,Fe)
	B00a	701-720	T	absolute; R-matrix; electron impact cross-section for Fe^{15+} (plasma)
	B00b	0.02-10 kV	T	absolute; 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; β 's; Cooper minimum
	KCF83	19-22	P	decay of 3d \rightarrow 3p resonance; CIS PES
Gd 4d	CP84	120-200	P	4d \rightarrow f continuum res., fit to C84 lineshape, compared to 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 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 \rightarrow f res.
	ND&90	45-54	P,T	laser dissociated I_2 , strong 4d-6s(^2D) 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, $N_{\text{eff}} < 10$
MNN92	44-60	P	laser produced I from I_2 ; PES, DES
NMC92	44-60	P	TIY, PES, DES, laser diss. I_2 ; 4d 6 5d
SM&96	45-300	P,T	laser plasma; I, I^+ , I^{++} absorption; MCI-HF calc; 4d 6 f dominates
AC&00b	40-136	T	absolute, I^0 , I^+ , I^{++} ; RPAE; com to NSM91; x3 deviation = unknown physics ?
KA&00	40-140	P	absolute; I^+ , I^{++} , PIY; giant resonances
W01	50-120	P,R	review of atom and ion photoionization
AC&02	40-150	T	absolute; I^0 , I^+ , I^{++} excitaiton; GRPAE, comp. to KA&00
DT02	60-130	T	absolute; I^0 , I^+ , I^{++} excitaiton; DFT, comp. to KA&00
KA&02a	40-160	P	absolute, I^+ , I^+ , I^{++} PIY; 4f collapse maaped; isonuclear identical; $\Sigma(\text{OOS}) \sim 10$ suggests little cross-shell correlation
In 4d	LOL84	P,T	abs.; sol.; comp. to $I_2(\text{CNS73})$ Xe(HK&69), 4d Cooper min.; struct. 4d-> ϵf
Ir 5p,4f	MS&97a	P,T	relative; atomic beam; Ir^+ , Ir^{++} yields; Fano profie
K 2p	M75	P	photographic
	MH&92	P	K^+ , K^{2+} , K^{3+} yield, cascade Auger and shake processes
	KK&92	P	relative, oven, photoion yield, comp. of (Ca,K,Mn,Fe)
	BRK00	E	metastable state detection; K^*
K 1s	BA&95	P	multicharge state yields, tail to low E of high charge states - virtual 1s
	ABZ96	T	comp. to Ar 1s; nucl. screening changes intensities; $I(\text{Ar}1s63p) < I(\text{K}1s63p)$
	PK&01	P	realtive, 1s3s3p doubly excited states
Kr 3d	CM64	P	photographic, Rydberg analysis IP (93.82, 95.04)
	LBZ64	P	absolute
	LZB64	P	photographic
	CM65	P	photographic
	MC68	T	ab initio calculation, delayed onset
	AG&69	E	angular dependence of inelastic scattering, differential cross-section
	HK&69a	P	absolute, gas-solid comparison
	ZG71	P,T	review, continuum res.
	CM75a	P	photographic, absolute
	GM&76	P	Rydberg structure, no analysis
	CM77a	P	photographic, correction to CM75a theory comparison
	KT&77	E	Rydberg analysis IP (93.79, 95.04), Z+1 analogy, <70meV FWHM res.
	EKK78	P	Auger decay of res. lines
	C84	T	res. width/energy relation
	HM&84	P	absolute, total and ion yield spectra, no P.C.I. detected
	AA&86b	P	energy dependence of Auger and AI spectra
	DSK86	E	high res. (65 meV), d-->s quadrupole transitions
	AA&87	P	partial and total PI X-sections, 4s Cooper minimum
	HL&87	P	threshold PES, shake-off at discrete res.
	LH&87	P	DES, partial yields at 5p, 6p res., X-sections, βs
	CM&88a	P	anisotropy of DES (AI) at 3d63p; parity forbidden transitions
	K88	P	partial PI X-sections
	AA&89b	P,T	DES, shake-up intensities
	CM&89	P	resonant Auger, ang. dist.; comp. of Ar,Kr,Xe
	MLL89	P	ionic yields, direct double ionis. versus 1- and 2-step autoionisation
	AA&90a	P,T	DES, shake-up fraction comp. of Ne1s, Ar2p, Kr3d, Xe4d
	BS90	P,R	DES at 5p Ryd; comp. of Kr, Ne, Ar DES
Kr 3d . .	HY&90a	P	ion yield spectra ($\text{Kr}^{2+}, \text{Kr}^{3+}, \text{Kr}^{4+}$)
	HY&90b	P	partial and total ion yields; (ZEKE,ion) coinc; PCI
	MH&90	P	absolute, partial ion yields, multiple ionis. ratios ($\text{Kr}^+ - \text{Kr}^{4+}$)
	R90	T	absolute; ion (1+, 2+); absorption; comp of Ba 4d, Xe4d, Kr3d
	VM&90	P	(hv,2e); 2-step autoionization decay of discrete states in Ar, Kr, Xe
	AH&91	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	Kr^+, 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; ΔBR at edges
	TA&92	95-260	P,T	absolute, partial 3d, 4s, 4p X-sect.; β , 5/2:3/2 branch. ratios, MMDF calc
	C93	100-5000	T	X-sect; β ; 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
Kr 3p	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, β -spectrum, interference with $4p^4 np$ 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 Kr^{4+}); Ryd. series in Kr^{4+} ; C-K Auger cascade
Kr 2p	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
	KNY93	1670-1760	T	HF-MC; multi-electron effects at L_3 and L_2 thresholds in Kr 2p and Xe 2p
Kr 2s	SG&95a	1660-1760	P	gas, cluster comparison, 3d exciton in cluster is 0.5 eV above gas
	HT&99	1660-1720	P,T	TIY, threshold ion coinc to Kr^{7+} , PCI (up to 8 eV)
Kr 1s	NI&00	1650-1800	P	TIY, resonant Auger; ang. Dist
	KM&07	1640-1780	P	absolute cross-section
Kr 1s . .	C93	100-5000	T	X-sect; β ; comp. of all rare gases; ang. cor. correct.; dipole breakdown
	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_2) comp., near-edge shape res. in solid
Kr 1s . .	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 ₃
	C82c	80-150	T	correlation effects at res.
	HM&87	100-150	P,T	partial and total; 4d6e giant res.
	HB&89	100-150	P,T	laser plasma, La ³⁺ 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 ³⁺ ; 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 ³⁺
	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 ₂ lines observed
	CP75	60-80	T	pre-edge structure
	ZBS75	50-70	P	core-excited states from H ⁺ ,He ⁺ 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 ⁺
	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)
	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
Li 1s . . .	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; 13 ² P, ² D states predicted;
	CD&96	140-147	P,T	absolute; hollow Li (1s ⁰ 2p ³); Fano resonance; R-matrix calcs.
	DC&96	143-154	P,T	PI line; 19 meV resolution; 118 meV natural linewidth
	JC&96	140-144	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.

	KL&96	62-76	P,T	absolute; absorption; Li^+ yields; high res. ($< 10 \text{ meV}$); compares Rydberg structure at Li^{K^+} , $\text{Li}^{KV^{++}}$ thresholds; R-matrix calc; window resonances
	KMC96	54-64	P,R	laser plasma; comp of Mg, Al ⁺ , Si ⁺⁺
	VF&96	60-180	T	absolute, photoionization cross-section
	DC&97a	150-175	P,T	Auger decay of hollow Li
	DC&97b	148-153	P,T	absolute; partial X-sections; triply excited states = hollow Li; extended Rydberg series; 2 core-excited electrons are strongly bound, 3rd weakly bound.
	KF&98	140-167	T	29 term R-matrix, hollow lithium ($\text{Li} 2l2l'$) state; comp. to expt. (DC&97)
	MC&00	60-180	P	relative, dual laser plasma, comp. to theory (VF&96)
	LM01	174-176	T	lineshapes for creating hollow Li^+ ($2s^2$) states
	WBW02	81-83	P	threshold for Li^{++} ; Wannier thoery compared
Li ⁻ 1s	Z99	55-75	T	absolute, Li^- core excited states
Mg 2p	KA&01	55-70	P	absolute, photodetachment involving $\text{Li}^- \rightarrow \text{Li}^+(1s^*)$
	N71b	16-62	P	photographic, Rydberg analysis IP's (57.544,57.822)
	EM74	55-70	P,T	photographic, compared to theory, Rydberg analysis
	WCK91	55-60	P	resonant AI; branching ratios
	WTA91	55-60	P	resonant AI; shake and PCI effects
	KH&92	60-130	T,P	RRPA, MBPT calc; ang. dist. for PE, Auger; expt-theory comp.
	KWM93	40-1000	T	RPA(E) calc. of σ , BR and β for all alkaline earths
	MB97	50-100	T	absolute OOS, GOS; HF-CI; Born approx.
Mg 2p ...	WD&97	140-160	P,T,R	partial cross-sections; R-matrix calculations
	KC&99	95-120	P,T	Mg^{++} , dual laser plasma
	W01	40-160	P,R	review of atom and ion photoionization
Mg 1s	GJ91	1310.6	T	IP.; f calc of common interstellar elements; KL structure
	BD&92	1.3-1.7kV	P	Mg^{7+} - Mg^{10+} K-shell absorption in plasma; X-ray emission
	MB97	1.30-1.31	T	absolute OOS, GOS; HF-CI; Born approx.
Mn 3p	KM&02b	100-2000	T	absolute, realxation effects; comp. of Ca, Mg, Sr
	CMM76	40-70	P	photographic, comparison to solid Mn, MnF_2 , MnCl_2 , MnBr_2
	DF76	50-90	T	interference lineshape, multiplet effects, compared to solid
	BSW78	40-60	P	photographic, gas-solid comparison
	CGM71	20-85	P,T	photographic, compared to theory
	AIC81	40-70	T	RPAE calculation, compared to experiment (BSW78)
	GB&83	40-100	T	absolute ($4s, 3d, 3p$), MBPT, compared to expt (BSW78)
	C84	40-100	T	res. width/energy relation
	SS&85	40-70	P	comparison of absorption (BSW78) with sum of partial cross-sections
	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^+ 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	$4s(^7S/{}^9S)$ BR; spin-pol. RPAE; matches expt. (Sonntag unpublished); strong $3p63d$, $4s62p$ coupling
	CK&91a	40-70	P	laser-plasma, relative, Mn, Mn^+ , comp. to metal and molecules (sol)
	CM&91	40-70	P	laser-plasma, Cr, Mn, Mn^+ compared
Mn 3p ...	KY91	45-70	T	absolute, p 6 ed resonance; effect of AI; PCI effect on position & width
	D92b	47-54	T	comp. of Mn^+ , Mn^{*+} ; spin-resolved X-sections
	SZ92	30-80	R	comp. of $3p$ edges of 3d-TM atoms; partial X-sect; Mn^{2+} , β s, calc.
	D93a	47-54	T	comp. of Mn^+ , Mn^{*+} , Mn; SP-RPAE; ($3d+4s$) 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	RPAE of $3p64s$ & $3p63d$ res.; reversal in PA ($4s < 3d$) relative to $\beta(3d)$ ($3d < 4s$)
	DBH96	32-46	P,T	R-matrix; Mn^+ 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 ($2p^1$, 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 ₂ , origin of σ^* res.
	GJ91	412.4	T	IP.; f calc of common interstellar elements; KL structure
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	$\sigma^{(++)}/\sigma(\text{TOT})$ 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
	YK&86b	1.07-1.08	T	ab initio, double excitation ($1s_1, 3p_{es}$; $1s_1 4s_{ep}$), 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 _n 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
Ne 1s ...	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 ₂ O, NH ₃ , CH ₄ , 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 ₀ = 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
	H90	860-900	E,R	absolute, comp. of Ne, NH ₃ , N ₂ H ₄ , N ₂ ; Ryd. vs. valence
	ST90	0-3000	E	absolute, double diff. (angle, E ₀), 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 _n series
	SI&92	860-980	P,T	gas,solid, theory comp.; Ne ₈₇ cluster gives good match to solid spectrum
	SS92a	810-1340	P	Ne ^{x+} 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) excitons 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 _n (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
	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 interereference; 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 spectrator Auger
	SP&00	865-871	P	SB7 LURE beamline tests; ΔE/E > 8500; 280 meV fwhm
Ne 1s ...	SY&00	870	P	resonant Auger Raman at 1s →3p; 100 meV fwhm; β
	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
	YO&02	840-880	P,T	relative; Ne ^{x+} (x=1-3) ion photoionization; MC-Dirac-Fock gets E right
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; β ; 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
O 1s	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	high res.; TIY; discharge mix of O ₂ /O; $\Gamma = 140(9)$ meV; HF calc.; 1s → π^* 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
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.
Pr 3d	GG&98b	100-140	P	relative, partial PI cross-sections; shape resonances in Pr, Nd
Pt 5p,4f	TL&85	920-960	P,T	electron yield (solid), comp to multiplet calc, full RE series
	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 ₊ , 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; $S^+ \rightarrow S^{++}$, S^{3+} ; x2 deviations with accepted astrophysics values
	BG&12	218-228	P	multi-electron photodetachment from S^-
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 ₅
	DC99	30-40	P,T	relative, dual plasma, HF calc; metastable; Sb, Sb ⁺ , Sb ⁺⁺ , Sb ³⁺
	AC&00c	30-100	P,T	relative, dual plasma, HF calc; metastable; Sb, Sb ⁺ , Sb ⁺⁺ , Sb ³⁺ , Sb ⁴⁺ ; 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^{3+} ; 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 coorelation effects; compare to W01
	SM&02b	28-45	P,T	absolute; $\text{Sc}^{++} \rightarrow \text{Sc}^{+++}$; 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_4 , SiF_4
	SK&95a	105-140	P,T	(Si^{2+}); dual plasma; HF-CI calc.
	KMC96	110-140	P,R	laser plasma; comp of Mg, Al^+ , Si^{++}
	CK&98a	93-113	P,T	relative; dual laser plasma; absorption from metastable Si^{*+} , Si^{2+} ; HF calc
	CK&98b	105-190	P, T	Si^+ ; dual laser plasma; ab initio calc.; comp. to Al
	KC&99	100-130	P,T	dual laser plasma
	W01	143-165	P,R	Si^+ excitation; review of atom and ion photoionization
Si 1s	GJ91	1848.6	T	IP, f calc of common interstellar elements; KL structure
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^{2+} - Sm^{4+}) 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	Sr^+ , Sr^{2+} yields at threshold
	KWM93	40-1000	T	RPA(E) cacl. of σ , BR and β 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 σ , BR and β for all alkaline earths
	MS&95a	135-300	P,T	dual laser; Sr^0 to Sr^{3+} ; HF-CI calc; cont. X-sect. depends on charge
	IK&95b	130-200	P	relative; Sr^+ Sr^2 , Sr^3 yields from Sr^+ ; 3d6ef giant res.; 4d orb. collapse
Sr 3p	KH&87	136-146	P	total and partial ion yields, no 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 σ , BR and β 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 (TbAl ₂ (sol)), comp to multiplet calc, full RE series
Te4d	M99	70-102	P,T	Te^{4+} , 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	Ti^{3+} ; dual laser plasma; RPAAE calc.
Ti 2p	GBP82	>450	T	inner-shell excitation contributions to total cross-section calculated

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.; ThF ₄ (CP&80), calc. (W84)
	CM&91	80-140	P,R	laser-plasma, comp. to 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, UF ₄ (CP&80)
U 5d	W84	80-160	T	non-relativistic RPA, non-statistical f(S-O); cont. res., comp. to expt (UF ₄ -CM&80; U(solid)-Cukier et al. J. Phys (Paris) 39 (1978) L315)
	CC87	70-150	P	relative, plasma continuum, compared to 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.
	KG&00	15-150	P,T	relative, total and partial yields (U ⁺ , U ⁺⁺ U ³⁺); dual laser plasma
V 1s	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 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
Xe 4d . . .	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%), β 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 $d \rightarrow \epsilon f$ 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 ϵf res.
	HM&86	138-152	P	absolute, partial & total ion yields; Ryd. series most visible in Xe^{4+}
	SKR86	63-70	E	high res. (65 meV), quadrupole $d \rightarrow s$ 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); βs ; enhanced 2+ at 4d giant res.
	LF&88	150-300	P	4p, 4d part. X-sect; rel; β 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, βs
	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 Cs^+ , Ba^{2+} , 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 β ; 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
	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	($h\nu, 2e$); 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; ΔBR at edges
	WC&92	64-70	P	CIS spectra; Auger- β ; 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 Xe:C_{60} inside cage; EXAFS
	C93	100-5000	T	X-sect; β ; 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
Xe 4d . . .	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) coine.; $4d_{5/2}:4d_{3/2}$ BR; PCI; comp. to theory
	BS96	50-1000	P,R	absolute, partial cross-sect. comp. to total; β '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; β 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; β 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 Xe, Xe^+ , 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 $Xe^+ \rightarrow Xe^{++}$; comp to expt
	AA&01	70-140	P,T	absolute; RPAE calc; Xe^+ , Xe^{++} excitation & ionization
	BA&01	105-127	P	threshold EY, ion coincidence
	II&01	50-150	P	absolute
	W01	70-130	P,R	review of atom and ion photoionization
	BF&02	40-180	E	absolute, GOS, ef shape resonance has minimum($K^2 = 3au$)/maximum($K^2 = 6au$)
	KA&02a	40-160	P	absolute, Xe^0 , Xe^+ , Xe^{++} PIY; 4f collapse mapped; isonuclear identical; $\Sigma(OOS) \sim 10$ suggests little cross-shell correlation
	LS&02	64-76	P,T	TPEPICO; PCI; dynamics of Auger decay via 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 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; β ; 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
Xe 3d ...	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 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 ~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
Xe 2s	IV&98	4.5-7.0	P	multi-electron excitation; three electron transitions
	DGT92	5.41-5.50	P	Rydberg, Z+1 comp.; LN double excit; compt. to KH&89
Xe 1s	MH&99	5.44-5.48	P	PIY, ERAMICO, PCI, multi-step Auger; modelled
	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 ($\text{Yb}_2\text{O}_3(\text{s})$), 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^{n^+} 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_3H_9	NKM90	40-120	P	$\text{Al}(\text{CH}_3)_3$, ion yield, PEPICO, PIPICO, DDI, selective fragm. at edge
	NK&91	40-120	P	ion yield, BR, PIPICO
$\text{Al}_2\text{C}_3\text{Cl}_3\text{H}_9$	NK&91	40-120	P	$\text{Al}_2(\text{CH}_3)_3\text{Cl}_3$, ion yield, ion branching ratios, PIPICO

Antimony 4d (35 eV)

Sb ₅	BC94	20-120	P,R	relative; comp. to atom, solid; giant resonances review
Sb _n	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 ₂	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 _n	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 _n ; 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 _n

	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, AEY as f(size); ZEKE; PEPIPICO
	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 _n	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 ₃	GDT97	1.31-1.39	P,T	relative; TIY, MS-X α ; pot. barr.; AsCl ₃ , PCl ₃ , GeCl ₄ , SnCl ₄ comp.
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Arsenic 1s (11.7 keV)

AsF ₃	MB&79	11.8-11.9	P	pot. bar. effects, comp. to AsF ₅ -doped polyacetylene
	MB&84	11.8-11.9	T	non-relativistic HF, comp. to expt (MB&79)
AsF ₅	MB&79	11.8-11.9	P	pot. bar. effects, comp. to AsF ₅ -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 ₆₀	PN&93	80-180	P	absolute; comp. of atomic and BaC ₆₀ - inside cage; EXAFS
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Beryllium 1s (110 eV)

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

Bismuth 5d (25 eV)

BiC ₃ H ₉	NS&90	16-42	P	Bi(Me) ₃ , ZEKE, PI yield, BR, comp. of methyl-metal fragmentation (Bi, Ga, Zn, Ge, Sn, Pb)
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Boron 1s (190 eV)

BBr ₃	II&80	170-280	P	absolute
	II&82	190-280	P,T	absolute, discrete shape res., ab initio calc.
BClF ₂	HD&92	190-220	P	partial IY; yield spectra distinguish mixed (BCl _x F _{3-x})
BCl ₂ F	HD&92	190-220	P	partial IY; yield spectra distinguish mixed (BCl _x F _{3-x})
BCl ₃	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 & participator at π*, σ*

BF₃	UT&00	195-199	P,T	TIY, relative, resonant Auger probe of Jahn-Teller coupling
	F68	190-210	P	pot. bar. effects, comp. to B, BN, B ₂ O ₃ - 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
	SDD81	190-225	T	MSM X- α 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 ₄ (s), CF ₄ ; expt (HB71, II&82)
	CF&84a	190-215	E	comp. of 2.5 and 15° spectra, σ^* (e) enhanced
	KI&84	190-225	P	relative, DES enhanced valence PES at discrete res.
	SSH84a	205	T	σ^* -res./bond length relationship
	VA&85	190-230	P,R	comp. to N ₂ , NO ₃ ⁻ , shape resonances
	KYK86	190-225	P,T	comp to II&82 BF ₄ ⁻ ; Ni(CN) ₄ ²⁻ Ni1s; Fe(CN) ₆ Fe,N1s; edg. geom.
	T86	150-200	T	X α ; comp of BF ₃ , B(OH) ₃ , C(OH) ₃ ⁺ XANES, R & symmetry effects
	HJ&87	190-220	P	partial ion yields, strong variation of σ^*/π^* with channel, QMS
	NAV88a	190-220	P	comp. to KNO ₃ , NaNO ₃ ; $\delta(\pi-\sigma)$ versus R
	NAV88b	190-220	P	comp. to KNO ₃ , NaNO ₃ ; $\delta(\pi-\sigma)$ versus R
	PV&90	190-210	P	comp. to NO ₂ ⁻ , NO ₃ ⁻ ; $\delta(\pi-\sigma)$ versus R
	EA&91	180-230	E,T	comp. to BF ₄ ⁻ , EHT calc; (np- π^*) distinguishes trigonal/non geom.
	NAV91	190-220	P	comp. of planar co-ordinated anions, π - σ bond length correlation
	U91	196,206	P,R	PE & Auger study of decay of a ₁ , 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; spectrator is 3x participator
	UC&94a	190-220	P	resonant Auger; 2a ["] 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 β 's; X-sections for F ⁺ ; 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
BF₃ . . .	TKU98	194-198	P,T	2a ₂ ["] 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
BF₄⁻	MF&02	195	P	resonant Auger Raman; mapping potential energy surfaces
	HS&81	190-210	P,T	ABF ₄ solid compounds (A=K,Na,NH ₄) comp. to BF ₃ , CF ₄
BHO	SM&83	190-215	P,T	solid state, res. structure, comp. to BF ₃ and CF ₄ .
	EH99	160-240	E,T	absolute; transient from H ₂ S+B+SiO ₂ ; comp of HBO, HBS, H ₃ B ₃ O ₃
BHS	H00	160-250	E,R	transient ISEELS; comp of HBO,HBS, H ₂ S
	HE&01	160-240	E	absolute; transient ISEELS
H₃O₃	EH99	160-240	E,T	absolute; transient from H ₂ S+B+SiO ₂ ; comp of HBO, HBS, H ₃ B ₃ O ₃
	H00	160-250	E,R	transient ISEELS; comp of HBO,HBS, H ₂ S
B₂H₆	HE&01	160-240	E	absolute; transient ISEELS
	T86	150-200	T	X α ; comp of BF ₃ , B(OH) ₃ , C(OH) ₃ ⁺ XANES; $\delta(R)$ & sym. eff.
	ZV72	185-210	P,R	relative intensities

B₃H₃O₃	EH99	185-210	E,T	absolute; from H ₂ O+B; comp of HBO, HBS, H ₃ B ₃ O ₃
B₃H₆N₃	DG&86	185-235	E	(borazine), comp. to Bz & cyclohexane, aromatic, split σ^* 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 ₃ H ₃ ⁺
	PV&03	188-204	P	TEY, resonant Auger, 30 meV fwhm, vibrational fine structure
B₄C₆H₁₄	HW&93	180-240	E,T	2,3-diethylcarborane, absolute, EHMO, MNDO; ref. for CVD of BC
B₅H₉	HW&93	180-240	E,T	pentaborane, absolute, EHMO, MNDO; ref. for CVD of BC
	LD&92a	180-280	E,T	EXELFS, MNDO geometry
B₅C₁₂H₁₈P	HLD91	160-220	E	Ph ₂ PB ₅ H ₈
B₅C₁₉FeH₁₇O₂P	HLD91	160-220	E	Cp(CO) ₂ FeB ₅ H ₂ P(Ph) ₂
B ₉ C ₂ H ₁₁	HW&93	180-270	E,T	nido-1,2-dicarbaundecaborane, absolute, EHMO, decomp. of Ni(M) ₂
B₁₀C₂H₁₂	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	ionoic fragmentation of clos-carborane
B₁₀C₂H₁₂	HU&97	185-220	E,P,T	m-carborane, absolute; ab initio; EELS, TIY comp. for isomers; ioniz. eff.
B₁₀C₂H₁₂	HU&97	185-220	E,P,T	p-carborane, absolute; ab initio; EELS, TIY comp. for isomers; ioniz. eff.
B₁₀H₁₄	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 ₁₈ C ₄ H ₂₂ Ni	HLD91	160-220	E	Ni(B ₉ C ₂ H ₁₁) ₂ , Ni bollyl complex (Cp-analog)

Bromine 3d (75 eV)

BrCClH ₂	SR&94	68-110	P	TIY; PEPICO; PEPI3CO; selective frag.; Br(CH ₂) _n Cl, n=1-3
	MS&98b	90	P	ES-AEPICO, PE, site-selective fragmentation & kinetics
BrCF ₃	JC&97	68-80	P	relative; PES, PA comp.; ligand field and spin-orbit splitting; same ligand field paramaters in excitation and ioniz.
BrCH ₃	HB78a	50-300	E	CH ₃ Br, cont. res.
	MN87	68-79	P	TPES, DES $\sigma^*(C-Br)$; PIPICO, partial dissociation prior to decay
	N88	63-79	P,R	$\sigma^*(C-Br)$; PIPICO, partial dissociation prior to decay
	NE&88	68-79	P	$\sigma^*(C-Br)$; 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	$\sigma^*(C-Br)$; 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 ₂ ClH ₄	SR&94	68-110	P	TIY; PEPICO; PEPI3CO; selective frag.; Br(CH ₂) _n Cl, n=1-3
BrC ₂ F ₄ I	NM&90	60-140	P	Auger, AI and ion yield (PIPICO); selective fragmentation
BrC ₂ H ₃	SBK88	60-100	E	v vinyl bromide, high res.
	MLL89	68-110	P	mass spectra, ion yields, selective fragmentation
BrC ₂ H ₅	MLL89	68-110	P	PIPICO spectra, ion yields, selective fragmentation
BrC ₃ ClH ₆	SR&94	68-110	P	TIY; PEPICO; PEPI3CO; selective frag.; Br(CH ₂) _n Cl, n=1-3
BrC ₆ H ₅	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 _{5/2} =77.12(3), 3d _{3/2} =78.23(3)]
	BI&85	60-100	E	absolute, photoionization and fragmentation, similar to CH ₃ 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 $\sigma^*(\text{H-Br})$; PIPICO, partial dissociation prior to decay
	NB87	68-80	P,R	$\sigma^*(\text{H-Br})$; dissociation prior to decay; review
	N88	63-79	P,R	$\sigma^*(\text{H-Br})$; PIPICO, electron and ion spectroscopy
	NM&88	68-79	P	$\sigma^*(\text{H-Br})$; 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^+ , ang. dist., KER etc from MRD-CI calc of HBr^{2+}
	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
	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.
Br ₂	PH&02	68-77	P	high res.; angle resolved (ion coinc.); symmetry-based re-assignments
	MM12	68-72	P,R	ultra-fast decay ($\text{HBr-Br}3d$; DCl , $\text{HCl-Cl}2p$; H_2S - $\text{S}2p$, $\text{O}_2-\text{O}1s$)
	SC&84	66-80	E	75 meV fwhm, strong res. 9.1eV 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 ₄ C	BS&02A	50-450	P,T	relative, TIY, PIY, compared to SiBr_4 , GeBr_4 , Me_3SiBr (BL&98)
Br ₄ Si	BL&98	50-450	P,T	relative, TIY, PIY

Bromine 3p (190,196 eV)

C ₂ H ₃ Br	SBK88	60-100	E	v vinyl bromide, high res., width of $3p_{3/2}>3p_{1/2}$ due to C-K
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Bromine 2s (1790 eV)

Br ₄ Si	BM&89a	1.75-1.90	P	SiBr ₄ ; broad line; no pre-edge feature
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Bromine 1s (13.5 keV)

BBr ₃	FA98	13.4-14.4	P	relative; EXAFS; MSx α calc; 0.1 pm accuracy claimed; compare to ED
BrC ₆ H ₅	OT&86	13.4-13.5	P	Bz-Br; comp of Br ₂ , Bz-Br and Br-polyacetylene
	O96	13.4-13.5	P,R	XAFS review; comp. to Br-polyacetylene
BrH	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 ₂	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 ₂ , Bz-Br and Br-polyacetylene
	FE&86	13.4-14.7	P	near edge and EXAFS, comp. to theory, Br ₂ 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 ₂ , GeCl ₄ , SF ₆
	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 ₄ C	FA98	13.4-14.4	P	relative; EXAFS; MS-X α calc; 0.1 pm accuracy claimed; compare to ED
	CEK76	13.4-14.6	P	extended fine structure (EXAFS)
<u>Calcium 2p (350 eV)</u>				
CaBr ₂	KR&02a	346-357	P, T	partial electron yield from 2D (hv, e) maps, relative; atomic multiplet
<u>Carbon 1s (290 eV)</u>				
B₄C₆H₁₄	HW&93	280-316	E,T	2,3-diethylcarborane, absolute, EHMO, MNDO; ref. for CVD of BC
B₅C₁₂H₁₈P	HLD91	280-316	E	Ph ₂ PB ₅ H ₈
B₅C₁₉FeH₁₇O₂P	HLD91	280-316	E	Cp(CO) ₂ FeB ₅ H ₂ P(Ph) ₂
B ₉ C ₂ H ₁₁	HW&93	280-316	E,T	nido-1,2-dicarbaundecaborane, absolute, EHMO, decomp. of Ni(M) ₂
B₁₀C₂H₁₂	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, PEPICICO; 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	ionoic fragmentation of clos-carborane
B₁₀C₂H₁₂	HU&97	280-305	E,P,T	m-carborane, absolute; ab initio; EELS, TIY comp. of isomers; ioniz. eff.
B₁₀C₂H₁₂	HU&97	280-305	E,P,T	p-carborane, absolute; ab initio; EELS, TIY comp. of isomers; ioniz. eff.
B ₁₈ C ₄ H ₂₂ Ni	HLD91	280-316	E	Ni(B ₉ H ₁₁ C ₂) ₂ , Ni bollyl complex (Cp-analog)
BrCD ₃	HB79c	285-290	E	vibrational structure, isotope shifts
BrCH ₃	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 ₂ H ₃	BMT88	280-310	E	comp. to ETS
	SKB88	275-320	E	high res., comp. to vinyl halides
Br ₄ C	BS&02A	50-450	P,T	relative, TIY, PIY, compared to SiBr ₄ , GeBr ₄ , Me ₃ SiBr (BL&98)
BrC₅MnO₅	HR89	280-320	E	Mn(CO) ₅ Br, absolute, π^* intensity as measure of d π -p π backbonding
	RH89a	275-330	E	comp. to CO, Mn(CO) ₁₀ & M(CO)s; E(ref); f(π^*) α backbond
	H90a	280-325	E,R	absolute; comp. to TM-COs; relaxation and δ (R) for $\sigma^*(CO)$
	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 $\rightarrow \pi^*$; orbital mapping
BrC ₆ H ₅	HP&78	283-295	E	XPS-EELS chemical shifts comp.
Br ₂ C ₁₂ H ₈	WC&05	284-308	E,T	o,o-dibromo-biphenyl, quantitative, GSCF ₃ , ring-ring-interactions
CClF ₃	CS90	292-301	P	high res. (50 meV); sharp $\sigma^*(C-Cl)$, broad $\sigma^*(C-F)$; comp of CCl _x F _{4-x}
	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 _x F _{4-x} , x=1-4	
YL94	285-330	E	absolute GOS; comp. of CF _{4-n} Cl _n (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	
CClH ₃	HB78a	180-350	E	vibrational structure
	HB78b	286-292	E	comp. through CH _x Cl _{4-x} 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 _x F _{4-x} , x=1-4	
CP&07	280-350	P	relative, TIY, PIY +ve, -ve; state-selective frag.	
CCl ₂ F ₂	CS90	291-299	P	$\sigma^*(C-Cl)$, $\sigma^*(C-F)$ slit; comp of CCl _x F _{4-x}
	ZIB92	280-330	E	absolute, high res. (70 meV), pot. bar., comp. of CCl _x F _{4-x} , x=1-4
BSS93b	50-1500	P	partial ion yields at coarse resolution	
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 $\text{CF}_{4-n}\text{Cl}_n$ ($n=0-4$); $\sigma^*(\text{C}-\text{Cl})$ GOS changes
CCl_2H_2	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_2O	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_3F	ZIB92	280-330	E	absolute, high res. (70 meV), pot. bar.
	YL94	285-330	E	absolute GOS; comp. of $\text{CF}_{4-n}\text{Cl}_n$ ($n=0-4$); $\sigma^*(\text{C}-\text{Cl})$ GOS changes
	SS97	290,310	P	PIPICO branching ratios; site-specific fragmentation; comp. to $\text{CF}_x\text{Cl}_{4-x}$
	SS98b	280-320	P	PIY, comp of C 1s, F1s, Cl 2p
CCl_3H	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 $\text{CCl}_x\text{F}_{4-x}$, $x=1-4$
CCl_4	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 $\text{CCl}_x\text{F}_{4-x}$, $x=1-4$
	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 $\text{CF}_{4-n}\text{Cl}_n$ ($n=0-4$); $\sigma^*(\text{C}-\text{Cl})$ GOS changes
	SC&02	288-296	P	absolute; high res.; weak Ryd.; $\Gamma \sim 72$ meV; comp. of CX_4 , $\text{X}=\text{H,Cl,F}$
CCuO	YA&97	287	T	$\text{Cu}-(\text{CO})$; STEX; π^* OS comp. of CO, CuCO, Cu_{17}CO , Cu_{50}Co ; initial and final state rules
CCu_{17}O	YA&97	287	T	$\text{Cu}-(\text{CO})$; STEX; π^* OS comp. of CO, CuCO, Cu_{17}CO , Cu_{50}Co ; initial and final state rules
	PA&96	280-340	T	absolute, STEX; comp. of CO, Cu_{17}CO , Cu_{50}Co ; models of CO/Cu(100)
CCu_{50}O	YA&97	287	T	$\text{Cu}-(\text{CO})$; STEX; π^* OS comp. of CO, CuCO, Cu_{17}CO , Cu_{50}Co ; initial and final state rules
	PA&96	280-340	T	absolute, STEX; comp. of CO, Cu_{17}CO , Cu_{50}Co ; models of CO/Cu(100)
CDHO_2	GM&06	280-340	P	(DCOOH), TIY, PIY, fragmentation, PEPIPICO, compare 4 isotopomers
CDHO_2	GM&06	280-340	P	(HCOOD), TIY, PIY, fragmentation, PEPIPICO, compare 4 isotopomers
CD_2O	RD&92	285-312	P	high res.; Franck-Condon analysis 6 geometry; E_{el} as f(isotope)
	PP&00	286	T	MC-SCF Z+1 calc; vibrational structure, XPS better than NEXAFS, comp. to expt (RD&92)
CD_2O_2	GM&06	280-340	P	(DCOOD), TIY, PIY, fragmentation, PEPIPICO, compare 4 isotopomers
CD_4	HPB77	285-293	E	vibn'l struct; isotope intensity effects (J-T vibronic coupling)
	HM&91b	287-294	P	ZEKE, 0.15 eV fwhm; comp. of CH_4 , CD_4 ; PCI modifies ZEKE; FC anal. of C_K^+ possible ($\Delta\Gamma = -0.052(7)\text{A}$; hole relax. $>$ internucl. rep.
	RDK93	286-291	P	high res (60 meV); $I^D/I^H(3s) = 0.57(5)$; B-O not H-T vibronic coupling; comp. of CH_4/CD_4 ; $\text{C}_2\text{H}_6/\text{C}_2\text{D}_6$; $\text{C}_3\text{H}_8/\text{C}_3\text{D}_8$
	ST&93	286-291	P,T	high res (60 meV); CH_4/CD_4 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. $\text{C } 1s^{-1}$
	KR&02b	260,350	P, T	ERAMICO, 2-step model of fragmentation
	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_4O	AJ&97a	278-293	P	CD_3OD ; relative, 45 meV fwhm; vibrational struct; comp to CH_3OH
CFH_3	BBB78	282-310	P	absolute, $\text{CH}_x\text{F}_{4-x}$
	HB78a	284-295	E	vibrational structure, comp. through CH_3X series
	HB79c	284-293	E	vibrational structure
	SSH84a	295	T	σ^* -res./bond length relationship

	RS&89	290-330	T	MS-X α calc. of f & β for ($\text{CF}_x\text{H}_{4-x}$, x=0-4); only CH_4 resonant
	LAL91	285-305	T	CNDO, systematic calc. of σ^* energies; ISEELS, ETS for param. det.
	S92	280-320	E,R	comp. of CH_3X , X=H, CH_3 , NH_2 , OH, F; $\sigma^*(\text{X}-\text{H})$
	KU+95	287-294	P,T	60 meV fhlm; ab initio $\Delta\text{SCF-Cl}$; resonant Auger; confirms $\sigma^*/3s$ but mixed; Rydberg structure very similar to CH_4 ; reassigned peaks
	US&96	285-305	P,T	high res (60 meV); comp. of $\text{CH}_x\text{F}_{4-x}$ (0<x<4); Auger and AI decay; SCF calculation; Rydberg vs. valence
CFHO	AM97	284-295	T	electronegativity correlations used for assignments; comp. to BBB78
	IH87	275-325	E	HCOF , absolute, comp. to (HCOX , X= NH_2 , OH), π^* mapping
	RI&88	275-336	E	absolute, per-fluoro effect
	S92	280-320	E,R	comp. of $\text{CH}_x\text{F}_{2-x}\text{O}$, $\sigma^*(\text{C}-\text{F})$ development
	SLD95	287	T	absolute, DF-LCAO; OS for C1s, O1s $\rightarrow \pi^*$; orbital mapping
CF_2H_2	HC96	290	T	DFT; singlet-triplet (0.90 eV)
	BBB78	282-310	P	absolute, pot. bar. effects
	SSH84a	295	T	σ^* -res./bond length relationship
	RS&89	290-330	T	MS-X α ; C1s X-sect. & β for ($\text{CF}_x\text{H}_{4-x}$, x=0-4); only CH_4 resonant
	US&96	285-305	P,T	high res (60 meV); comp. of $\text{CH}_x\text{F}_{4-x}$ (0<x<4); Auger and AI decay; SCF calculation; Rydberg vs. valence
CF₂O	AM97	284-295	T	electronegativity correlations used for assignments; comp. to BBB78
	RI&88	275-325	E	carbonyl fluoride, C-F σ^* res., absolute, perfluoro effect
	S92	280-320	E,R	comp. of $\text{CH}_x\text{F}_{2-x}\text{O}$, $\sigma^*(\text{C}-\text{F})$ development
	SLD95	287	T	absolute, DF-LCAO; OS for C1s, O1s $\rightarrow \pi^*$; orbital mapping
	HC96	290	T	DFT; singlet-triplet (1.04 eV)
CF₃H	BBB78	282-310	P	absolute, pot. bar. effects
	SSH84a	295	T	σ^* -res./bond length relationship
	HN86	275-330	E	absolute
	RS&89	290-330	T	MS-X α ; C1s X-sect. & β for ($\text{CF}_x\text{H}_{4-x}$, x=0-4); only CH_4 resonant
	LAL91	285-305	T	CNDO, systematic calc. of σ^* energies; ISEELS, ETS for param. det.
CF₃NO	US&96	285-305	P,T	high res (60 meV); comp. of $\text{CH}_x\text{F}_{4-x}$ (0<x<4); Auger and AI decay; SCF calculation; Rydberg vs. valence
	AM97	284-295	T	electronegativity correlations used for assignments; comp. to BBB78
	HIR89	280-340	E	absolute, weak bond effect

CF₄	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- α , comp. to BBB78; BF ₄ ⁻ (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	σ^* -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 ₂) & 1s6e3p pred; corr. with LiF, K ₂ BeF ₄ & KBF ₄ (A1s)
	HI86	300-1000	E	extended fine structure, comp. to BBB78
	SA&86b	250-780	P	absolute, comp. to CH ₄ ; transfer of OS (cont'd discrete)
	SDD86	300-330	T	MS-X α , 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 ₄ , CO ₂
	LM&89	290-345	P	total ion yield, TOF mass spec at sel. E; no sel. frag.; comp. to SiF ₄
	RS&89	290-330	T	MS-X α ; X-sect, β for (CF _x H _{4-x} ,x=0-4); CH ₄ 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 _{2+x} F _{4-x} , x=0-2
	H90a	290-320	E,R	absolute, pot. bar. effect on I{ $\sigma^*(C-F)$ } through CF _x series
	HW&90	300-700	E	EXELFS, comp. to PA (BBB78)
	LAL91	285-305	T	CNDO, systematic calc. of σ^* energies; ISEELS, ETS for param. det.
	ZIB92	280-330	E	absolute, high res. (70 meV), pot. bar., comp. of CCl _x F _{4-x} , x=1-4
	HM94	270-410	E,R	absolute; improved osc. str. conversion; this bibliography!!
	SBS94b	44-1500	P	partial and total ion yields; PEPICO; site selective fragmentation
	YL94	285-330	E	absolute GOS; comp. of CF _{4-n} Cl _n (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 _x F _{4-x} (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 ₂) 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 dissoc.
	US&99b	295-302	P,T	absolute; high res.; $\Gamma \sim 74$ meV; comp. of CX ₄ , X=H,Cl,F
	SC&02	288-296	P	TIY, resonant 2D Auger maps. Ultra-fast dynamics, Jahn-Teller (1s, 3p) t ₂
	PG&12	295-302	P	resonant (Auger,ion) coincidence
	IIS12b	299	P	CF ₃ OF, low-lying $\sigma^*(F-O)$
CF₄O	IM&87	290-330	E	PEPICO, PIPICO, site-selective fragmentation
CF ₈ 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	σ^* -res./bond length relationship
	SSH84a	300	T	σ^* shape res.; position & shape as f(R); approx. cyl. well & ab initio
	SG&89	290-330	T	CNDO, systematic calc. of σ^* energies; ISEELS, ETS for param. det.
	LAL91	285-305	T	

CHN ...	ZZ&92	285-300	T	Δ SCF; explicit core hole; localisation; rules for E(MO) for 2nd row
CH ₂	CG&80	283-300	T	ab initio calc.
CH ₂ O	HB80b	280-320	E	formaldehyde; vibrational structure, cont. res., Z+1 analogy
	SSH84a	300	T	σ^* -res./bond length relationship
	RI&88	270-330	E	absolute, comp. to H _x F _{2-x} CO, perfluoro effect
	SBT88	285-293	T	absolute; ab initio; low-lying double excitation; comp to HB80b
	SG&89	290-330	T	σ^* shape res.; position & shape as f(R); approx. cyl. well & ab initio
	LAL91	285-305	T	CNDO, systematic calc. of σ^* energies; ISEELS, ETS for param. det.
	RD&92	285-312	P	high res.; Franck-Condon analysis 6 geometry; E _{el} as f(isotope)
	S92	280-320	E,R	comp. of CH _x F _{2-x} O, $\sigma^*(C-F)$ development
	KS&93	295-350	P	absolute; partial PI X-sect.; β ; 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; β s
	SCT96	295-320	T	core-valence double ionisation; $^1\pi$, $^3\pi$ states; comp. of CO, H ₂ CO, N ₂
	YA&96	280-320	T	STEX; comp. to expt. and other theory; R ₂ CO species
	TPA98	280-320	T	absolute; DFT vs. STEX, compares CO and R ₂ CO, R = H, Me
	YA&97	287	T	π^* 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 ($1s^{-1}$, π^{-1} , π^2) state predicted
	TMG01	285-292	T	absolute; AC2, MRCI; comp. to RD&92
	TM&01b	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 π^*
	CT06	284-296	T	ADF-DFT, compared to experiment, agree within 0.3 eV
CH ₂ O ₂	IH87	275-325	E	(formic acid), absolute, π^* 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 σ^* energies; ISEELS, ETS for param. det.
	S92	280-325	E,R	comp. of HCO ₂ H, HCO ₂ CH ₃ and PMMA nEXAFS
	GM&06	280-340	P	TIY, PIY, fragmentation, PEPIPICO, comparison of 4 isotopomers
CH ₃ I	HB78a	50-350	E	cont. res.
	HB79c	284-293	E	vibrational structure
	OCB98	5-480	E	absolute; (e,2e); (e,e+ion); ion yields, dipole induced breakdown
CH ₃ NO	IH86	275-325	E	HCONH ₂ formamide, comp. to (HCOX, X=F,OH)
CH ₃ NO ₂	VA&92	280-750	P	absolute; analysed as (CH ₃ ⁺ , NO ₂ ⁻); bond length corr.
CH ₃ NS ₂	TV93	285-295	T	NH ₃ CS ₂ ; ab initio-SCF-EICVOM; pre-edge res. (π^* , σ^*_{O-O} , σ^*_{S-S})
CH ₃ O ₃	T86	290-310	T	C(OH) ₃ ⁺ ; X α calc; comp of BF ₃ , B(OH) ₃ , C(OH) ₃ ⁺ , $\delta(R)$ – symmetry
CH ₄	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
	DC76	285-295	T	ab initio calc.
	EH&76	280-300	P	photoelectric yield

(CH ₄ cont'd)	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 ₃ ,H ₂ 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 ₂ H ₆ (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 ₄ ; transfer of OS (cont'd discrete in CF ₄)
	SS86a	240-390	P	total (e ⁻ ,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 ₃), comp. to other alkanes
	SAV87	280-320	P	absolute; thr. integrated OS comp. to CF ₄ , CO ₂
	RS&89	290-330	T	MS-Xα; C1s X-sect. & β for (CF _x H _{4-x} ,x=0-4); only CH ₄ res.!
	MR&90	280-320	P	ion desorption (H ⁺ from ice); comp. to TEY; gas (WB74b)
	RC&90	280-320	P	comp. of gas, solid; ion yields, H ⁺ ultrafast diss.
	HM&91b	287-294	P	ZEKE, 0.15 ev fwhm; comp. of CH ₄ , CD ₄ ; PCI modifies ZEKE; FC analysis of C _K ⁺ (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 ₃ X, X=H, CH ₃ , NH ₂ , OH, F; σ*(X-H)
	RDK93	286-291	P	high res (60 meV); I ^D /I ^H (3s) = 0.57(5); B-O not H-T vibronic coupling; comp. of CH ₄ /CD ₄ , C ₂ H ₆ /C ₂ D ₆ ; C ₃ H ₈ /C ₃ D ₈
	ST&93	286-291	P,T	high res (60 meV); ab initio; CH ₄ /CD ₄ comp; 3s/3p (D/H) is 0.65; comp of H ₂ O, NH ₃ , CH ₄ - 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 ₁ ,t ₂) are mixed with Rydbergs
	US&96	285-305	P,T	high res (60 meV); comp. of CH _x F _{4-x} (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 ₄ , 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
(CH ₄) _n	KB&97	284-296	P	NEXAFS as f(cluster size); gas-solid evolution
CH ₄ O	WB74b	282-325	E	(CH ₃ 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)
(CH ₄ O cont'd)	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_3X , X=H, $\text{CH}_3\text{ NH}_2$, OH, F; $\sigma^*(\text{X-H})$
	AJ&97a	278-293	P	relative, 45 meV fwhm; vibrational struct; comp to CD_3OD
	HP&99	287-298	P	relative, TIY, PIY, PEPICO yields, site specific fragmentation
	SO&02	285-298	P	relative, anion PIY, OH ⁻ 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
CH₄S	DTH90	275-325	E	CH_3SH ; absolute, comp. to other RSH, RSR'; $\sigma^*(\text{C-S})$
	TV93	285-295	T	ab initio-SCF-EICVOM; pre-edge res. ($\pi^*, \sigma^*_{\text{o-o}}, \sigma^*_{\text{s-s}}$); comp to DTH90
CH₅N	WB74b	280-320	E	(CH_3NH_2 - methylamine) res. at thr.
	SSH84a	295	T	σ^* -res./bond length relationship
	SB85b	285-335	E	σ^* res. at thr., comp. to $(\text{CH}_3)_x\text{NH}_{3-x}, x=0-3$
	LAL91	285-305	T	CNDO, systematic calc. of σ^* energies; ISEELS, ETS for param. det.
	S92	280-320	E,R	comp. of CH_3X , X=H, $\text{CH}_3\text{ NH}_2$, OH, F; $\sigma^*(\text{X-H})$
CNiO	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; $f(\pi^*)=0.24$; no reduction in $f(\pi^*)$ relative to free CO (.239 6 .234)
CO	SLD95	287	T	absolute, DF-LCAO; OS for C1s, O1s $\rightarrow \pi^*$; orbital mapping
	WSB70	280-310	E	ionic fragmentation (C^+ , CO_2^+ 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 β s
	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 effFects, comp. to N_2
	BD&82	285-290	E,R	calibration ($\pi^*=287.40\text{eV}$)
	ES&83a	284-302	P	total ion yield and fragmentation (PIMS), comp. to KLW776
	GN&83	280-320	P,T	comparison of core and valence cont. shapes
	KK83	285-289	T	ab initio (Z+1) basis calc. of (1s, π^*) energy, comp. to expt (HB80a)
	SK&83	280-300	E	dipole forbidden transitions
	TS&83	270-320	P	absolute, cont. X-sect., Auger yield, β value, shape res.
	UT83	280-290	E	$^3\pi$ state observed in ELS ($E_0=400\text{eV}$) and Auger-ELS (e,2e)
	ZMP83	280-500	E	appearance pot.s, π^* at 287.3
	AA84	285-310	T	ab initio, CI, all 1-e & 2-e transitions, oscillator strength
	CF&84b	287	P	DES, π^* AI; comp. to $\text{Cr}(\text{CO})_6$, $\text{CO}/\text{Cu}(100)$; $^1\pi \rightarrow ^3\pi$ before AI on surf.?
	EC&84	280-340	P	ion yield, ion KE, comp. to DES, CO/Cu and Mn,Co,Fe carbonyls
(CO cont' d)	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 (π^* 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) ($^3\pi^-$ $^1\pi$ =1.45 eV)	
SK&84b	270-320	P	absolute, Auger (AI) X-sect.; comp. to KLW77a, calc.	
SSH84a	295	T	σ^* -res./bond length relationship	
TL&84	280-320	P	Auger on π^* , cont; PES X-sect. & β 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 π^* , comp. to TKR79	
RL&85	280-320	P	comp. of multilayer PSID and ISEELS; comp. of CO, N ₂ , NO, N ₂ O	
UT85	275-315	E	autoionization and Auger decay by (e,2e)	
BH&86	285-320	P	β s change at π^* but not σ^* res.	
HI86	280-530	E	weak EXAFS	
HK86	283-290	E	5-40 eV constant final energy scans, $^3\pi^-$ / $^1\pi$ ratio, σ^* negative ion res. at 14 eV excitation	
KS&86	287	T	DV-X α , 1s--> π^* , comp. to IPES, NiCO, sensitive to R(Ni-C)	
RS&86	300-400	P	partial X-sections, β s for main line & sat.(S ₁ , S ₂); S ₁ (308 eV) displaced $\sigma^*(C-O)$; S ₂ (315 eV) - no shape res., diff. β 2e- excited states (1s ⁻¹ , val ⁻¹ , π^* ²)	
AWS87	303-308	T	IYs; (e,ion) coinc.; ion KE, comp. to TM COs & chemisorbed CO	
E87	285-340	P	XPS satellite part. X-sect.; S1 - displaced res.; S2 - no σ^*	
FR&87	300-400	P	ab initio, CI, absolute dipole, comp. to expt	
K87	287-295	T	absolute, test of EELS6PA conversion	
MC&87	280-330	E	review of electron-beam core excitation spectroscopies (Aussois)	
H89	280-320	E,R	thr. excited Auger, PCI, negative ion res.	
HKA88	280-300	E	absolute, total & part. IY; PIPICO, ion breakdown patterns	
HL&88	260-360	P	ZEKE; XPS-sat & EELS/PA, higher Ryd., 2e & shake-up, PCI	
MF&88	280-320	P	PIPICO, comp. to valence & O1s double ionisation	
NE&88	287,305	P	comp. to Ni(CO) ₄ ; vibrations resolved on π^*	
CSB89	280-335	E	σ^* shape res.; pos. & shape as f(R); approx. cyl. well; ab initio	
SG&89	290-330	T	comp to EELS, lower discrete/cont.; cont. flatter; O1s 2nd order	
SY&89	280-320	P	satellite line X-sect; comp. to atomic and N ₂	
BS90	296-400	P	85 meV fwhm; vibn struct. in 2-e- transitions	
DX&90	285-310	P	absolute; comp. to TM-COs; relaxation and $\delta(R)$ for $\sigma^*(CO)$	
H90a	280-325	E,R	absolute; comp. to TM-COs; f(π^*) vs. extent of backbonding	
HWR90a	280-325	E	RCHF calc, improved agreement with experiment [LT&84]	
SBM90	292-322	T	re. absorption vs. ion yields, PCI effects, comp. to N ₂	
BH91	280-320	E,R	ab initio; XAS and XRF; comp. to expt. (HB80a)	
FA91	287-290	T	β -parameter; comp. to DS&80	
L91	295-320	T	CNDO, systematic calc. of σ^* energies; ISEELS, ETS for param. det.	
LAL91	285-305	T	150 meV fwhm; isotope effect on π^* , Ryd vib'n; comp to N ₂ ;	
MC&91	285-304	P	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) ₅	
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	
(CO cont' d)	RS&92a	280-330	P	TEY, TIY; comp. of CO ⁺ and (CO) ₂ ⁺ from (CO) _n , n to 8;

			cont. incr. in CO^+ ; ms; PIPICO
SK&92a	298-322	P	cross-sect. & β from PES; (1s^{-1}) 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	ΔSCF ; 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	β -values for C^+ and Auger; $\beta>1$ at 305 (σ^*) in both; $\pi\text{-}\sigma$ 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; σ^* 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^+, O^+ ; relaxed core HF calc; effect of C 1s shake-up on β
DK94	286,287.4	E	autoioniz. decay of ${}^3\pi$ ($E_0=315$ eV); PCI shifts (95 mV- ${}^1\pi$; 115 mV- ${}^3\pi$)
DRK94	286-291	P,R	SX700 high res. studies; vibrational structure in small mols.
FKH94	284-288	E,T	angle and E_0 study of ${}^3\pi$; ab initio CI potential curves; ${}^1\pi$ and ${}^3\pi$ differ
FE&94	285-290	E,T	triplet π^* ; INDO calc; correlation of S-T split. and $f({}^1\pi^*)$
HH&94	285-320	P	Auger anisotropy at σ^*
NR&94	287.4	P,T	DES; v of CO^+ (val) depends on v of ($\text{C}1\text{s}^{-1}, \pi^*$); comp. to N_2, O_2
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; ΔSCF 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°), β ; initial state alignment produces anisotropic Auger; effect stronger at π^* than σ^*
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 σ^* SR only seen in parallel
HW&95	330	P	ang.dist. of shake-up; participant 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: $\text{C}1\sigma^*=86(10)$ mV; $\text{C}1\text{s}^{-1}=97(10)$ 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 π^* , Ryd.
EK&96	286-294	P	partial ion yields; KERDs; frag. mechanisms; enhanced $v=4$ of π^* 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_{17}CO , Cu_{50}Co ; models of CO/Cu(100)
(CO cont ' d)	SB&96	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 ₂ CO, N ₂
SH&96b	287-287	P	(C ⁺ ,O ⁺) angular and KE distributions; β 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; π^* , σ^* res. rel. position; comp. of π - σ sep. in CO, C ₂ H ₂ , C ₂ H ₄ , N ₂ , O ₂
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 π^* , σ^* ; (C,O ⁺) NOT detected, contrary to HL&88
YA&96	280-320	T	STEX; comp. to expt. and other theory; R ₂ CO species
AK&97	285-289	P	angle-resolved ion yields; ion β 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) ⁻¹ and resonant interference ; PE branching ratios as f(E) from interference absolute; STEX; resonant elastic scatt.; vib'n α detuning in REXS
GA97	280-340	T	mass & angle resolved PEPICO; TOF e-,ion; forward/backward asymmetry due to multiple scattering; agrees with DSD76
HG&97	321,326	P	relative; 12500 resolving power; 25 meV fwhm instrumental
JA&97b	286-297	P	resonant X-ray emission (RIXS); ang. dep. at 3s, 3p, Ryd; v-dependent
NG&97	287-296	P,R	relative; high-res.; vibrationally resolved AI decay; ab initio calcs;
PN&97	287-289	P,T	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'l struct. α 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	π^* 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 α 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 σ^*
SA&98a	300-340	P	fixed-in-space molecule; symmetry repsolved PA and PI; Angular distribution.; forward scattering effect
SA&98b	305,330	PT	σ^* 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 ₂ 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
BW&99	287, 350	P	PEPICO; Auger-ion coinc; 2-step (C ⁺ ,O ⁺) at π^* ; wall coll. & KERD
HH&99	290-300	P	Ryd states; angle rresolved resonant Auger; β 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	π^* (79(5) and Ryd (3s 92(5), 3p 108(20)) lifetime widths
SS&99	287-292	P	resonant Auger at π , 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
(CO cont'd)	FK&00	287	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 ₂
	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 ₀)
	KS01	296-1000	E	electron impact excited Auger-ion coincidence; comp to CO ⁺⁺ 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 – vib'n'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
	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 ⁻ 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
	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 ₂ , N ₂ , N ₂ O
	PN&15	856	P	2-site double core hole IP (ts-DCH), SR, not FEL, coincidences
	TKU15	855	T	(XH _m -YH _n) 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 → π*; orbital mapping
COPt	SLD95	287	T	absolute, DF-LCAO; OS for C1s, O1s → π*; orbital mapping
COS	WB74e	282-328	E	pot. bar. effects
	TKR79	288-289	E	<70meV FWHM res., vibrational structure
	SSH84a	295	T	σ*-res./bond length relationship, anomalus
	TL&84	280-320	P	Auger on π*, Auger, PES cross-sections, βs, absolute
	HK87	285-297	E	singlet-triplet (π) = 1.13 eV, σ*(C-S) = 0.3 eV
	HI88b	280-530	E	near edge and EXELFS; comp to calc (unpublished)
	NE&88	305	P	PIPICO, ion kinetic energies, comp. to valence, O1s ionization
	NH&88	285-325	R	comp. of ETS, all edges, CO ₂ , CS ₂ re localization of σ*, decay
	MH&89	275-340	E,T	absolute, ab initio, comp. of CO ₂ , COS & CS ₂ - 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 π* state of CO ₂ , COS, CS ₂ ; ion yield polarization
	EK&97a	287-297	P	TIY, PEPICO; β ; high res.; PEPIPICO
	EK&97b	286-296	P	TIY, PEPICO; fragmentation mechanisms
	EK&97c	286-296	P	TIY, PIY; PE3PICO; fragmentation mechanisms
(COS con't)	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 σ*

	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 α
	GA&05b	298-335	P, T	AR-PEPICO, comp of S2p, C1s, O1s at selected energies, MS-X α
CO₂	WB74a	285-328	E	cont. res., Z+1 analogy
	SB76	285-330	T	geometry corrected, Z+1 analogy calc., E(¹ π - ³ π)=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 ⁻¹ width = 0.07(2) eV
	KK83	285-289	T	ab initio (Z+1) basis calc. of (1s, π^*) energy, comp. to expt (WB74a)
	SK&83	280-300	E	dipole forbidden transitions
	ZMP83	280-500	E	appearance pot.s, π^* 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	σ^* -res./bond length relationship, anomalous
	TL&84	280-320	P	Auger on π^* , Auger, PES cross-sections, β 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 π - ³ π)=1.48eV, comp. to theory (SB76)
	HK87	288-299	E	singlet-triplet (π^*) = 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- α ; thr. inte. OS comp. to CH ₄ , CF ₄
	NH&88	285-325	R	comp. of ETS, all edges, CO ₂ , CS ₂ re localization of σ^* , decay
	MH&89	275-340	E,T	absolute, ab initio, comp. of CO ₂ , COS & CS ₂ - all edges
	SG&89	290-330	T	σ^* 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,2e); DES comp. to Auger, theory [Phys. Rev. B 41 (90) 10510]
	LAL91	285-305	T	CNDO, systematic calc. of σ^* energies; ISEELS, ETS for param. det.
	MC&91	292-297	P	50 meV; vibrations in Ryd. states
	BBS91	260-380	E,T	GOS (π^*); ab initio Δ 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 ₂) _n
	SK&92a	298-340	P	cross-sect. & β from PES; (1s ⁻¹) 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 α ; comp. to WB74
	BD93	288-292	E	near threshold (0°) excit.; σ^* res. in I(¹ π / ³ π); δ E(¹ - ³)=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 ₂ , N ₂ O, Fe(CO ₂ (NO) ₂
	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, β s; 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; β s for main & satellite lines; coupling prevents use of main lines to identify SR; strong conjugate shake-up
(CO ₂ cont' d)	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 ² =0; comp. to BBS91
	HC&96	300	P	triple coincidence (C+,O+,O+) PIPICO
	K96b	292-298	P,R	symmetry resolved; 3sσ _g shows anisotropy assoc. with bending; vibronic coupling in antisym. mode; strong effect on 3p,3d; no axial recoil approx. O ⁻ yield; compared to cation and TIY; O ⁻ from primary process
	RJ96	280-330	P	STEX; comp. to expt. and other theory; R ₂ CO species
	YA&96	280-320	T	Renner-Teller split π* state of CO ₂ , COS, CS ₂ ; ion yield polarization
	AK&97a	291	P,T	resonant X-ray emission (RIXS)
	NG&97	291	P,R	π* OS; test of initial and final state sum rules; comp to expt.
	YA&97	287	T	Ryd (3s100(10), 3p 90(10), 4p (80(20)) lifetime widths
	PV&99	290-296	P	methods; GOS at π*, Ryd; MC-GMS calc
	ET&00	280-296	E,T	dipole, non-dipole spectra; π* GOS; parallel detection evaluation
	H00	282-330	E,T,R	high res.; resonant Auger; Renner-Teller; participator decay to A state; potential energy curves derived
	KBB00	289-292	P,T	E-PEPICO; bending mode affects ionic frag; more (O ⁺ ,CO) on low-E side sub-natural linewidths by resonant Auger
	MS&00	290-298	P	GOS at π*, Ryd; MC-GMS calc
	SO&01	290.7	P	fixed-in-space PE ang. dist.; f,p,h waves similar intensity at σ*
	TE&01b	280-340	E,T	threshold yield; shake-up satellites; time domain analysis
	AM&02	288-325	P	symmetry resolved, high resolution; review
	HR&02	285-320	P,T	Auger-ion imaging; bent-linear changes fragmentation, ES-AEPICO
	K02	284-298	P,TR	symmetry-resolved Renner-Teller, A ₁ , B ₁ potentials and spectra; vibrational structure; comp to YN&02
	MC&02	290-292	P	relative, Anion, cation PIY; only O ⁻ at (C1s ⁻¹ ,π*); O ⁻ , C ⁻ at O1s edge
	N02	290-292	T	GOS computed with vibronic contributions
	OS&02	288-312	P	COLTRIMS, ion-ion correlation, geometry deformation in (1s ⁻¹ , π*) symmetry-resolved Renner-Teller; separation of A ₁ , B ₁ signals
	RB02	292	T	fixed-in-space ang. dist.; RCHF calc agree with measurements
	SM&02	291	P, T	GOS and incident energy (Jubilee) resonances calculated
	YN&02	290-292	P	PIPIPICO (-ve, +ve) at π*; mechanism via (CO ⁺⁺ ,O ⁻)
	SF&03	285-335	P,T	GOS; oscillations from Young-type interference; comp to ET&00
	KM&03	290	T	ion angular dist; fixed-molecule PAD spectra, review
	RF04	290	P	PE ang. dist., expt'l dipole matrix elements, shape resonance @ 315 eV
	BRB05	292-296	T	Auger-ion-ion coincidence, [Auger, metastable CO ₂ ²⁺] coinc.
	YHA05	315	P,R	in-situ catalysis tracking (CO oxidation) in a E-TEM
	TA&07	300-325	P,T	(CO ⁺ , O ⁺) ang. dist in coinc with PE; bend angle geometric effect
	SS&12	320	P	double core hole (DCH) PES&Auger; compare CO, CO ₂ , N ₂ , N ₂ O
(CO ₂) _n	MC14	275-285	E	ZEKE, (ZEKE, ion,ion) yield; threshold ion-pairs with atomic ions are quenched in cluster; fast charge transfer; participator val. Auger
	TK&14	320	P,T	H ₂ CO ₃ ; ab initio-SCF-EICVOM; pre-edge res. (π*, σ* _{O-O} ,σ* _{S-S}) pot. bar. effects
	BF15	664	P,T	anomalous σ*-res./bond length relationship
	DJ&92	295-320	P	H87 relative yields of CS ₂ ⁺ , CS ⁺ , CS ₂ ²⁺ ; ion state decay, quadrupole MS
	CO ₃ H ₂	TV93	285-295	HK87 singlet-triplet (π*) = 0.9 eV, σ* = 0.8 eV
	CS ₂	WB74e	280-325	comp. of ETS, all edges, CO ₂ , CS ₂ re localization of σ*, decay
	SSH84a	295	E	absolute, ab initio, comp. of CO ₂ , COS & CS ₂ - all edges
	H87	270-310	P	Renner-Teller split π* state of CO ₂ , COS, CS ₂ ; ion yield polarization
	HK87	284-297	E	TIY, angle-resolved PEPICO; β = -0.65 for S ⁺ at π*; doubly excited states; anisotropy as f(KE); 80 meV fwhm
	NH&88	285-325	R	FE&99 TIY; ionic frag; branching ratios; state selective fragmentation
	MH&89	275-340	E,T	YE&99 TIY; ionic frag; branching ratios; state selective fragmentation
	AK&97a	286	P,T	K02 symmetry resolved, high resolution; review
	KE&98	280-320	P	KM&03 GOS and incident energy (Jubilee) resonances calculated
(CS ₂ cont'd)	FE&99	283-320	P	
	YE&99	283-320	P	
	K02	284-298	P,TR	
	KM&03	286	T	

	ET&07	280-310	E,T	absolute, OOS, , non-dipole, triplet states
	TR&07	280-310	E,T	absolute, OOS, GOS to 30 a.u. ⁻¹ , MP-CI calc
C ₂	SG&89	290-330	T	σ^* shape res.; pos. & shape as f(R); approx. cyl. well & ab initio
C ₂ ClH ₃	BMT88	280-310	E	comp. to ETS
	SKB88	275-320	E	high res., comp. to vinyl halides
C ₂ ClH ₅	HB78b	284-300	E	ethyl chloride; test of spectral additivity
	FL02	284-299	E	absolute, GOS profiles compared of C 1s, Cl 2p & valence
C ₂ Cl ₂ H ₂	CT&12	283-291	P, T	iso-dichloroethylene, PEY, resonant Auger, ADC Green's fn. calc.
C ₂ Cl ₂ H ₄	H92a	280-340	E	1,2-dichloroethene, absolute, comp. to NEXAFS (W. Walter)
C ₂ Cl ₃ H	WH90	275-340	E	trichloroethene
C ₂ DH	KI&97	282-292	P,T	high res. (20 meV); isotopomer comp.; vibronic coupling at π^* ; bending modes excited; ab initio calc.
C ₂ D ₂	MC&91	284-291	P	50 meV fwhm; π^* & Ryd vibns; comp of C ₂ H _x , C ₂ D _x (isotope eff.)
	KI&97	282-292	P,T	high res. (20 meV); isotopomer comp.; vibronic coupling at π^* ; bending modes excited; ab initio calc.
C ₂ D ₂ H ₂	KI&95b	283-291	P	CD ₂ CH ₂ ; absolute; ethene isotopomers 40 meV fwhm; vibn'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 ₂ D ₄ , C ₂ H ₄ ,CH ₂ CD ₂ , cis-CHDCHD)
C ₂ D ₂ H ₂	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 ₂ D ₄ , C ₂ H ₄ ,CH ₂ CD ₂ , cis-CHDCHD)
C ₂ D ₄	CS90	284-287	P	π^* vib'n'l isotope effect; symmetry breaking; localised core hole
	MS&89	284-287	P	π^* vib'n'l isotope effect; symmetry breaking; localised core hole
	MS&90	284-287	P	π^* vib'n'l isotope effect; symmetry breaking; localised core hole
	MC&91	286-291	P	50 meV fwhm; π^* & Ryd vibns; comp of C ₂ H _x & C ₂ D _x (isotope eff.)
	RA&92	284-286	P	high. res. (<90meV); vibn'l; comp. to C ₂ H ₄
	KI&95b	283-291	P	40 meV fwhm; π^* vibn's in isotopomers; hole localiz.
	KG&97	283-287	T	vibronic coupling; symmetry breaking and core hole localization; comparison of isotopomers (C ₂ D ₄ , C ₂ H ₄ ,CH ₂ CD ₂ , cis-CHDCHD)
C ₂ D ₆	MC&91	287-291	P	50 meV fwhm; π^* & Ryd vibns; comp of C ₂ H _x & C ₂ D _x (isotope eff.)
	RDK93	286-291	P	high res (60 meV); comp. of CH ₄ /CD ₄ ; C ₂ H ₆ /C ₂ D ₆ ; C ₃ H ₈ /C ₃ D ₈
C ₂ FH ₃	BB&85	280-296	P	parent ion yields, distorted cont./discrete intensities; QMS
	MC&87	275-325	E	absolute, comp. to C ₂ H _x F _{4-x} , development of pot. bar.
	HFM87	280-320	E	comp. to other fluorocarbons; $\sigma^*(C-F)$ 'giant shape res.'
	BMT88	280-310	E	comp. to ETS
	RI&88	275-325	E	perfluoro effect, $\sigma^*(C-F)$
	SKB88	275-320	E	high res., comp. to vinyl halides
C ₂ FeN ₂ O ₄	SL&92	280-300	P	Fe(CO) ₂ (NO); PEPICO; stewise fragmentation; non-selective
	ML&93	285-320	P	ionic fragmentation mechanisms; comp. of CO ₂ , N ₂ O, Fe(CO ₂ (NO)) ₂
	L95	320	P,R	PEPICO dissoc.; review of coinc. studies of DI dynamics
	NM96	320	P,R	PEPICO; review of fragmentation
C ₂ F ₂ H ₂	BB&85	280-296	P	1,1-CH ₂ =CF ₂ , 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; $\sigma^*(C-F)$ 'giant shape res.'
	MC&87	275-325	E	absolute, comp. to C ₂ H _x F _{4-x} , C-F σ^* res., pot. bar.
	RI&88	275-325	E	perfluoro effect, $\sigma^*(C-F)$
	JS&90	285-306	P	ZEKE, PE-PI coinc.; sel. frag.; comp. of CF ₂ CH ₂ , CF ₃ CH ₃
	HB&91	285-310	P	ZEKE, TEY, TIY; TOF-MS; site-selective frag.; "memory-eff."
(C ₂ F ₂ H ₂ cont'd)	OY&05	283-308	P	absolute, PIY, KE distributions of CFH ₂ ⁺ , CH ₂ ⁺ , vibrational effects
C ₂ F ₂ H ₂	MC&87	275-325	E	1,2-CHF=CHF; absolute, comp. to C ₂ H _x F _{4-x} , C-F σ^* res., pot. bar.
C ₂ F ₃ H	BB&85	280-296	P	parent ion yields, distorted cont./discrete intensities; QMS

	HFM87	280-320	E	comp. to other fluorocarbons; $\sigma^*(C-F)$ 'giant shape res.'
	MC&87	275-325	E	absolute, comp. to $C_2H_xF_{4-x}$, $C_2H_xF_{4-x}$, pot. bar.
	RI&88	275-325	E	perfluoro effect, $\sigma^*(C-F)$
$C_2F_3HO_2$	RI&88	280-330	E	CF_3COOH , comp. to other acids
$C_2F_3H_3$	MS&84	280-309	P	CH_3CF_3 ; thr. e^- , 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_2H_6 , CH_3CF_3 , C_2F_6 ; partial pot. barr.
	JS&90	285-306	P	ZEKE, PE-PI coinc.; sel. frag.; comp. of CF_2CH_2 , CF_3CH_3
	HB&91	285-310	P	ZEKE, TEY, TIY; TOF-MS; site-selective frag.; "memory-eff."
	SSL91	290-300	T	site-selective frag. at CF_3 ; but stat. redist. int. energy in M^{2+}
$C_2F_3H_4N$	HC&87b	278-305	P	$CF_3CH_2NH_2$, thr. e^- , TOF-MS, claims selective fragmentation
C_2F_3N	HS90	280-340	E	CF_3CN , absolute; comp. to other triply bonded species
C_2F_4	BB&85	280-296	P	parent ion yields, distorted cont./discrete intensities; QMS
	HFM87	280-320	E	comp. to other fluorocarbons; $\sigma^*(C-F)$ 'giant shape res.'
	MC&87	275-325	E	absolute, comp. to $C_2H_xF_{4-x}$, $C-F \sigma^*$ res.
	RI&88	275-325	E	perfluoro effect, $\sigma^*(C-F)$
	H90a	290-320	E,R	absolute, pot. bar. effect on $I\{\sigma^*(C-F)\}$ through CF_x series
	LAL91	285-305	T	CNDO, systematic calc. of σ^* energies; ISEELS, ETS for param. det.
C_2F_6	HFM87	280-320	E	comp. to other fluorocarbons; $\sigma^*(C-F)$ 'giant shape res.'
	IM&88	275-325	E	$C-F \sigma^*$ res.
	H90a	284-320	E	absolute; comp. of C_2H_6 , CH_3CF_3 , C_2F_6 and CF_x ; pot. barr.
	AC&95	290-315	T	STEX ab initio; absolute; growth of poly ($CF_2)_n$ by $C_{2n}F_{4n+2}$, $n=1-5$
$C_2F_6O_2$	H86b	285-335	E,R	orbital mapping
	IM&87	285-335	E	$CF_3-O-O-CF_3$, long O-O bond = low σ^*
	HM&89	275-350	P	absolute; total, partial ion yields; PIPICO, diss. IY; sel. frag.
C_2H_2	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
	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	σ^* -res./bond length relationship
	HK87	283-293	E	$Eo=120$ eV, no triplets resolved, π^* broader, Rydbergs modified
	AR&89	280-320	P,E,T	curve fit of HB77; comp. to NEXAFS; theor. (SW) lineshape; multi e- σ^* 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^2 , delocal. hole; C_2H_x ($x=2,4,6$); $\sigma^*(C-H)/\sigma^*(C-C)$ reversal
	FSL91	290-390	T	CNDO, systematic calc. of σ^* energies; ISEELS, ETS for param. det.
	LAL91	285-305	T	50 meV fwhm; π^* & Ryd vibns; comp of C_2H_2 & C_2D_2 (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_2H_x , $x=2,4,6$; $\sigma^*(C-C)$
	S92	280-330	E,R	$^3\pi^*$; INDO calc; correl. of $\Delta(1,3)$ and π^* osc. str.
	FE&94	284-286	E,T	absolute; improved method for X-section detection; this bibliography!!
	HM94	270-350	E,R	GOS for $^1\pi^*$; relax., corr. & core-hole local. considered; OOS=0.147
	MB&94a	280-292	E,T	coupled cluster abi initio; S-T splittings of Rydberg states
	NB95	284-292	T	local density; Hedin-Lundquist potential needed to match expt.
	STS95	284-310	T	DFT calc.; $^3\pi^-1\pi$ split = 0.50 eV
(C_2H_2 cont'd)	HC96	285-286	T	constant chemical potential LDA; π^* , σ^* res. rel. position; comp. of $\pi-\sigma$ sep. in CO , C_2H_2 , C_2H_4 , N_2 , O_2
	SST96	285-315	T	

	KI&97	282-292	P,T	high res. (20 meV); isotopomer comp.; vibronic coupling at π^* ; bending modes excited; ab initio calc.
	KK&97a	280-350	P	main line cross-sections; comp. to absorption; weak peak at C ₂ H ₂ abs. max; comp. of C ₂ H _x , x=2,4,6; disputing existence of shape resonances
	KK&97b	290-360	P,T	absolute; C 1s ₋₁ main line & satellite X-sections; broad 310 eV peak assigned to shake-up NOT σ^* ; smooth main line β at 310 eV 6 no σ^*
	KK&97c	298, 338	P,T	XPS, g-u splitting = 0.05(1) eV; vibrational and 2 state fit
	KN&97b	280-340	P	resonance Auger, well-resolved Rydberg spectrum; angle resolved; π^*, σ^* anisotropic; double excitation
	TPA98	280-320	T	absolute; DFT vs. STEX, comparison of C ₂ H _{2x} , x=1,2,3; comp. to C ₂ H ₂ /Cu
	GG&99	284-292	P,T	core hole localization in C ₂ 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 C ₂ H ₆
	TB&99	297-348	P,T	σ_g & σ_u partial X-sections; resonance in ratio of X-sect.; disputes KK&97b
	HC&00	280-340	T	shape resonances from MS (Feff8) in C ₂ H _{2x} ; ang. dep; IPs good to 0.5 eV
	LL00	290-360	T	absolute; partial channel; β ; comp. to KK&97a; σ^* overlaps 2-electron
	HJ&02	278-330	E,T	absolute GOS; calculated strong quadrupole π^* not observed
	K02	284-298	P,TR	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 σ^*_{C-C} in C ₂ H _x
	K04	287-292	P,T	symmetry resolved Ryd states; g-u splitting, Ryd-val. Exchange
	MTU04	298-356	P	vibrationally & σ_g/σ_u resolved PI X-sections; SR only in σ_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 ⁻² , ³ π^* , ¹ π^*
	SF&05	270,286,540	P	momentum imaging, (H ⁺ , H ⁺ , C ₂ ⁺) newton diagram at C1s ⁻¹ , π^*
	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 ₂ H ₂ O ₂ S ₄	PN&15	597,654	P	1-site, 2-site double core hole IP (ts-DCH), SR, not FEL, coincidences
C ₂ H ₃ I	TV93	285-295	T	(OHCS ₂) ₂ ; ab initio-SCF-EICVOM; pre-edge res. (π^* , σ^*_{O-O} , σ^*_{S-S})
C ₂ H ₃ N	BMT88	280-310	E	comp. to ETS
	SBK88	275-320	E	high res., comp. to vinyl halides
C ₂ H ₃ N	HTM89	275-325	E,P	(CH ₃ CN), comp. to solid, σ^* res./bond length
C ₂ H ₃ NS	HM&89	275-350	P	absolute; total, partial ion yields; PIPICO, diss. IY; sel. frag.
C ₂ H ₃ NS	S92	280-320	E,R	comp. of gas, sol. monolayer(Pt)
C ₂ H ₄	PS&01	280-315	T	STEX, comp. to expt.; extensive series of C-N compounds
	HTM89	275-340	E	(CH ₃ NC), comp to CH ₃ CN, vibrational ELS
	HTM89	275-340	E	(CH ₃ SCN), comp to CH ₃ NCS, vibrational ELS
	HTM89	275-340	E	(CH ₃ NCS), comp to CH ₃ SCN, vibrational ELS
	EH&76	280-300	P	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	σ^* -res./bond length relationship
	HR87	280-300	E	use of core excitation (HB77) to interpret Auger satellites (DES)
(C ₂ H ₄ cont'd)	MC&87	275-325	E	absolute, comp. to C ₂ H _x F _{4-x}
	SS87b	269-324	P	8% modulation of W-value (energy/ion pair); Ryd., cont. struct; weak π^* , prominent σ^* , 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_2D_4 , sym. breakdown, local. hole	
PF&89	280-360	P	partial X-sect., σ^* at 302 eV	
CS90	284-287	P	π^* 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	π^* vib'nl isotope effect; symmetry breaking; localised core hole	
FSL91	290-390	T	absolute; L^2 , delocal. hole; C_2H_x ($x=2,4,6$); $\sigma^*(C-H)/\sigma^*(C-C)$ reversal	
GK&91	283-291	P,T	40 meV fwhm; (${}^1B_{1u}, {}^1B_{2g}$) vibronic coupling; 0.02 eV sep.; dynamic hole localisation by vibronic-coupled symmetry breaking	
LAL91	285-305	T	CNDO, systematic calc. of σ^* energies; ISEELS, ETS for param. det.	
MC&91	284-291	P	50 meV fwhm; π^* & Ryd vibns; comp of C_2H_x & C_2D_x (isotope eff.)	
TF&91	280-300	T	MS (cluster); calc. of pol. dep. on Cu(100); C-H res. (288 eV) with σ -pol.; comp. to expt. (SSH84a)	
RA&92	284-286	P	high. res. (<90meV); vib'n'l; comp. to C_2D_4 ; M- C_2H_4 bond mod. vib.	
S92	280-330	E,R	comp. of C_2H_x , $x=2,4,6$; $\sigma^*(C-C)$	
KS&93	290-350	P	absolute; partial PI, β ; 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_2H_4 , C_4H_6 , C_6H_8 ; comp. to GK&91 (solid); claims relaxation shifts dominate; π^* split small.	
FE&94	284-287	E,T	${}^3\pi^*$; INDO calc; correl. of $\Delta(1,3)$ and π^* 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 $H-(CH=CH)_n-H$, $n=1-5$	
KI&95b	283-291	P	40 meV fwhm; π^* 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); π -exciton effects; $H(C_2H_2)_nH$, $n=1,10$	
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; π^* , σ^* res. rel. position; comp. of π - σ sep. in CO , C_2H_2 , C_2H_4 , N_2 , O_2	
YA96	290-315	T	STEX; shake-up spectra related to NEXAFS; $H(C_2H_2)_nH$, $n=1-5$	
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_2D_4 , C_2H_4 , CH_2CD_2 , cis-CHDCHD)	
KK&97a	280-350	P	main line cross-sections; comp. to absorption; weak peak at C_2H_4 abs. max; comp. of C_2H_x , $x=2,4,6$; disputing existence of shape resonances	
KK&98c	284-350	P	absorption; PES; $C1s^{-1}$ & satellite partials; disputes shape resonance	
TPA98	280-320	T	absolute; DFT vs. STEX, comparison of C_2H_x , $x=1,2,3$	
GG&99	284-292	P,T	core hole localization in C_2H_x ; 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_2H_6	
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	
(C_2H_4 cont'd)	SF&99	283-292	P, T	reonant Auger at π^* 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_2H_{2x} ; ang. dep; IPs good to 0.5 eV
	RB00	285-289	T	absolute; GMS-ab initio; GOS for π^* , Ryd

	HJ&02	278-322	E,T	absolute GOS; calculated strong quadrupole π^* 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 σ^*_{C-C} in C_2H_x
	IH07	284-302	T	relative, Gaussian augmented plane wave (GAPW) - DFT; (-5 to +3 eV errors on 14 small molecules
$(C_2H_4)_n$	PN&15	595,652	P	1-site, 2-site double core hole IP (ts-DCH), SR, not FEL, coincidences
	RS&92b	280-320	P	clustered ethylene; comp. of partial, total yield channels
C_2H_4O	HR96	282-296	P,R	clustered ethylene; comp. of partial, total yield channels
	HB80b	280-320	E	$(CH_3CHO$ - acetaldehyde) cont. res.
C_2H_4O	SSH84a	295	T	σ^* -res./bond length relationship
	YA&96	280-320	T	STEX; comp. to expt. and other theory; R_2CO species
$C_2H_4O_2$	YA&97	287	T	π^* OS; test of initial and final state sum rules; comp to expt.
	TJ&99	284-300	P	relative; TIY; participator decay; 2 states in π^*
$C_2H_4O_2$	SB91a	280-410	P	ethylene oxide; high res.; Ryd. vib'nl resolved; comp to C_3H_6
	ES84	270-310	P	$(CH_3COOH$, acetic acid), partial & total ion yields, mass spectra
$C_2H_4O_2$	RI&88	270-330	E	$C-F \sigma^*$ res., absolute, perfluoro effect
	S92	280-325	E,R	comp. of HCO_2H , HCO_2CH_3 and PMMA NEXAFS
$C_2H_5NO_2$	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
$C_2H_5NO_2$	IH88	275-325	E	$HCOOCH_3$, methyl formate, absolute, spectral aditivity tested
	JT94b	275-316	E,T	ISEELS as f(resolution); DES by (e,2e); strong participator
$C_2H_5N_3O_2$	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
C_2H_6	IK&14	330	P	fragmentation of ionized glycine
	UA&99	280-340	E	biuret; $(NH_2(CO)NH(CO)NH_2)$; absolute; polymer model
C_2H_6	LC&07	280-320	E,T	comp. of di-carbonyls; charge shifts for fingerprinting, GSCF3
	EH&76	280-300	P	photoelectric yield
C_2H_6	HB77	280-340	E	comp. to CH_4 & EH&76 C_2H_6 data
	HB&84	280-320	E	comp. to CH_4 (WB74b), (HB77) data, $\sigma^*(C-C)$ res. at thr.
C_2H_6	SSH84a	295	T	σ^* -res./bond length relationship
	HI87	275-325	E	$\pi^*(CH_3)$, comp. to other alkanes
C_2H_6	HR87	280-300	E	use of core excitation (HB77) to interpret Auger satellites (DES)
	IM&88	275-325	E	absolute OS, comp. to C_2F_6
C_2H_6	AR&89	280-320	P,E,T	curve fit of HB77; comp. to NEXAFS; theor. asymmetric σ^* lineshape
	SG&89	290-330	T	σ^* shape res.; pos. & shape as f(R); approx. cyl. well & ab initio
C_2H_6	H90a	284-316	E,R	absolute; comp. of C_2H_6 , CH_3CF_3 , C_2F_6 ; partial pot. barr.
	FSL91	290-390	T	absolute; L^2 , delocal. hole; C_2H_x ($x=2,4,6$); $\sigma^*(C-H)/\sigma^*(C-C)$ reversal
C_2H_6	LAL91	285-305	T	CNDO, systematic calc. of σ^* energies; ISEELS, ETS for param. det.
	MC&91	284-291	P	50 meV fwhm; π^* & Ryd vibns; comp of C_2H_x & C_2D_x (isotope eff)
C_2H_6	S92	280-320	T,R	MS-X α ; comp. of propane, ethane
	RDK93	286-291	P	high res (60 meV); comp. of CH_4/CD_4 ; C_2H_6/C_2D_6 ; C_3H_8/C_3D_8
$(C_2H_6 \text{ cont'd})$	KK&97a	280-350	P	main line cross-sections; comp. to absorption; no peak at claimed position of σ^* in abs. (but main line cross-section does not reach); comp. of C_2H_x , $x=2,4,6$; disputing existence of shape resonances
	TPA98	280-320	T	absolute; DFT vs. STEX, comparison of C_2H_{2x} , $x=1,2,3$
$(C_2H_6 \text{ cont'd})$	GG&99	284-292	P,T	core hole localization in C_2H_{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 C_2H_6
$(C_2H_6 \text{ cont'd})$	RK&99	250-560	P	absolute; true absorption; vibn'l resolved PES; $C1s^{-1}$, Sat., X-sect
	HC&00	280-340	T	shape resonances from MS (Feff8) in C_2H_{2x} ; ang. dep; IPs good to 0.5 eV
$(C_2H_6 \text{ cont'd})$	ZTC03	280-320	T	MS-cluster calc, C-H resonances in near continuum, $\delta(R)$ for σ^*_{C-C} in C_2H_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	(XH _m -YH _n) X,Y = C,N,O,F; m,n = 0-3 – 2-site double core hole IPs
C₂H₅NO₂	CG&04	282-304	E	(glycine), comp. of Gly, Gly-gly, Gly ₃ , gas-solid
C₂H₆O	WB74b	285-325	E	(CH ₃ OCH ₃ - dimethyl ether)
	SSH84a	295	T	σ*-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 σ* energies; ISEELS, ETS for param. det.
C₂H₆O	SY&89	280-320	P	(C ₂ H ₅ OH), lower discrete/cont. ratio, cont. flatter, O1s 2nd order
C ₂ H ₆ O ₂	EUH98	280-320	E	ethylene glycol; (CH ₂ OH-CH ₂ OH); absolute; comp to PEO
C ₂ H ₆ O ₃	HW&91	280-340	E	(CH ₃ O) ₂ C=O; absolute; comp. to phenyl carbonate
C ₂ H ₆ OS	TB&88	280-320	E	(CH ₃) ₂ S=O, DMSO, comp. to S1s
C ₂ H ₇ N	SB85b	285-335	E	σ* res. at thr., comp. to (CH ₃) _x NH _{3-x} ,x=0-3
C ₂ H ₈ O ₂	IH07	284-302	T	methanol dimer; relative, Gaussian augmented plane wave (GAPW) - DFT; (-5 to +3 eV errors on 14 small molecules
C ₂ N ₂	HB79b	280-320	E	cont. res.
	SSH84a	295	T	σ*-res./bond length relationship
	SG&89	290-330	T	σ* shape res.; pos. & shape as f(R); approx. cyl. well & ab initio
C ₃ D ₈	RDK93	286-291	P	high res (60 meV); comp. of CH ₄ /CD ₄ ; C ₂ H ₆ /C ₂ D ₆ ; C ₃ H ₈ /C ₃ D ₈
C₃F₃H	HS90	280-340	E	CF ₃ C:::CH, absolute; comp. to other triply bonded species
C ₃ F ₃ H ₃ O	HC&87b	280-310	P	CF ₃ COCH ₃ , thr. e-, TOF-MS, claims selective fragmentation
C₃F₆O	RI&88	280-325	E	(perfluoroacetone), C-F σ* res., absolute, perfluoro effect
C₃F₆	IM&88	275-325	E	perfluoro-cyclopropane, C _x F _{2n} series, σ*(C-F) dominated
C₃F₈	HFM87	280-320	E	comp. to other fluorocarbons; σ*(C-F)'giant shape res.'
	IM&88	275-325	E	perfluoropropane, C _x F _{2n+2} series, σ*(C-F) dominated
C₃H₂O₂	IH88	275-325	E	(propionic acid), comp. to solid, absolute
C ₃ H ₃ N ₂ O ₂	IH&11	330	P	(uracil), site-selective fragmentation after C 1s ionization, PEPICO
C ₃ H ₂ N ₂ OBr	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
C ₃ H ₃	SC95	288	T	c-C ₃ H ₃ ⁺ ;ADC local/delocal calc; Jahn-Teller localis.; comp. to B ₃ H ₃ N ₆
C ₃ H ₃ N	MB&94b	280-320	P,T	C ₂ H ₃ CN - acrylonitrile; <100 mV fwhm; ab initio; vibrational structure; comp. of C ₂ H ₄ , C ₃ H ₃ N,C ₄ H ₆ ,C ₄ H ₈
	HA&97	282-307	E,T	relative; 0.25 eV fwhm; Z+1 calc'n; π* interactions; comp. of CH ₂ =CHCN, C ₂ H ₂ (CN) ₂ , CH ₂ =CHCH ₂ CN
	DS&05	282-318	E,T	assignments revised;
C₃H₃N₃	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
C₃H₄	SB85a	280-320	E	CH ₂ =C=CH ₂ (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)
C ₃ H ₄	HI88a	275-325	E	CH ₃ 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
C₃H₄N₂	AGH93	280-320	E,P	imidazole; absolute; gas-EELS; comp. to sol.-NEXAFS
	CPA01	280-310	T	STEX with screening; comp. to expt. (AGH93)
C ₃ H ₄ N ₂	DH&98	280-330	E,T	pyrazole, relative, 0.2 eV fwhm, Z+1 HONDO, pyrrole vs. pyrazole
C₃H₄O	IH88	275-325	E	(propionic alcohol), comp. to solid, absolute, group analysis
C ₃ H ₄ O	SB92	280-320	E	ethylene oxide; high. res.; comp. to cyclopropane
C ₃ H ₄ O	DF&03	280-320	E	CH ₂ =CH-CHO, acrolein; π* delocalisation; ab initio GAMES
C₃H₄O₂	IH88	275-325	E	(acrylic acid), comp. to solid, absolute, group analysis
C ₃ ClH ₅ O	LDN07	283-298	P	epichlorohydrin – CH ₃ (CH-O-CH ₂); TIY, PEPICO, site selective

C₃H₆	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 ₂ H ₄ O
	S92	280-320	E,T,R	MS-X α ; comp. of cyclic-C _n alkanes
	SB92	280-320	E	ethylene oxide; high. res.; comp. to cyclopropane
	FL96	282-294	T	absolute; Δ SCF-CI; comp. to XPS shake-up and expt. [S92]; n-C _n H _{2n} , n=3,4,5,6 compared
C₃H₆	HS90	280-340	E	propene; absolute; comp. to calc. (S92)
	S92	280-320	T,R	MS-X α ; site-selected calc.
	PN&15	645	P	2-site double core hole IP (ts-DCH), SR, not FEL, coincidences
C₃H₆NO₂	GH01	280-320	E	alanine; absolute; comp of amino acids
C₃H₆NO₂S	PC&98	285-315	T	cysteine; (D,L) STEX; comp. of NEXAFS, circ. Dichr. of amino acids
C₃H₆N₂O₂	LC&07	280-320	E,T	malonamide; comp.of di-carbonyls; charge shifts for fingerprinting, GSCF3
C₃H₆O	IH88	275-325	E	(acrylic alcohol), comp. to solid, absolute, group analysis
C₃H₆O	WB74c	282-328	E	((CH ₃) ₂ 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 ₃) ₂ C=O re perfluro effect
	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 ₂ 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
C₃H₆O	YA&96	280-320	T	propaldehyde; absolute; STEX; R ₂ CO comparison
	YA&97	287	T	π^* OS; test of initial and final state sum rules; comp to expt.
	TJ&99b	284-300	P	relative, TIY
C₃H₆O	PL&07	285-295	P, T	methyloxirane CH ₃ -[CHOCH ₂]; TIY; XPS, calc; resonant Auger
C₃H₆O₂	IH88	275-325	E	(propionic acid), comp. to solid, absolute, group analysis
C₃H₆O₃	HW&91	275-325	E	(CH ₃ O) ₂ C=O, methyl carbonate; absolute, comp. to PEELS
C₃H₆O₃	LC&07	280-320	E,T	(dimethoxymethanone)comp.of di-carbonyls; charge shifts for fingerprinting, GSCF3
C₃H₆O₃	H01	280-320	E	lactic acid; Me(CHOH(COOH); absolute
C₃H₇NO₂	CG&04	282-304	E	(alanine), comp. of alanine, benzene, phenylalanine - additivity
C₃H₇NO₂	UH&95a	280-320	E,T	NH ₂ CO ₂ Et, urethane; absolute; comp. to model polyurethane polymers
C₃H₇NO₂	UH&95b	280-320	E,T	NH ₂ CO ₂ Et, urethane; absolute; EHMO; dist. urethane & ureas
C₃H₇NO₂	PC&98	285-315	T	alanine; (D,L-) STEX; comp. of NEXAFS, circ. Dichr.of amino acids
	PV&04	280-310	P	TIY, PIY, CD asymmetry <1e-3; <1e-2 for fixed-in-space
C₃H₇NO₃	PC&98	285-315	T	serine; (D,L-) STEX; comp. of NEXAFS, circ. Dichr. of amino acids
	PV&04	280-310	P	TIY, PIY, CD asymmetry <1e-3; <1e-2 for fixed-in-space
C₃H₈	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 α -SW, molecular orientation
	LAL91	285-305	T	CNDO, systematic calc. of σ^* energies; ISEELS, ETS for param. det.
(C ₃ H ₈ cont'd)	S92	280-320	T,R	MS-X α ; comp. of propane, ethane
	RDK93	286-291	P	high res (60 meV); comp. of CH ₄ /CD ₄ ; C ₂ H ₆ /C ₂ D ₆ ; C ₃ H ₈ /C ₃ D ₈
	VF&98	285-320	T	comp. to HI87, X α -SW; long-chain alkanes; σ^* along C-C bonds
	WBW99	280-320	T	ab initio Δ SCF; comp to solid & clusters; conformational dep; Ryd persist in condensed phase

C₃H₈O	UG05	286-292	P,T	high-res, 40 meV; comparison of small alkanes; Ryd-val mix; GSCF3
	IH88	275-325	E	(n-propanol), absolute, group analysis
	TH&98	285-295	P	threshold e-; TIY; TPEPICO; triple coinc; isomer study
C ₃ H ₈ O	TH&98	285-295	P	(isoproponol); threshold e-; TIY; TPEPICO; triple coinc; isomer study
C ₃ H ₈ O ₂	LB764	30-620	P	(CH ₂ (OCH ₃) ₂ - methylal), absolute
C ₃ H ₈ O ₂	EUH98	280-320	E	1,2-propane diol; absolute; comp to PPO
C ₃ H ₉ P	SB85c	280-330	E	(Me) ₃ P
	HH&98	284-304	E	absolute; comp. to (t-Bu) ₂ PCl
C ₃ H ₉ N	SB85b	285-335	E	(Me) ₃ N, σ^* res. at thr., comp. to (CH ₃) _x NH _{3-x} , x=0-3
C₃H₇NO₂	UH&95b	280-330	E	NH2-CO ₂ Et, absolute; modelling of polyurethane PEELS
C ₄ F ₃ H ₉ O ₃ SSi	UH94a	280-330	E	Me ₃ SiOSO ₂ CF ₃ ; comp of Si-O-X species; inductive, resonance effects
C ₄ F ₃ H ₅ O ₂	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
C₄F₆	MC&87	275-325	E	perfluorobutadiene, absolute
	RI&88	275-325	E	absolute, comp. to C ₄ H ₆ re perfluoro effect
C₄F₆	RI&88	275-325	E	CF ₃ C::CCF ₃ , comp. to C ₄ H ₆ , perfluoro effect
C₄F₆H₂	IO&12	297	P	cis-cyclic-C4F ₆ H ₂ , resonant Auger - ion coincidence, site specific frag.
C₄F₈	HB&84	280-325	E	(CF ₃ CFCFCF ₃) - strong $\sigma^*(C-F)$ res.
	SSH84b	290-300	T	test of bond length determination from σ^* res.
	RI&88	280-340	E	reassigned HB&84
	LAL91	285-305	T	CNDO, systematic calc. of σ^* energies; ISEELS, ETS for param. det.
C₄F₈	IM&88	275-325	E	perfluoro-cyclobutane, C _x F _{2x} series, $\sigma^*(C-F)$ dominated
C₄F₁₀	HFM87	280-320	E	comp. to other fluorocarbons; $\sigma^*(C-F)$ 'giant shape res.'
	IM&88	275-325	E	perfluorobutane, absolute, comp to C _x F _{x+2}
	AC&95	290-315	T	STEX ab initio; absolute; growth of poly-(CF ₂) _n by C _{2n} F _{4n+2} , n=1-5
C ₄ GeH ₁₂	BS&02B	50-450	P, T	GeMe ₄ ; PEPICO, PIPICO, partial ion yields; EICVOM calc
C ₄ H ₂ N ₂	HA&97	282-307	E,T	trans-dicyanoethylene; relative; 0.25 eV fwhm; Z+1 calc'n; π^* interactions; comp. of CH ₂ =CHCN, C ₂ H ₂ (CN) ₂ , CH ₂ =CHCH ₂ CN
C ₄ H ₄ N ₂	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
C ₄ H ₄ N ₂	PS&01	280-315	T	(pyrimidine), STEX, extensive series of C-N compounds
	VC&06	280-320	P	, TIY vs. vis-UV fluorescencence yield; state selective decay
	VG&08	284-330	P,T	relative, transmission, double ion cell, DEMON calc, comp of 5 aza-rings
C ₄ H ₄ N ₂	PS&01	280-315	T	(pyridazine), 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
C ₄ H ₆ N ₂ O ₂	IH&10	330	P	(thymine), site-selective fragmentation after C 1s ionization, PEPICO
	IH&11	330	P	site-selective fragmentation after C 1s ionization, PEPICO
C ₄ H ₄ O	NIH86	275-325	E	(furan)
	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
C₄H₄S	H86b	275-325	E,R	(thiophene), comp. to thiolane, other heterocyclics
	HNS86	275-325	E,P	comp. to thiolane, solid, monolayer; MS-X α calc
	HT&90	275-325	E	absolute, 3-alkyl-thiophenes; no mod. of π^* (cf. polymer cond.)
	HE91	(white)	P	(hv;e _{Auger} ,ion) coinc.; mass spectra at C1s, S2p with Auger
C₄H₄Se	HTB89	275-325	E	(selenophene), comp to solid
C ₄ H ₅ N	HA&97	282-307	E,T	allyl-cyanide; relative; 0.25 eV fwhm; Z+1 calc'n; π^* interactions; comp. of CH ₂ =CHCN, C ₂ H ₂ (CN) ₂ , CH ₂ =CHCH ₂ CN
	PS&01	280-315	T	STEX, extensive series of C-N compounds
C₄H₅N	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
C ₄ H ₅ N	PS&01	280-315	T	(1,3-pyrrole), STEX, extensive series of C-N compounds
C ₄ H ₅ N	PS&01	280-315	T	(2,4-pyrrole), STEX, extensive series of C-N compounds
C₄H₆	HB&84	280-325	E	(cis, trans-1,3-butadiene CH ₂ CHCHCH ₂)
	SB85a	280-320	E	0.07eVFWHM, two π^* levels observed
	L86	284-290	T	HAM/3 electron affinities, reassigned π^* levels, comp. to HB&84
	MC&87	284-296	E	comp. to C ₄ F ₆ , reassigned 1s6 π^* s
	RI&88	275-325	E	absolute, comp. to C ₄ H ₆ re perfluoro effect
	NS&92	280-330	P,T	ab initio, π^* vib'n 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 ₂ H ₄ , C ₄ H ₆ ,C ₆ H ₈ ; comp. to NS&92 (solid); claims relaxation shifts dominate; π^* split small.
	MB&94b	280-320	P,T	<100 mV fwhm; ab initio; vibrn=l str.; comp. of C ₂ H ₄ , C ₃ H ₃ N,C ₄ H ₆ ,C ₄ H ₈
	GA95	284-290	T	delocalization in polyenes; comp. of H-(CH=CH) _n -H, n=1-5
	CA&95	280-320	T	polyenes, STEX, π/σ convergence
	GYA96	285	T	X-ray emission as f(conjugation); π -exciton effects; H(C ₂ H ₂) _n H, n=1,10
	YA96	290-315	T	STEX; shake-up spectra related to NEXAFS; H(C ₂ H ₂) _n H, n=1-5
	SO&96	284-286	P,T	decay of π^* 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 ₄ H ₆	RI&88	275-325	E	CH ₃ C:::CCH ₃ , 2-butyne, absolute, ref. per-F-2-butyne re per-F eff.
	S92	280-320	E,R	comp. to polymer NEXAFS
C₄H₆O₃	LC&07	280-320	E,T	acetic anhydride; di-carbonyls; charge shifts for fingerprinting, GSCF3
C₄H₆O₅	LC&07	280-320	E,T	MeO(CO)O(CO)OMe; di-carbonyls; charge shifts, GSCF3
C ₄ H ₇ N	PS&01	280-315	T	(2-pyrroline), STEX, extensive series of C-N compounds
C ₄ H ₇ N	PS&01	280-315	T	(3-pyrroline), STEX, extensive series of C-N compounds
C₄H₇NO₂	LC&07	280-320	E,T	Me(CO)N(CO)Me; di-acetamide; di-carbonyls; charge shifts, GSCF3
C₄H₇NO₄	UA&99	280-320	E	ethyl allophanate (NH ₂ (CO)O(CO)OEt); absolute; polymer model
	UH&99	280-320	E,T	ethyl allophanate; absolute; GSCF3; comp. of urethane species
C ₄ H ₈	HB&84	280-325	E	(1-butene CH ₂ CHCH ₂ CH ₃)
	MB&94b	280-320	P,T	<100 mV fwhm; ab initio; vib. structure; comp. of C ₂ H ₄ , C ₃ H ₃ N,C ₄ H ₆ ,C ₄ H ₈
	FL96	282-294	T	absolute; Δ SCF-CI; comp. to XPS shake-up and expt. [S92]; n-C _n H _{2n} , n=3,4,5,6 compared
C ₄ H ₈	HB&84	280-325	E	(cis-2-butene CH ₃ CHCHCH ₃)
C ₄ H ₈	HB&84	280-325	E	(trans-2-butene CH ₃ CHCHCH ₃)
C₄H₈	HN&86	275-325	EPT	(cyclobutane), comp. to other cyclics, sol., calc., E(σ^*) α R
	H86	280-320	E,R	comp. to n-butane
	S92	280-320	E,R	comp. to polymer NEXAFS
C₄H₈N₂O₄	CG&04	282-304	E	(glycyl-glycine), comp. of Gly, Gly-gly, Gly ₃ , gas-solid
C₄H₈N₂O₃	GC&03	283-310	E,T	absolute, comp Gly, Gly-Gly; tri-gly(s); peptide bonds; GSCF3
C₄H₈O	NIH86	275-325	E	(tetrahydrofuran)
	SY&89	280-320	P	comp to EELS, lower discrete/cont.; cont. flatter, O1s 2nd order
C ₄ H ₈ O	YA&96	280-320	T	iso-butanaldehyde; absolute; STEX; R ₂ CO comparison
	YA&97	287	T	π^* OS; test of initial and final state sum rules; comp to expt.
C ₄ H ₈ O ₂	SY&89	280-320	P	(p-dioxane), lower discrete/cont.; cont. flatter, O1s 2nd order
C ₄ H ₈ S	H86b	275-325	E,R	(thiolane), comp. to thiophene, other heterocyclics
	HNS86	275-325	E,P	$\sigma^*(C-S)$, comp. to C ₄ H ₄ S
	HE91	(white)	P	(hv; e_{Auger} ,ion) coinc.; mass spectra at C1s, S2p with Auger
C₄H₉N	NIH86	275-325	E	(pyrrolidine)
	PS&01	280-315	T	STEX, extensive series of C-N compounds
C₄H₁₀	HI87	275-325	E	n-butane

	H86	280-320	E,R	comp. to cyclo-butane
	S92	280-320	E,T,R	MS-X α ; comp. of cyclic-C _n alkanes
	WBW99	280-320	T	ab initio ASCF; comp to solid & clusters; conformational dep; Ryd persist in condensed phase
C₄H₁₀	HI87	275-325	E	iso-butane
	UG05	286-292	P,T	high-res, 40 meV; comparison of small alkanes; Ryd-val mix; GSCF3
C₄H₁₀O	IM&87	275-325	E	t-butanol, comp. to t-butyl-peroxide
C₄H₁₀O	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
C₄H₁₂OSi	UH94a	280-330	E	Me ₃ Si(OMe);comp of Si-O-X species; inductive, resonance effects
	UT&97	283-303	P	absolute; Si-Si & Si-O-R
C ₄ H ₁₂ Pb	NK&89	50-600	P	Pb(CH ₃) ₄ ; total & partial ion d; no C1s signal (!); contaminated optics; core-site dependent fragmentation
C₄H₁₂Si	SD&84	280-380	E	(Me) ₄ Si-TMS, methane-like spectrum
	SD&85	280-380	E	methane-like spectrum
	W92	280-320	E	absolute; comp. of Si(CH ₃) ₄ , Si ₂ (CH ₃) ₆ and Si ₆ (CH ₃) ₆ ; σ^* (Si-Si)
	UX&94	280-330	E	absolute; comp. of edges of Si-Si compounds
C ₄ H ₁₂ OSi	UH94a	280-330	E	Me ₃ Si(OMe);comp of Si-O-X species; inductive, resonance effects
C ₄ NiO ₄	CSB89	280-335	E	Ni(CO) ₄ , high res., comp. to CO; vibrations resolved on π^*
	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(π^*) vs. extent of backbonding
	SLD95	287	T	absolute, DF-LCAO; OS for C1s, O1s $\rightarrow \pi^*$; orbital mapping
C ₄ N ₂ O	UH&95b	280-320	E,T	(NH ₂) ₂ C=O, urea; absolute; EHMO; comp. to polyurethanes
C₅Cl₃H₅Ti	WH93	280-335	E	CpTiCl ₃ , abs. comp. of Cp _x TiCl _{4-x} , x=0-2; diff '10Dq' at each edge
C₅F₈	RI&88	280-330	E	perfluor-cyclopentene, absolute
C₅F₁₀	IM&88	280-330	E	perfluoro-cyclopentane, comp. to per-F c-C ₂ H _{2n+2} ; strong $\sigma^*(C-F)$
C₅F₁₂	HFM87	280-320	E	comp. to other fluorocarbons; $\sigma^*(C-F)$ 'giant shape res.'
	IM&88	275-325	E	perfluoropentane, C _x F _{2x+2} series, $\sigma^*(C-F)$ dominated
C₅F₁₂	IM&88	275-325	E	perfluoro-neo-pentane, $\sigma^*(C-F)$ dom.; comp. to C ₂ F ₆ , extra $\sigma^*(C-F)$
C₅FeO₅	EC&85	280-340	P	Fe(CO) ₅ , ion & electron yield, comp. to free CO, CO/Cu, Cr(CO) ₆
	E87	280-340	P	ion yields, DES
	MSN89	270-520	P	total, partial ion yields; comp to CO, Fe ₂ (CO), EXAFS?
	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(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 ³ π - ¹ π split. in CO and Fe(CO) ₅ (1.30 eV); core hole relaxation investigated via EHMO calc
	WRH92	280-330	E	absolute, comp. to CxFe(CO) ₃ , COTFe(CO) ₃ , Fe(Cp) ₂ ; mix. lig. effect
	SLD95	287	T	absolute, DF-LCAO; OS for C1s, O1s $\rightarrow \pi^*$; orbital mapping
C₅H₂N₄	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)
C₅H₅N	AV&85	285-305	P	(pyridine), absolute; comp. benzene, toluene & styrene; 1 π^* 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
(C ₅ H ₅ N cont'd)	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
C₅H₆	H90a	272-320	E,R	cyclopentadiene, comp to Fe,Co,Ni metallocenes

	RWH91	280-320	E	absolute, comp. of CpH, di-CpH, C ₅ H ₈ re π^* of Cp ⁻
	PS&01	280-315	T	STEX, comp. to expt.; extensive series of C-N compounds
C ₅ H ₆ S	HT&90	280-330	E	3-Me-thiophene; absolute, comp. 3-alkylthiophenes; NEXAFS of poly.
C₅H₆Se	HTB89	275-325	E	(3-Me-selenophene), absolute, comp. to selenophene, solid
C ₅ H ₇ N	PS&01	280-315	T	(1,4-dihydropyridine), STEX, extensive series of C-N compounds
C₅H₈	H86b	280-320	E,R	comp. to solid, monolayer
	HN&86	275-325	E,P	(cyclopentene), σ^* res./bond length, solid, monolayer comp.
	RWH91	280-320	E	absolute, comp. of CpH, di-CpH, C ₅ H ₈ re π^* of Cp ⁻
	PS&01	280-315	T	STEX, comp. to expt.; extensive series of C-N compounds
C₅H₈O	HI88a	275-325	E	(1,3-dihydropyran)
C₅H₈O₂	LC&07	280-320	E,T	Me(CO)Me(CO)Me; di-carbonyls; charge shifts, GSCF3
C₅H₈O₄	LC&07	280-320	E,T	MeO(CO)Me(CO)OMe; di-carbonyls; charge shifts, GSCF3
C ₅ H ₉ N	PS&01	280-315	T	(1,2,3,4-tetrahydropyridine), STEX, extensive series of C-N compounds
C ₅ H ₉ N	PS&01	280-315	T	(1,2,3,6-tetrahydropyridine), STEX, extensive series of C-N compounds
C₅H₁₀	HN&86	275-325	E,P	(cyclopentane), σ^* res./bond length, solid, monolayer comp.
	S92	280-320	E,T,R	MS-X α ; comp. of cyclic-C _n alkanes
	PS&01	280-315	T	STEX, comp. to expt.; extensive series of C-N compounds
C ₅ H ₁₀	FL96	282-294	T	1-pentene; absolute; Δ SCF-Cl; comp. to XPS shake-up and expt. [S92]; n-C _n H _{2n} , n=3,4,5,6 compared
C₅H₁₀O	NIH86	275-325	E	(tetrahydropyran)
C ₅ H ₁₀ O	YA&96	280-320	T	diethylketone; absolute; STEX; R ₂ CO comparison
	YA&97	287	T	π^* OS; test of initial and final state sum rules; comp to expt.
C ₅ H ₁₀ N ₂	HE&01	280-305	E	methyl-carbene; thermal decomposition of tetra-amino ethylene
C₅H₁₁N	NIH86	275-325	E	(piperidine)
	PS&01	280-315	T	STEX, extensive series of C-N compounds
C ₅ H ₁₁ NO ₂	PC&98	285-315	T	valine; (D,L-) STEX; comp. of NEXAFS, circ. Dichroism of amino acids
C₅H₁₂	HI87	275-325	E	n-pentane
	LAL91	285-305	T	CNDO, systematic calc. of σ^* energies; ISEELS, ETS for param. det.
	S92	280-320	E,T,R	MS-X α ; comp. of cyclic-C _n alkanes
C₅H₁₂	HI87	275-325	E	iso-pentane
C₅H₁₂	HI87	275-325	E	neo-pentane
	UG05	286-292	P,T	high-res, 40 meV; comparison of small alkanes; Ryd-val mix; GSCF3
C ₅ H ₁₄ O	UHR95	280-320	E	sec-butyl ethyl ether; absolute
C ₅ H ₁₄ OSi	TC&02	280-320	E	Me ₃ SiOEt; absolute; comp. to vinyl silanes
C ₅ H ₁₅ NSi	UH94b	280-330	E	Me ₃ Si(NMe ₂) ₂ ; comp. of Si-N cmpds; models for SiN _x O _y films
C₅MnO₅H	HR89	280-320	E	Mn(CO) ₅ H, absolute, π^* intensity as measure of d π -p π backbonding
	RH89a	275-330	E	comp. to CO, Mn(CO) ₁₀ & M(CO)s; E(ref); f(π^*) α backbond
	SLD95	287	T	absolute, DF-LCAO; OS for C1s, O1s \rightarrow π^* ; orbital mapping
C ₆ ClH ₅	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)
C ₆ CrO ₆	EC&84	287	P	Cr(CO) ₆ , ion & electron yield, comp. to free CO, CO/Cu, Fe(CO) ₅
	CSB90	275-325	E	comp. of M(CO) ₆ , M=Cr, Mo, W
	SLD95	287	T	absolute, DF-LCAO; OS for C1s, O1s \rightarrow π^* ; orbital mapping
C ₆ D ₆	CS90	284-287	P	π^* 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 ₆ D ₆ cont'd)	MS&90	284-287	P	40 meV fwhm; π^* vib'nl isotope eff; symmetry breaking; local hole
	MC&91	284-291	P	50 meV fwhm; π^* & Ryd vibns; comp of C ₂ H _x &C ₂ D _x (isotope effect)
C₆FH₅	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 σ^* res.
	PY&97	280-310	T	STEX; C ₆ H _x F _{6-x} isomers; comp to HF&87; test of building block; C-R shift; (C ₆ H ₅ X, X=F,NH ₂ ,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	
C₆F₂H₄	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 ₆ H _x F _{6-x} isomers; comp to HF&87; test of building block	
C₆F₃H₃	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 ₆ H _x F _{6-x} isomers; comp to HF&87; test of building block	
C₆F₄H₂	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 ₆ H _x F _{6-x} isomers; comp to HF&87; test of building block	
C₆F₅H	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 ₆ H _x F _{6-x} isomers; comp to HF&87; test of building block	
C₆F₆	YP&97	280-310	T	comp. of phenol, aniline, fluorobenzene; substituent effects	
	HI86	290-700	E	extended fine structure	
	HFM87	280-320	E	comp. to other fluorocarbons; σ*(C-F) 'giant shape res.'	
C₆F₁₂	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 _x series	
C₆F₁₄	D92a	270-320	P,R	PEPICO, PEPIPICO; fragmentation mechanisms	
	PY&97	280-310	T	STEX; C ₆ H _x F _{6-x} isomers; comp to HF&87; test of building block	
	IM&88	275-325	E	(perfluoro-cyclohexane), σ*(C-F) dominated	
C₆H₄N₂S	OS&90	280-320	P,T	PTFE(s), EY-NEXAFS, comp. to gas (IM&88); reassigned σ*s	
	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	
C₆H₄N₂S₂	AC&95	290-315	T	STEX ab initio; absolute; growth of poly-(CF ₂) _n by C _{2n} F _{4n+2} , n=1-5	
	HD&91	275-320	E	Bz(N-S) ring; comp. of S-N heterocycles, aromaticity	
	HD&91	275-320	E	Bz(N-S) ring; comp. of S-N heterocycles, aromaticity	
C₆H₄N₂S₃	HD&91	275-320	E	Bz(N-S) ring; comp. of S-N heterocycles, aromaticity	
	FH92	280-330	E,T	O=Bz=O; absolute; EHMO; comp. of BzOH, Bz(OH) ₂ and quinone	
	C ₆ H ₅ I	HP&78	283-295	E	XPS-EELS chemical shifts comp.
C₆H₅NO₂	TUH96	280-320	E,T	absolute; EHMO; comp. to aniline, benzene and nitroanilines	
	C ₆ H ₆	HS90	280-345	E	CH ₃ C/C-C/CCH ₃ ; absolute; comp. to other X:::X species; conj.
	S92	280-320	E,T,R	MS-Xα; comp to propyne, solid	
C₆H₆	EH&76	280-300	P	benzene, photoelectric yield	
	HB77	280-340	E	cont. res.	
	ES84	270-310	P	partial & total ion yields, e _u π* res. anomalously weak	
(C₆H₆ .cont'd)	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 ₂ (b _{2g}), comp. to ETS	
(C₆H₆ .cont'd)	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	
(C₆H₆ .cont'd)	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.	
(C₆H₆ .cont'd)	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 ₆ hydrocarbons; develop. of π* & σ* conjugation	
(C₆H₆ .cont'd)	MS&89	284-287	P	30 meV fwhm, vib'ns; comp. to C ₂ D ₄ ; 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	E- yield NEXAFS of H-(C ₆ H ₄) _n -H (N=1,3-6); comp. to benzene (HS&85), π* localisation, CNDO/S calc. (Z+1)
	CS90	284-287	P	π* 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; π* vib'nl isotope eff.; symmetry breaking; local. hole (e,2e); comp. to calc.; suggests R-dependent interference in I(q)
	BG&91	291	E	comp. of c-C ₆ HCs; development of π* & σ* conjugation
	H91	280-320	E	comp. of c-C ₆ HCs; development of π* & σ* conjugation
	LAL91	285-305	T	CNDO, systematic calc. of σ* energies; ISEELS, ETS for param. det.
	MC&91	284-291	P	50 meV fwhm; π* & Ryd vibns; comp of C ₂ H _x &C ₂ D _x (isotope effect)
	VNP91	280-320	P	comp. of BF ₃ , BN(s) & borazine; edge resonances
	ME&92	282-292	P	comp. of gas (HB77) & sol.; H ⁺ 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 ₂ H _x , x=2,4,6; σ*(C-C)
	FE&94	284-286	E,T	³ π*; INDO calc; correl. of Δ(1,3) and π* osc. str.
	AVC95	280-314	T	absolute; ΔSCF with Stieltjes continuum; comp. of benzene, naphthalene, anthracene, tetracene and pyrene; comp. to expt. reinterpret HS&85 resonant X-ray emission (RIXS); unbroken symmetry; states assigned
	SG&95b	284-310	P,T	DFT calc.; ³ π ⁻¹ π split = 0.41 eV
	HC96	285	T	absolute, EHMO, comp. to aniline, nitrobenzene and nitroanilines
	TUH96	280-320	E,T	STEX; C ₆ H _x F _{6-x} isomers; comp to HF&87
	PY&97	280-310	T	absolute; reference for Ph ₃ Si-X, Me ₃ Si-X
	UT&97	282-303	P	GSCF3; DOUS modified by core hole effect; compared to condensed ring systems: chrysene, perylene, coronene
	OM&98	280-310	T	absolute; main line partial cross-sections; disputes shape res. existence
	KK&99	290-360	P	relative, Z+1 ab initio; C _{2v} sym. Ass.; Ryd-val mix; 289 peak = 2e-
	DF&00	280-320	E,T	absolute; high-res (50 meV), partial X-sect; β; EXAFS; resonant Auger; no SR; explains 298 continuum peak
	RK&00a	282-800	P	STEX, comp. to expt.; extensive series of C-N compounds
	PS&01	280-315	T	partial ion yield; molecule, di-cluster compared, 90 meV shift
	FG&03b	284-286	P	absolute; comp. to X-ray Raman spectra
	GT&03a	280-320	E	comp. of alanine, benzene, phenylalanine - additivity
	CG&04	282-304	E	relative, hi-res; comp. of C ₆ -ring molecules; DFT-TS accurate to 0.2 eV
	KP&06	283-293	P, T	(1,2)-nitroaniline; absolute, EHMO, comp. to aniline, nitrobenzene
C₆H₆N₂O₂	TUH96	280-320	E,T	(1,3)-nitroaniline; isomer effects on spectra; EHMO calculations
C₆H₆N₂O₂	H00	282-298	E,T,R	(1,3)-nitroaniline; absolute, EHMO, comp. to aniline, nitrobenzene
C₆H₆N₂O₂	TUH96	280-320	E,T	isomer effects on spectra; EHMO calculations
C₆H₆N₂O₂	H00	282-298	E,T,R	(1,4)-nitroaniline; absolute, EHMO, comp. to aniline, nitrobenzene
C₆H₆O	FH92	280-330	E,T	isomer effects on spectra; EHMO calculations
C₆H₆O	PY&97	280-310	T	phenol; absolute; EHMO; comp. of BzOH, Bz(OH) ₂ and quinone
C₆H₆O	YP&97	280-310	T	STEX; C-R shift; (C ₆ H ₅ X, X=F,NH ₂ ,OH)
C₆H₆O	PP&00	285	T	comp. of phenol, aniline, fluorobenzene; substituent effects
C₆H₆O₂	FH92	280-330	E,T	MC-SCF Z+1 calc; vibrational structure, XPS better than NEXAFS
C₆H₇N	HUR93	280-330	E	HO-Bz-OH; EHMO; comp. of BzOH, Bz(OH) ₂ and quinone
C₆H₇N	LA&95	284-296	P,T	aniline, comp. to dimethylaniline
C₆H₇N	LAG96	284-294	T	RIXS; comp. to benzene; interference between (C-H, C-R) π* states
C₆H₇N	TUH96	280-320	E,T	absorption; RIXS; polarisation anisotropy
C₆H₇N	NG&97	284-294	P,R	absolute, EHMO, comp. to nitrobenzene and nitroanilines
C₆H₇N	PY&97	280-310	T	resonant X-ray emission (RIXS); comp. to benzene
C₆H₇N	YP&97	280-310	T	STEX; C-R shift; (C ₆ H ₅ X, X=F,NH ₂ ,OH)
C₆H₇N	PP&00	285	T	comp. of phenol, aniline, fluorobenzene; substituent effects
C₆H₇N	CPA01	280-320	T	MC-SCF Z+1 calc; vibrational structure, XPS better than NEXAFS
C₆H₇N				STEX with screening; comp. to expt. (HUR93)

C₆H₈	HR89	280-320	E	(1,3-cyclohexadiene), comp. of c-C ₆ HCs; π^* & σ^* conjugation
	H91	275-335	E	comp. of c-C ₆ HCs; development of π^* & σ^* conjugation
	KP&06	283-293	P, T	relative, hi-res; comp. of C ₆ -ring molecules; DFT-TS accurate to 0.2 eV
	CA&95	280-320	T	polyenes, STEX, π/σ convergence
	PS&01	280-315	T	STEX, comp. to expt.; extensive series of C-N compounds
C₆H₈	HR89	280-320	E	(1,4-cyclohexadiene), comp. of c-C ₆ HCs; π^* & σ^* conjugation
	H91	275-335	E	comp. of c-C ₆ HCs; development of π^* & σ^* 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 ₆ -ring molecules; DFT-TS accurate to 0.2 eV
C₆H₈	NS&92	280-330	P,T	1,3,5-hexatriene; solid NEXAFS; vib'n'l struct., ab initio
	LA93	282-292	T	1-particle Green's function; comp. of C ₂ H ₄ , C ₄ H ₆ , C ₆ H ₈ ; comp. to NS&92 (solid); claims relaxation shifts dominate; π^* split small.
	GA95	284-290	T	delocalization in polyenes; comp. of H-(CH=CH) _n -H, n=1-5
	GYA96	285	T	X-ray emission as f(conjugation); π -exciton effects; H(C ₂ H ₂) _n H, n=1,10
	YA96	290-315	T	STEX; shake-up spectra related to NEXAFS; H(C ₂ H ₂) _n H, n=1-5
C₆H₈O	UHR99	280-320	E	2-cyclohexene-1-one; absolute; conjugation test
C₆H₈O₂	FH94	280-330	E,T	1,2-chclohexanedione, absolute; eff. of cong.; enol-form
C₆H₈O₂	FH94	280-330	E,T	1,3-chclohexanedione, absolute; eff. of cong.; keto-form
C₆H₈O₂	FH94	280-330	E,T	1,4-chclohexanedione, absolute; eff. of cong.; keto-form
C₆H₉N₃O₃	UA&99	280-340	E	trimethyl-isocyanurate; absolute; polymer model
C₆H₉S	HT&90	275-325	E	3-Ethyl-thiophene; absolute, no mod. of π^* (cf. polymer cond.)
C₆H₁₀	HN&86	275-325	E,P	(cyclohexene), res./bond length
	HR89	280-320	E	comp. of c-C ₆ hydrocarbons; development of π^* & σ^* conjugation
	H91	275-335	E	absolute, comp. of c-C ₆ hydrocarbons; π^* & σ^* 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 ₆ -ring molecules; DFT-TS accurate to 0.2 eV
C₆H₁₀	EL&98	280-320	E	dimethylcyclobutene; absolute; comp with tetramethylcyclobutene
C₆H₁₀O	FH94	280-330	E,T	(cyclohexanone); absolute; comp. to o,m,p-cyclohexanediol
C₆H₁₀O	UHR99	280-320	E	4-hexene-3-one; absolute; conjugation test
C₆H₁₂	DG&86	280-330	E	(cyclohexane), comp. to borazine, benzene, claims giant resonance
	HN&86	275-325	E,P	δ -R; solid, monolayer comp., MS-X α 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 ₆ hydrocarbons; development of π^* & σ^* conjugation
	H91	275-335	E	absolute, comp. of cyclic-hexa-hydrocarbons; π^* & σ^* conjugation
	LAL91	285-305	T	CNDO, systematic calc. of σ^* energies; ISEELS, ETS for param. det.
	S92	280-320	E,T,R	MS-X α ; comp. of cyclic-C _n 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 ₆ -ring molecules; DFT-TS accurate to 0.2 eV
C₆H₁₂	FL96	282-294	T	1-hexene; absolute; Δ SCF-CI; comp. to XPS shake-up and expt. [S92]; n-C _n H _{2n} , n=3,4,5,6 compared
C₆H₁₂N₂	RUH95	280-320	E	DABCO; absolute
C₆H₁₄	HI87	275-325	E	n-hexane, C _x H _{2x+2} series
	HI88b	275-335	E	absolute, comp. to c-C ₆ H _x , evolution of conjugation
C₆H₁₄O	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
C₆H₁₆N₂Si	UH&94b	390-420	E	bis(dimethylamino)dimethylsilane; explore Si-N bond
C₆H₁₆OSi	UH94a	280-330	E	Et ₃ SiOH; comp of Si-O-X species; inductive, resonance effects
C₆H₁₈OSi₂	UH94a	280-330	E	Me ₃ SiOSiMe ₃ ; comp of Si-O-X species; inductive, resonance effects
	UT&97	282-303	P	absolute; Ph ₃ Si-X. Me ₃ Si-X

C₆H₁₈O₃Si₃	UH94a	280-330	E	c-(SiMe ₂ O) ₃ ; comp of Si-O-X species; inductive, resonance effects
C₆H₁₈Si₂	W92	280-320	E	absolute; comp. of Si(CH ₃) ₄ , Si ₂ (CH ₃) ₆ and Si ₆ (CH ₃) ₆ ; 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 ₃ Si-X, Me ₃ Si-X
C₆MoO₆	CSB90	275-325	E	comp. of M(CO) ₆ , M=Cr, Mo, W
	SLD95	287	T	absolute, DF-LCAO; OS for C1s, O1s → π*; orbital mapping
C₆O₆V	TD&92a	280-330	P,E	V(CO) ₆ , absolute
C₆O₆W	CSB90	275-325	E	W(CO) ₆ , comp. of M(CO) ₆ , M=Cr, Mo, W
C₇CoH₅O₂	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) ₂ , Co ₂ (CO) ₈ and Co(Cp) ₂
C₇F₅N	IO&99	278-292	P	C ₆ F ₅ CN; TIY; mass spec at π* _{ring}
C₇FeH₆O₃	RH92	280-330	E	C ₄ H ₆ -Fe(CO) ₃ ; comp. of Fe(CO) ₅ , RFe(CO) ₃ , Fe(Cp) ₂ ; mix. lig. effect
C₇H₅N	H92a	275-340	E,T	(benzonitrile), absolute; EHMO
	PS&01	280-315	T	STEX, extensive series of C-N compounds
C₇H₆O	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
C₇H₇NO₂	UH&95b	280-330	E	NH ₂ -CO ₂ Ph, absolute; modelling of polyurethane PEELS
C₇H₈	AV&85	285-305	P	toluene; absolute, comp. of benzene, polystyrene & toluene
C₇H₈	HS90	275-340	E	1,6-heptadiyne; absolute; conjugation as f(chain length)
C₇H₈O	HU97	280-320	E	anisole (Ph-OMe); absolute
C₇H₈N₂O	UH&95a	280-320	E	phenylurea; absolute; modelling of polyurethane PEELS
	UH&95b	280-320	E	phenylurea; absolute; distinguishing urea/urethane
C₇H₉N	UH96	280-320	E	N-methyl aniline; absolute
C₇H₁₀	WH&90	280-320	E	norbornene; absolute; comp. of NB, 2-CH ₃ -NB & 2-CF ₃ -NB
	H92b	280-320	E,R	comp. of NB, 2-Me-NB, 2-CF ₃ -NB; core vs. valence
C₇H₁₂O₂	LUH97	280-320	E	butyl acrylate; absolute; polymer model
C₇H₁₂O₄	LC&07	280-320	E, T	(dimethyl malonate), comp of di-carbonyls, GSCF3
C₇H₁₄O	YA&96	280-320	T	dipropylketone; absolute; STEX; R ₂ CO comparison
	YA&97	287	T	π* OS; test of initial and final state sum rules; comp to expt.
C₇H₁₈N₃Si	UH&94b	280-320	E	tris(dimethylamino)methylsilane; exploring Si-N bond
C₈Cl₂H₆O₂	HUR92	275-340	E	CICO-Bz-CICO (terphthalic Cl); absolute; comp. to polymer EELS
	RY&92	280-320	E	comp. of small mol. analogs with PET polymer
C₈ClH₁₈P	HH&98	284-304	E	(tBu) ₂ PCl; absolute; comp. to PMe ₃
C₈Co₂O₈	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 ₂ (CO) ₈ ; absolute; comp. to mixed-Cp, CO species
	H92b	281-307	E,R	absolute, comp. of CpCo(CO) ₂ , Co ₂ (CO) ₈ and Co(Cp) ₂
C₈F₃H₉	WH&90	280-320	E	CF ₃ -norbornene; absolute; comp. of NB, 2-CH ₃ -NB & 2-CF ₃ -NB
	H92b	280-320	E,R	comp. of NB, 2-Me-NB, 2-CF ₃ -NB; core vs. valence
C₈F₁₈	AC&95	290-315	T	STEX ab initio; absolute; growth of poly-(CF ₂) _n by C _{2n} F _{4n+2} , n=1-5
C₈H₆	LUH99	280-320	E,T	phenylacetylene; absolute; GSCF3, low-lying π*
C₈H₆O₂	HUR92	275-340	E	CHO-Bz-CHO (Terphthaldehyde); absolute; comp. to polymer EELS
	RY&92	280-320	E	comp. of small mol. analogs with PET polymer
	YP&97	280-320	T	ortho, para terphthaldehyde; substituent effects; comp. to HUR92
C₈H₈	HN&86	275-325	E,P	(cyclo-octatetraene), σ*-E,R; solid, monolayer comp.
C₈H₈	AV&85	285-305	P	(C ₆ H ₅ CH-CH ₂ -), polystyrene, comp. to benzene, pyridine & toluene
	KP&06	283-293	P, T	relative, hi-res; comp. of C ₆ -ring molecules; DFT-TS accurate to 0.2 eV
C₈H₉NO	UH&95b	275-330	E	benzyl carbamate; absolute; modelling polyurethanes
C₈H₉NO₂	GH01	280-320	E	phenylalanine, comp. of amino acids
C₈H₁₀	CA&95	280-320	T	polyenes, STEX, π/σ convergence
	GA95	284-290	T	delocalization in polyenes; comp. of H-(CH=CH) _n -H, n=1-5

	GYA96	285	T	X-ray emission as f(conjugation); π -exciton effects; H(C ₂ H ₂) _n H, n=1,10
	YA96	290-315	T	STEX; shake-up spectra related to NEXAFS; H(C ₂ H ₂) _n H, n=1-5
C₈H₁₀	EH&98	275-325	E	o-xylene (Me-C ₆ H ₄ -Me); absolute; weak ring substitution effects
	HE&98	284-388	E,T	m-xylene; absolute; subst. isomer effects on π^* shape
C₈H₁₀	EH&98	275-325	E	m-xylene (Me-C ₆ H ₄ -Me); absolute; weak ring substitution effects
	HE&98	284-388	E,T	m-xylene; absolute; subst. isomer effects on π^* shape
C₈H₁₀	EH&98	275-325	E	p-xylene (Me-C ₆ H ₄ -Me); absolute; weak ring substitution effects
	HE&98	284-388	E,T	m-xylene; absolute; subst. isomer effects on π^* shape
C₈H₁₀	KP&06	283-293	P, T	(ethylbenzene- C ₆ H ₅ -CH ₂ CH ₃); relative, hi-res; comp. of C ₆ -ring molecules; DFT-TS accurate to 0.2 eV
C₈H₁₁N	HUR93	275-330	E	N,N-dimethylaniline, absolute
C₈H₁₂	WH&90	280-320	E	CH ₃ -norbornene; absolute; comp. of NB, 2-CH ₃ -NB & 2-CF ₃ -NB
	H92b	280-320	E,R	comp. of NB, 2-Me-NB, 2-CF ₃ -NB; core vs. valence
C ₈ H ₁₂ O ₃ Si	TC&02	280-320	E	(CH ₂ =CH)Si(OAc) ₃ ; absolute; vinyl silanes
C₈H₁₂S	HT&90	275-325	E	3-butyl thiophene; absolute; no mod. of π^* (cf. polymer cond.)
C₈H₁₂Si	HS90	280-345	E	HC/C-CH ₂ -C/CSi(CH ₃) ₃ ; absolute; comp. of X:::X species
C₈H₁₄	EL&98	280-320	E	cis-tetramethylcyclobutene; comp of cis, trans, dimethylcyclobutene
C₈H₁₄	EL&98	280-320	E	trans-tetramethylcyclobutene; comp of cis, trans, dimethylcyclobutene
C ₈ H ₁₆ O	UHR92	280-330	E	di(sec-butyl)ether; absolute; modelling of polyurethane PEELS
C₈H₁₈O₂	IM&87	275-325	E	(bis-(t-Bu)peroxide) low-lying $\sigma^*(O-O)$
C ₈ H ₁₈ O ₃ Si	TC&02	280-320	E	(CH ₂ =CH)Si(OEt) ₃ ; absolute
C ₈ H ₂₄ N ₄ Si	UH94b	280-330	E	Si(NMe ₂) ₄ ; comp. of Si-N cmpds; models for SiN _x O _y films
C₈H₂₄O₄Si₄	UH94a	280-330	E	c-(SiMe ₂ O) ₄ ; comp of Si-O-X species; inductive, resonance effects
C ₉ CrH ₆ O ₃	W92	280-330	E	BzCr(CO) ₃ , absolute; comp to CrBz ₂
	WHR92	280-330	E	BzCr(CO) ₃ , absolute; comp to CrBz ₂
C₉FeH₈O₃	WRH92	280-330	E	CxFe(CO) ₃ ; comp. of Fe(CO) ₅ , RFe(CO) ₃ , Fe(Cp) ₂ ; mix. lig. effect
C ₉ Fe ₂ O ₉	MSN89	270-520	P	total, partial ion yields; comp to Fe(CO) ₅ ; EXAFS?
	WRH92	280-330	E	absolute, comp. with Fe(CO) ₅ , RFe(CO) ₃ , Fe(Cp) ₂ ; mix. lig. effect
C₉H₅O₄V	WHR92	280-320	E	cyclopentadienyl vanadium tetracarbonyl
C₉H₆N₂O₂	UHR99	280-320	E,T	2,4-TDI, absolute; isomeric effect
C₉H₆N₂O₂	UHR99	280-320	E,T	2,6-TDI, absolute; isomeric effect
C₉H₇MnO₃	W92	280-330	E	Me-CpMn(CO) ₃ , absolute
C₉H₈O₂	LUH97	280-320	E	vinyl benzoate; absolute; model for PET X-ray damage
C₉H₁₀O₂	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
C₉H₁₁NO₂	CG&04	282-304	E	(phenylalanine), comp. of alanine, benzene, phenylalanine - additivity
C₉H₁₁NO₂	UH&95b	280-330	E	Ph-NH-CO ₂ Et, absolute; modelling of polyurethane PEELS
C ₉ H ₂₇ NSi ₃	UH94b	280-330	E	N(SiMe ₃) ₃ ; comp. of Si-N cmpds; models for SiN _x O _y films
C₁₀ClCo₃O₉	HM&93	280-330	E,P,T	Cl-C-[Co(CO) ₃] ₃ , abs.; gas(E,P-ions), sol(P); PIPICO, TOF-MS
C₁₀Cl₂H₁₀Ti	WH93	280-335	E	Cp ₂ TiCl ₂ , abs. comp. of Cp _x TiCl _{4-x} , x=0-2; diff '10Dq' at each edge
C₁₀Cl₂H₁₀V	WRH89	274-340	E	Cp ₂ TiCl ₂ , absolute
C₁₀CoH₁₀	HR89	280-320	E	cobaltocene, absolute, strong C1s6e _{1g} (M3d)
	RH89b	275-325	E	comp. of Fe, Co, Ni metallocenes
	H92b	281-307	E,R	absolute, comp. of CpCo(CO) ₂ , Co ₂ (CO) ₈ and Co(Cp) ₂
C₁₀CrH₈O₃	WRH89	280-330	E	toluene-Cr(CO) ₃ , comp. to Bz ₂ Cr
C₁₀CrH₁₀	HWR89	275-325	E	chromocene, comp. of V, Cr, Mn
C₁₀F₄H₈	UH96	280-320	E	dimethyl-tetrafluoro-benzocyclobutane; model for dielectric polymer
C₁₀F₁₆	HI88a	275-335	E	per-fluoro-adamantine, strong $\sigma^*(C-F)$
C₁₀F₈	RI&88	275-325	E	per-fluoro-naphthalene, low-lying $\sigma^*(C-F)$, perfluoro-effect
	LAL91	280-300	T	CNDO, pred. of π^* and σ^* energies
C ₁₀ F ₂₂	AC&95	290-315	T	STEX ab initio; absolute; growth of poly-(CF ₂) _n by C _{2n} F _{4n+2} , n=1-5

C₁₀FeH₁₀	HR89	280-320	E	ferrocene, absolute, strong C1s6e _{1g} (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
C₁₀GeH₂₀N₂	LU&99	282-309	E,T	c-Ge(RNCH=CHNR), R=tBu, comp. cyclic diamino C; Si; Ge; ; GSCF3
C₁₀GeH₂₂N₂	LU&99	282-309	E,T	c-Ge(RNCH ₂ CH ₂ NR), R=tBu, comp. cyclic diamino C; Si; Ge; ; GSCF3
C₁₀GeH₂₂N₂	LU&99	282-309	E,T	c-H ₂ Ge(RNCH=CHNR), R=tBu, comp. cyclic diamino C; Si; Ge; ; GSCF3
C₁₀GeH₂₄N₂	LU&99	282-309	E,T	c-H ₂ Ge(RNCH ₂ CH ₂ NR), R=tBu, comp. cyclic diamino C; Si; Ge; GSCF3
C₁₀H₈	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; Δ SCF with Stieljes 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, ν_{C-C} 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
C₁₀H₈	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.
C₁₀H₁₀Mg	WRH89	274-340	E	Cp ₂ Mn, absolute
C₁₀H₁₀Mn	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; $\sigma^*(CO)$ shift
C₁₀H₁₀Ni	HR89	280-320	E	absolute, strong C1s6e _{1g} (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
C₁₀H₁₀O₄	UH&96	280-296	E,T	p-dimethylphthalate (MeO ₂ C-C ₆ H ₄ -CO ₂ 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
C₁₀H₁₀O₄	UH&96	280-296	E,T	o-dimethylphthalate (MeO ₂ C-C ₆ H ₄ -CO ₂ 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
C₁₀H₁₀O₄	UH&96	280-296	E,T	m-dimethylphthalate (MeO ₂ C-C ₆ H ₄ -CO ₂ 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
C₁₀H₁₀V	HWR89	275-325	E	vanadocene, comp. of V, Cr, Mn
C₁₀H₁₂	CA&95	280-320	T	polyenes, STEX, π/σ convergence
	GA95	284-290	T	delocalization in polyenes; comp. of H-(CH=CH) _n -H, n=1-5
(C ₁₀ H ₁₂ cont'd)	GYA96	285	T	X-ray emission as f(conjugation); π -exciton effects; H(C ₂ H ₂) _n H, n=1,10
	YA96	290-315	T	STEX; shake-up spectra related to NEXAFS; H(C ₂ H ₂) _n H, n=1-5
C₁₀H₁₂	RWH91	280-320	E	(CpH) ₂ (Diels-alder dimer); comp. of CpH, di-CpH, C ₅ H ₈ ; Cp ⁻ (π^*)
C₁₀H₁₃NO₂	UH&95b	280-330	E	Ph-N(CH ₃)-CO ₂ Et, absolute; modelling of polyurethane PEELS
C₁₀H₁₆	HI88a	275-325	E	adamantane, (tri-cyclo 3,3,1 ^{3,7})-decane
C₁₀H₁₇S	HT&90	275-325	E	3-hexyl-thiophene; absolute; no mod. of π^* (cf. polymer cond.)
C₁₀H₁₉O₄	LC&07	280-320	E,T	'BuO(CO)NH(CO)O'Bu; di-carbonyls; charge shifts, GSCF3
C₁₀H₂₀N₂	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
C₁₀H₂₀N₂Si	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

C ₁₀ H ₂₂ N ₂	LU&99	280-305	E	tBu-NCH ₂ CH ₂ N-tBu; absolute; ligand rel. to cyclic diamino C;Si:,Ge.
C ₁₀ H ₂₂ N ₄	HE&01	280-305	E	tetra-amino ethylene; used for thermal decomposition to form carbene
C₁₀H₂₂N₂Si	UH&98	283-302	E,T	c-Si(RNCH ₂ CH ₂ NR), R=tBu, unsat. silylene; absolute;
	LU&99	280-305	E,T	absolute; comparison of cyclic diamino C:, Si:, Ge: ; GSCF3 ab initio
C₁₀H₂₂N₂Si	UH&98	283-302	E,T	c-H ₂ 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
C₁₀H₂₄N₂Si	UH&98	283-302	E,T	c-H ₂ Si(RNCH ₂ CH ₂ NR), R=tBu, unsat. silylene; absolute;
	LU&99	280-305	E,T	absolute; comparison of cyclic diamino C:, Si:, Ge: ; GSCF3 ab initio
C₁₀H₂₂O	HI88a	275-325	E	decyl alcohol
C₁₀Mn₂O₁₀	HR89	280-320	E	absolute, π^* intensity as measure of d π -p π backbonding
	RH89a	275-330	E	Mn ₂ (CO) ₁₀ , comp. CO, other M(CO)s; E(ref); f(π^*) α backbond
C₁₁Co₃H₃O₁₀	HM&93	280-330	E,P	CH ₃ O-C-[Co(CO) ₃] ₃ ; abs.; comp. of gas (E), sol (P-TEY)
C₁₁FeH₈O₃	WRH92	280-330	E	COT-Fe(CO) ₃ ; comp. of Fe(CO) ₅ , RFe(CO) ₃ , Fe(Cp) ₂ ; mix. lig. effect
C₁₁H₁₄N₂O₄	UHR99	280-320	E	TDI-bis-methyl urethane; absolute
C ₁₁ H ₂₀ N ₂	LU&99	282-309	E,T	c-C:(RNCH=CHNR), R=tBu, carbene; absolute;
C ₁₁ H ₂₂ N ₂	LU&99	282-309	E,T	c-C:(RNCH ₂ CH ₂ NR), R=tBu, absolute;
C ₁₁ H ₂₄ N ₂	LU&99	282-309	E,T	c-H ₂ C:(RNCH ₂ CH ₂ NR), R=tBu, hydrogenated carbene (ref.)
C₁₂CrH₁₂	W92	280-330	E	CrBz ₂ ; absolute; comp to BzCr(CO) ₃
	WRH92	275-330	E	CrBz ₂ ; comp. to benzene
C₁₂FeH₁₂	WRH92	280-330	E	CH ₂ =CH-CpFeCp; comp. of organo-irons; ligand interaction effects
C ₁₂ Fe ₃ O ₁₂	EC&84	280-340	P	Fe ₃ (CO) ₁₂ , ion & electron yield, comp. to free CO, CO/Cu, Cr(CO) ₆
C₁₂F₁₀	WC&05	284-308	E,T	biphenyl, absolute, GSCF ₃ , ring-ring-interactions (comp to o,o-dibromo)
C₁₂H₁₀	WC&05	284-308	E,T	biphenyl, absolute, GSCF ₃ , ring-ring-interactions (comp to o,o-dibromo), compared to hexa-phenylbenzene (s)
	FM&04	280-320	P,T	50 meV, ν_{C-C} vibrational progressions in π^* ; comp. to hi-res XPS; no dihedral modes (weakening ring-ring delocalization does not excite torsion) (BzO) ₂ CO (phenyl carbonate); absolute; comp. to polymer EELS
C ₁₂ H ₁₀ O ₃	HUR92	275-340	E	X-ray emission as f(conjugation); π -exciton effects; H(C ₂ H ₂) _n H, n=1,10
C ₁₂ H ₁₄	GYA96	285	T	C π^* ReN ₂ O ₂ , abs.; mixed ligand; chem. shift of N _a -N _b diphenylether, TIY, TD-DFT (Q-CHEM-4.1)
C₁₂H₁₅N₂O₂Re	HS92	280-330	E	3-octyl-thiophene; absolute, no mod. of π^* (cf. polymer cond.)
C ₁₂ H ₁₈ O	LL&14	284-299	P,T	absolute; comp. of Si(CH ₃) ₄ , Si ₂ (CH ₃) ₆ and Si ₆ (CH ₃) ₁₂ ; σ^* (Si-Si)
C₁₂H₂₁S	HT&90	275-325	E	absolute; comp. of edges of Si-Si compounds
C₁₂H₃₆Si₅	W92	280-320	E	c-(SiMe ₂) ₆ ; comp. of edges of Si-Si compounds
C ₁₂ H ₃₆ Si ₆	UX&94	280-330	E	relative, electron yield, multiple π^* res.; relaxation
C ₁₂ O ₁₂ Ru ₃	SF&90	275-325	P	(C ₆ H ₅ O) ₂ C=O; absolute; comp. to methyl carbonate (diphenoxymethanone), comp of di-carbonyls, GSCF ₃ (Ph-NH) ₂ C=O, absolute; modelling of polyurethane PEELS
C₁₃H₁₀O₃	HW&91	280-340	E	Ph-CH ₂ -Ph; absolute; modelling of polyurethane PEELS
C₁₃H₁₀O₃	LC&07	280-320	E, T	C π^* Mn(CO) ₃ ; absolute
C₁₃H₁₂N₂O	UH&95b	280-330	E	Bu-cpFeCp; organo-iron complexes, ligand interaction effects
C₁₃H₁₂	UH&93	280-330	E	anthracene; absolute; Δ SCF with Stieltjes cont.; comp. of aromatics
C ₁₃ H ₁₅ MnO ₃	WRH89	275-325	E	absolute; GSCF ₃ ; comp. to X-ray Raman spectra
C₁₄FeH₁₈	WRH92	280-330	E	phenanthracene; absolute; GSCF ₃ ; comp. to X-ray Raman spectra
C ₁₄ H ₁₀	AVC95	280-314	T	benzoic anhydride; absolute; polymer model
	GT&03a	280-320	E, T	3-decyl-thiophene, absolute, comp. of 3-alkyl-thiophenes; no change of π^* (polymer cond.)
C ₁₄ H ₁₀	GT&03a	280-320	E, T	butylated hydroxy toluene; absolute; polymer model
C₁₄H₁₀O₃	LUH97	280-320	E	tetracene; absolute; Δ SCF with Stieltjes cont.; comp. of aromatics
C₁₄H₂₅S	HT&90	275-325	E	X-ray emission as f(conjugation); π -exciton effects; H(C ₂ H ₂) _n H, n=1,10
C₁₅H₂₄O	LUH97	280-320	E	pyrene; absolute; Δ SCF with Stieltjes cont.; comp. of aromatics
C ₁₆ H ₁₀	AVC95	280-314	T	absolute; comp. to X-ray Raman spectra
C ₁₆ H ₁₈	GYA96	285	T	
C₁₈H₁₂	AVC95	280-314	T	
	GT&03a	280-320	E	

C₁₈H₁₂	GT&03a	280-320	E, T	triphenylene. absolute; GSCF3; comp. to X-ray Raman spectra
C₁₈H₁₂	GT&03a	280-320	E, T	1,2-benzanthracene. absolute; GSCF3; comp. to X-ray Raman spectra
C₁₈H₁₂	OM&96	280-294	P,T	chrysene; GSCF3 calc. of DOUS and excitation; comp. to solid, pol. dep. (π^* most intense at normal incidence); large core-hole effect
C₁₈H₁₄O₂	OM&98	280-310	T	GSCF3; DOUS mod. by core hole; comp.of chrysene, perylene, coronene
C₁₈H₁₆OSi	LL&14	284-301	P,T	1,3-diphenoxylbenzene, TIY, TD-DFT (Q-CHEM-4.1)
C₂₀H₁₂	UT&97	280-320	E	triphenylsilanol; absolute; Si-Si, Si-O-R systems
C₂₀H₁₂	OM&96	280-294	P,T	perylene; GSCF3 calc. of DOUS and excitation; comp. to solid, pol. dep. (π^* most intense at normal incidence); large core-hole effect
C₂₀H₂₂	OM&98	280-310	T	GSCF3; DOUS modified by core hole effect; compared to condensed ring systems: chrysene, perylene, coronene
C₂₀H₂₂	GA95	284-290	T	delocalization in polyenes; comp. to H-(CH=CH) _n -H, n=1-5
C₂₀H₂₂	GYA96	285	T	X-ray emission as f(conjugation); π -exciton effects; H(C ₂ H ₂) _n H, n=1,10
C₂₁H₁₅N₃O₃	UHR92	275-325	E	(Bz-O) ₃ C3N3 (tri-phenoxy-triazine); polyurethane modelling
C₂₄H₁₂	UA&99	280-320	E	tritylilisocyanurate; absolute, polymer model
C₂₄H₁₂	OM&96	280-294	P,T	coronene; GSCF3 calc. of DOUS and excitation; comp. to solid, pol. dep. (π^* most intense at normal incidence); large core-hole effect
C₂₄H₂₁N₃O₃	OM&98	280-310	T	GSCF3; DOUS mod. by core hole; comp.of chrysene, perylene, coronene
C₂₉H₂₀O	UA&99	280-320	E	tritylilisocyanurate; absolute, polymer model
C₃₀H₃₀Si₂	LUH99	280-320	E,T	tetraphenyl-cyclopentadienone; low-lying π^*
C₃₂H₁₆N₈	UT&97	282-303	P	Ph ₃ Si-SiPh ₃ ; absolute; reference for Ph ₃ Si-X, Me ₃ Si-X
C₃₂H₁₆N₈Fe	RSH93	280-316	E	phythalocyanine; compared to solid
C₃₂H₁₆N₈Fe	RSH93	280-316	E	Fe-phythalocyanine; compared to solid
C₃₂H₁₆N₈Ni	RSH93	50-450	E	Ni-phythalocyanine; compared to solid
C₃₂H₁₆N₈Zn	RSH93	280-316	E	Zn-phythalocyanine; compared to solid
C₆₀	KB&93a	280-296	P	gas, solid essentially identical; intramolecular e- correl.; XPS, Auger
C₆₀	KB&93b	280-296	P	gas comp. to EELS of solid; plasmon at 6 eV higher in gas
C₆₀	JT94a	284-290	T	relative, π^* transitions; minimal many-electron effects
C₆₀	AN&95	280-313	P	TOF mass spec; partial ion yields; (C ₂) _n losses dominate
C₆₀	LP&95	290-320	P	partial PI X-sect (main, sat.); β s; $\beta < 2$ at 300 eV interpreted as SR
C₆₀	BS96	290-320	P,R	absolute; cross-sections, β 's compared to solid
C₆₀	B97	270-320	P	total and partial ion yields; lumiescence; plasmasa resonance sought
C₆₀	KN&97a	280-296	P	pulse, PEPICO TOF; discrete, cont. frag; plasmon res. ~20 eV > IP; PCI

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)

BCl₃	FB70	190-210	P	pressure dependence
	II&80	190-280	P	absolute
	UC&94b	190-208	P	absolute, resonance Auger; spectator only; localised decay
BrCClH₂	SR&94	195-225	P	TIY; PEPICO; PEPI3CO; selective fragment.; Br(CH ₂) _n Cl, n=1-3
	NM96	220	P,R	mass spectra; comp. of Br 3d/Cl2p for Br(CH ₂) _n 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
BrC₂ClH₄	SR&94	195-225	P	TIY; PEPICO; PEPI3CO; selective fragment.; Br(CH ₂) _n Cl, n=1-3

	NM96	220	P,R	mass spectra; comp. of Br 3d/Cl2p for Br(CH ₂) _n Cl n=1-3
BrC ₃ ClH ₆	SR&94	195-225	P	TIY; PEPICO; PEPI3CO; selective fragment.; Br(CH ₂) _n Cl, n=1-3
	NM96	220	P,R	mass spectra; comp. of Br 3d/Cl2p for Br(CH ₂) _n Cl n=1-3
CClF ₂ H	CD78	120-270	P	absolute
CClF ₃	CD78	120-270	P	absolute
	ZIB92	190-290	E	absolute, high res. (70 meV), pot. bar., comp. of CCl _x F _{4-x} , x=1-4
	YL94	195-240	E	absolute GOS; comp. of CF _{4-n} Cl _n (n=0-4); σ*(C-Cl) GOS changes
	SS&95	190-280	P	PIPICO; start = selective ion gate; PIPICO yields; comp of Cl2p, Cls, F1s edges; only selective at Cl 2p edge
	SSB99	200-220	P	TIY, PIY; comp of CF _x Cl _{4-x} x=1-3; site selective fragmentation
CClH ₃	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 ₂ F ₂	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 _x F _{4-x} , 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 _{4-n} Cl _n (n=0-4); σ*(C-Cl) GOS changes
	SSB99	200-220	P	TIY, PIY; comp of CF _x Cl _{4-x} x=1-3; site selective fragmentation
CCl ₂ F ₂ H	CD78	120-270	P	absolute
CCl ₂ F ₃ P	HBC96	190-240	P	TIY, PIY, PEPICO; comp. of PCl ₃ , PF ₃ , CF ₃ PCl ₂
	NJ&98	180-240	P,T	absolute; GSCF3 calc.; LS-state; comp of PX ₃ , YPF ₃ . X=Cl,F, Y=O,S)
CCl ₂ H ₂	HB78b	190-290	E	extended fine structure (EXAFS)
	CG&88	160-240	P	DES, resonant Auger, βs, spectator dominates
CCl ₂ O	HUR92	180-290	E	absolute, comp. to terphthaloylchloride; EHMO
CCl ₃ F	CD78	120-270	P	absolute
	ZIB92	190-290	E	absolute, high res. (70 meV), pot. bar., comp. of CCl _x F _{4-x} , x=1-4
	YL94	195-240	E	absolute GOS; comp. of CF _{4-n} Cl _n (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 _x Cl _{4-x} x=1-3; site selective fragmentation
CCl ₃ 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 ₄	P34	180-300	P	photographic; FIRST MOLECULAR CORE EXCITATION
	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, βs, spectator dominates
	ZIB92	190-290	E	absolute, high res. (70 meV), pot. bar., comp. of CCl _x F _{4-x} , 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 _{4-n} Cl _n (n=0-4); σ*(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)
C₂ClF₅	CD78	120-270	P	absolute
C ₂ ClH ₃	SBK88	190-260	E	v vinyl chloride, comp. other vinyl halides, strong cont. res. $\sigma^*(C=C)$?
C ₂ ClH ₅	FL02	190-220	E	absolute, GOS profiles compared of C 1s, Cl 2p & valence
C ₂ Cl ₂ F ₄	CD78	120-270	P	absolute
C ₂ Cl ₂ H ₄	H92	120-270	P	dichloroethane; comp. to NEXAFS
C ₂ Cl ₂ H ₆ Si	CL&05	190-230	P	SiMe ₂ Cl ₂ , luminescence yield, Si*, Si ⁺ , CH*, H*, excited diatomic
C ₂ Cl ₃ H	WH90	160-280	E	Cl ₂ C=CClH
C ₂ Cl ₃ N	IO&99	190-280	P	absolute; selected E mass spec; no site-specific fragmentation
C₅Cl₃H₅Ti	W92	196-250	E	CpTiCl₃, absolute
	WH93	196-250	E	abs. comp. of Cp _x TiCl _{4-x} , x=0-2; diff '10Dq' at each edge
C ₆ H ₅ Cl	HP&78	195-215	E	comp. with carbon 1s near-edge features
C ₈ Cl ₂ H ₄ O	HUR92	180-290	E	para-Bz(COCl) ₂ ; absolute, comp. to phosgene
C ₈ ClH ₁₈ P	HH&98	130-220	E	(t-Bu) ₂ PCl; comp. to PCl ₃
C₁₀ClCo₃O₉	HM&93	180-280	E	Cl-C-[Co(CO)₃]₃, abs.; gas(E,P-ions), sol(P); PIPICO, TOF-MS
C₁₀Cl₂H₁₀Ti	WH93	196-250	E	Cp₂TiCl₂, abs.; comp. of Cp_xTiCl_{4-x}, x=0-2; diff '10Dq' at each edge
ClD	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 $2p^{-1}\sigma^*$ state; in Auger the valence, core holes are aligned
	MM12	68-72	P,R	ultra-fast decay (HBr-Br3d; DCl, HCl-Cl2p; H ₂ S - S2p, O ₂ -O1s)
ClF	FSD99	200-300	T	absolute; ab initio CI; DFT for cont.; comp of ClF, ClF ₃ ; F-cage effects
ClF ₃	BS87	190-230	E	high res.
	SB89	190-230	E	high res., partial bar. Effects
	FSD99	200-300	T	absolute; ab initio CI; DFT for cont.; comp of ClF, ClF ₃ ; 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 ₂ 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
(HCl cont'd)	SC&84	198-209	E	75meVFWHM, Rydberg IP [3/2=207.40(3), 1/2=209.03(3),
	AA&90b	200-202	P,T	DES at σ^* ; ultra-fast decay and normal compete
	YPD91	200-230	T	SCF-CI; vib'n'l effects; comp. to expt. (SC&84)
	AA&92a	198-214	P,T	PIPICO; partial & total ion yields; σ^* , Ryd. differ; HCl ²⁺ pot. curves
	AA&92c	200-203	P	resonant AI; comp. of HCl, Cl ₂ , H ₂ 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 α ; comp. of XH _n (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 σ not σ^* ; reflects relative widths of Franck-Condon to dissociate 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 σ^*)

	SA97	201,204	P	Auger resonant Raman; line narrowing at $4s\sigma$ but not at σ^*
	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; β 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 $2p^1\sigma^*$ 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 ₂	MM12	68-72	P,R	ultra-fast decay (HBr-Br3d; DCI, HCl-Cl2p; H ₂ S - S2p, O ₂ -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 ₂ , H ₂ S
	LB&95	195-250	T	MS-X α ; comp. to XH _n (X=Si,P,S,Cl)
Cl ₂ Fe	SG&02	195-215	P	TIY, angle resolved, exchange & S-O splittings,
Cl ₃ OP	CK&83	200-240	T	absolute, energy dependent Dirac calc, spin-dependence
	TKM82	198-215	T	X- α (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.
ClO ₂	NJ&98	180-240	P,T	absolute; GSCF3 calc.; LS-state; comp of PX ₃ , YPF ₃ . X=Cl,F, Y=O,S)
	FPR06	200-260	P	PIY, TIY; ionization yield; PEPICO, PIPICO
Cl ₃ 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 ₃ 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 ₃ , PF ₃ , CF ₃ PCl ₂
	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) ₂ PCI
Cl ₃ PS	TKM82	198-215	T	X- α (MSM calc.), comp. to expt (K77)
	NJ&98	180-240	P,T	absolute; GSCF3 calc.; LS-state; comp of PX ₃ , YPF ₃ . X=Cl,F, Y=O,S)
Cl ₄ Ge	GD&96	100-300	E	non-statistical 3/2:1/2 intensities; comp. to Cl 1s, Ce2p/3p of GeCl ₄
Cl ₄ Na ₄	YS&02	190-230	T	relative; MS-X α plus DFT; geometry dependence
(ClNa) _n	MC&99	190-235	P	relative, PIY, comp. to thin film, solid TEY
	NR&99	190-235	P,T	relative, PIY, comp. to thin film, solid TEY; MS cluster calc
Cl ₄ Si	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, β s, spectator dominates
	TL&89	190-240	T	absolute, X- α calc; cont. & discrete; Rydbergs
	W92	190-240	E	comp of SiCl ₄ and Si ₂ Cl ₆
Cl ₄ Ti	W92	196-250	E	TiCl ₄ , absolute, comp. to CpTiCl ₃
	WH93	196-250	E,T	absolute; comp. of Cp _x TiCl _{4-x} , x=0-2; diff '10Dq' at each edge
Cl ₆ Si ₂	W92	190-240	E	comp of SiCl ₄ and Si ₂ Cl ₆

Chlorine 1s (2830 eV)

AsCl₃ GDT97 2.81-2.85 P,T relative; TIY, MS-X α ; pot. barr.; AsCl₃, PCl₃, GeCl₄, SnCl₄ comp.; $\sigma^*(X-$

				Cl) bond length correlation
CClH ₃	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 $\sigma^*(C-Cl)$
	PF&94	2.80-2.93	P	thresh. PES; comp. of CH_xCl_{4-x} , x=0-3; CF_xCl_{4-x} , x=1-3; I(IP) α #-Cl
CCl ₂ H ₂	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_xCl_{4-x} , x=0-3; CF_xCl_{4-x} , 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
	ZK&15	2.82-2.83	P	nexafs & RIXS, core hole clock; compare 11 Cl compounds
CCl ₂ F ₂	HG76	2.81-2.84	P	absolute
	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; $\sigma^*(C-Cl)$
	PF&94	2.80-2.93	P	thresh. PES; comp. of CH_xCl_{4-x} , x=0-3; CF_xCl_{4-x} , 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 ₃ F	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; $\sigma^*(C-Cl)$
	PF&94	2.80-2.93	P	thresh. PES; comp. of CH_xCl_{4-x} , x=0-3; CF_xCl_{4-x} , x=1-3; I(IP) α #-Cl
CCl ₃ 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_xCl_{4-x} , x=0-3; CF_xCl_{4-x} , 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 ₃ H ₃ Si	FBN90	2.81-2.89	P	MeCl ₃ Si, discrete & cont. shape res.; strong double excitation
CCl ₄	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_xCl_{4-x} , x=0-3; CF_xCl_{4-x} , x=1-3; I(IP) α #-Cl
	ZK&15	2.82-2.83	P	nexafs & RIXS, core hole clock; compare 11 Cl compounds
C ₂ ClH ₅	ZK&15	2.82-2.83	P	Chloroethane, nexafs & RIXS, core hole clock; compare 11 Cl compounds
C ₂ Cl ₂ H ₆ Si	FBN90	2.81-2.89	P	Me ₂ Cl ₂ Si, discrete & cont. shape res.; strong double excitation
C ₂ Cl ₂ H ₂	ZK&15	2.82-2.83	P	chloro-ethene, nexafs & RIXS, core hole clock; compare 11 Cl compounds
C ₂ Cl ₂ H ₄	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 ₂ Cl ₃ H	HG76	2.81-2.84	P	absolute
C ₂ Cl ₃ H ₃	ZK&15	2.82-2.83	P	nexafs & RIXS, core hole clock; compare 11 Cl compounds
C ₂ Cl ₅ H	HG76	2.81-2.84	P	absolute
C ₃ ClH ₅ O	LDN07	2.81-2.85	P	epichlorohyrin – CH ₃ (CH-O-CH ₂); TIY, PEPICO, possible alignment
C ₃ ClH ₉ Si	FBN90	2.81-2.89	P	Me ₃ ClSi; discrete & cont. shape res.; strong double excitation
C ₆ H ₅ 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; β for fragmentation
CIF	FSD99	2.81-2.85	T	absolute; ab initio CI, DFT continuum; comp of ClF, ClF ₃ ; F-cage
ClF ₃	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
	PC&91	2.81-2.84	P
	LM&94	2.824	P
	PF&94	2.80-2.93	P
	LAG96	2.81-2.85	T
ClH	LN43	2.8-3.2	P
	SKN51	2.81-2.83	P
	BN66	2.81-2.85	P
	SBB68	2.81-2.85	P
	BS&69	2.81-2.85	P
	G70	2.81-2.84	P
	SM&70	2.81-2.85	P
	MN&75	2.81-2.85	T
	SYD82	2.81-2.85	T
	D86b	2.81-2.84	P
	BM&90	2.81-2.86	P
	LM&94	2.824	P
	FPS95b	2.82-2.83	T
	DA&98c	2.82-2.84	P
	FS&98	2.81-1.85	T
	HA&98a	2.82-2.85	P
	HA&98b	2.82-2.84	P
ClF ₅ S	RB&92	2.8-3.1	P,T
Cl ₂	LN43	2.81-3.20	P
	SKN51	2.81-2.84	P
	SBB68	2.81-2.85	P
	BS&69	2.81-2.85	P
	SM&70	2.81-2.85	P
	MS&73	2.81-2.85	T
	B80	2.81-3.20	P,R
	LG&86	2.8 -3.0	P
	BM&90	2.81-2.86	P
	FPS95a	2.82-2.83	T
	NM96	2.81-2.86	P,R
(Cl ₂ cont'd)	MS&97b	2.81-2.86	P,T
Cl ₂ OS	HBT87	2.81-2.86	P
Cl ₂ OS ₂	HBT87	2.81-2.86	P
Cl ₂ S	HBT87	2.81-2.86	P
Cl ₂ S ₂	HBT87	2.81-2.86	P
Cl ₃ P	GDT97	2.81-2.85	P,T
Cl ₄ Ge	GD&96	2.81-2.85	P,T
	GDT97	2.81-2.85	P,T
Cl ₄ Si	BF&87	2.81-2.88	P
	TL&89	2.81-2.88	T
	FBN90	2.81-2.89	P
	GDT97	2.81-2.85	P,T

Cl ₄ Sn	GDT97	2.81-2.85	P,T	relative; TIY, MS-X α ; pot. barr.; AsCl ₃ , PCl ₃ , GeCl ₄ , SnCl ₄ comp.; $\sigma^*(X-Cl)$ bond length correlation
<u>Chromium 2p (574, 584 eV)</u>				
CrCl ₂ O ₂	DF&94	570-575	T	ab initio CI; relaxed orb.; MO _x X _y (Ti,V,Cr,Mn); covalency incr. as Cl 6 F
CrF ₂ O ₂	DF&94	570-575	T	ab initio CI; relaxed orb.; MO _x X _y (Ti,V,Cr,Mn); covalency incr. as Cl 6 F
CrN ₄ O ₄	DFL92	570-575	T	Cr(NO) ₄ ; absolute; ab initio-SCF-CI; comp. of 3d spectra of 5 TM compounds; supports MO-model for edge structure
	FD&93	570-575	T	LCAO-SCF-CI; comp. of L-edges of organometallics
<u>Chromium 1s (5.99 keV)</u>				
Cr(CO) ₆	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 _x X _y (Ti,V,Cr,Mn); covalency incr. as Cl 6 F
CrCl ₂ O ₂	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 _x X _y (Ti,V,Cr,Mn); covalency incr. as Cl 6 F
CrF ₂ O ₂	DF&94	5.98-6.00	T	ab initio CI; relaxed orb.; MO _x X _y (Ti,V,Cr,Mn); covalency incr. as Cl 6 F
Cr(NO) ₄	FDL93	5.98-6.04	T	absolute; LCAO-SCF-CI; comp. to Cr 2p results; Ni, Fe, Cr cmpds
<u>Cobalt 3p (55 eV)</u>				
C ₇ CoH ₅ O ₂	HWR90b	30-280	E	CoCp(CO) ₂ ; absolute; comp. to other mixed-Cp, CO species
C ₈ CoO ₈	HWR90b	30-280	E	Co ₂ (CO) ₈ ; absolute; comp. to mixed-Cp, CO species
C ₁₀ ClCoO ₉	HM&93	30-280	E,P,T	Cl-C-[Co(CO) ₃] ₃ , abs.; gas(E,P-ions), sol(P); PIPICO, TOF-MS
C ₁₀ CoH ₁₀	HWR90b	30-280	E	CoCp ₂ ; absolute; comp. to mixed-Cp, CO species
C ₁₁ Co ₃ H ₃ O ₁₀	HM&93	30-280	E,P	CH ₃ O-C-[Co(CO) ₃] ₃ ; abs.; comp. of gas (E), sol (P-TEY)
<u>Cobalt 2p (775, 790 eV)</u>				
C ₇ CoH ₅ O ₂	WRH89	750-820	E	CoCp(CO) ₂ ; absolute; comp. to other mixed-Cp, CO species
C ₈ Co ₂ O ₈	WRH89	750-820	E	Co ₂ (CO) ₈ ; absolute; comp. to mixed-Cp, CO species
C ₁₀ ClCo ₃ O ₉	HM&93	750-820	E,P,T	Cl-C-[Co(CO) ₃] ₃ , abs.; gas(E,P-ions), sol(P); PIPICO, TOF-MS
C ₁₀ CoH ₁₀	HWR90b	750-820	E	CoCp ₂ ; absolute; comp. to mixed-Cp, CO species
C ₁₁ Co ₃ H ₃ O ₁₀	HM&93	750-820	E,P	CH ₃ O-C-[Co(CO) ₃] ₃ ; abs.; comp. of gas (E), sol (P-TEY)
<u>Cobalt 1s (7709 keV)</u>				
Co ₂	WRE89a	7.70-7.74	T	DVM-X α ; XANES; comp. of Co ₂ , Mn ₂ , Ni ₂
<u>Fluorine 1s (690 eV)</u>				
BF ₃	ZV72	680-710	P,R	pot. bar. effects
	SDD81	680-715	T	MSM X- α calc., shape res., comp. to experiment(ZV72)
	SSH84a	690	T	σ^* -res./bond length relationship
	VA&85	680-720	P,R	comp. of BF ₃ , N ₂ , NO ₃ ⁻ ; shape resonances
	NAV88a	688-708	P	comp. to KNO ₃ , NaNO ₃ (O1s - sol); $\delta(\pi-\sigma)$ versus R
	NAV88b	688-708	P	comp. to KNO ₃ , NaNO ₃ (O1s - sol); $\delta(\pi-\sigma)$ versus R
	PV&90	680-700	P	comp. to NO ₂ ⁻ , NO ₃ ⁻ ; $\delta(\pi-\sigma)$ versus R
	SU&97	680-710	P	PEPICO - E-resolved; partial X-sect.; ang. dist.; dynamics of 2a ₂ state
BeF ₂	CC84	686	T	delta SCF, F1s->5 σ^* at 685.3 (T=6.27eV), excited & ion state diss.
CCl ₃ F	ZIB92	680-740	E	absolute, high res. (70 meV), pot. bar., comp. of CCl _x F _{4-x} , x=1-4

	SS&95	290-325	P	PIPICO; start = selective ion gate; PIPICO yields; comp of Cl2p, C1s, F1s edges; only selective at Cl 2p edge
	SS97a	680-750	P	PIPICO, BR and X-sect.; site-specific fragmentation
	SSB99	680-710	P	TIY, PIY; comp of $\text{CF}_x\text{Cl}_{4-x}$ $x=1-3$; site selective fragmentation
CCl_2F_2	ZIB92	680-740	E	absolute, high res. (70 meV), pot. bar., comp. of $\text{CCl}_x\text{F}_{4-x}$, $x=1-4$
	BSS93b	50-1500	P	partial ion yields at coarse resolution
	SBS94a	670-730	P	partial ion yields; site-selective frag. at C 1s, Cl 2p, F 1s
	SSB94	670-730	P	partial ion-pair yields; site-selective frag.
	SS97	680-750	P	PIPICO, BR and X-sect.; site-specific fragmentation
	SSB99	680-710	P	TIY, PIY; comp of $\text{CF}_x\text{Cl}_{4-x}$ $x=1-3$; site selective fragmentation
$\text{CCl}_2\text{F}_3\text{P}$	HBC96	670-740	P	TIY, PIY, PEPIPICO; comp. of PCl_3 , PF_3 , CF_3PCl_2
CCl_3F	ZIB92	680-740	E	absolute, high res. (70 meV), pot. bar., comp. of $\text{CCl}_x\text{F}_{4-x}$, $x=1-4$
	SS97	680-750	P	PIPICO, BR and X-sect.; site-specific fragmentation
	SS98b	680-730	P	PIY, comp of C 1s, F1s, Cl 2p
	SSB99	680-710	P	TIY, PIY; comp of $\text{CF}_x\text{Cl}_{4-x}$ $x=1-3$; site selective fragmentation
CFHO	IH87	670-730	E	HCOF - formyl fluoride
	RI&88	670-730	E	absolute
	HC96	688	T	DFT, $\Delta^3\pi^{-1}\pi = 0.10$ eV
CFH₃	L73	670-780	P	res. at thr.
	HB78a	680-700	E	res. at thr.
	SSH84a	690	T	σ^* -res./bond length relationship
	US&96	682-696	P,T	TEY; Auger, AI; ultrafast decay proposed; SCF calc.
CF_2H_2	L73	670-780	P	res. at thr.
	SSH84a	690	T	σ^* -res./bond length relationship
	US&96	682-696	P,T	TEY; Auger, AI; ultrafast decay proposed; SCF calc.
CF₂O	RI&88	680-730	E	C-F σ^* res., absolute, perfluoro effect
	HC96	688	T	DFT, $\Delta^3\pi^{-1}\pi = 0.010$ eV
CF₃H	L73	670-780	P	res. at thr., extended fine structure (EXAFS)
	SSH84a	690	T	σ^* -res./bond length relationship
	HN86	680-720	E	absolute
	US&96	682-696	P,T	TEY; Auger, AI; ultrafast decay proposed; SCF calc.
CF₃NO	HIR89	680-730	E	absolute, $\sigma^*(\text{C-F})$ dominates
CF₄	L73	670-780	P	absolute, res. at thr., extended fine structure (EXAFS)
	WB74d	685-725	E	strong t_2 res.
	BH81	680-740	E,R	wide range
(CF ₄ cont'd)	HS&81	685-705	T	X- α calc, comp. to WB74d
	SSH84a	690	T	σ^* -res./bond length relationship
	SA&86b	690-780	P	absolute, t_2 res., comp. to C 1s
	SDD86	690-720	T	MS-X α calc, β , 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; PEPIPICO; (F^+ , CF_2^+), (F^+ , CF^+) only produced at F 1s edge
	SBS95	684-718	P	PEPIPICO 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 $\rightarrow \sigma^*\text{CF}$ anisotropic; 42% core-hole localization; symmetry breaking
	TF&99	688-703	P	relative; TIY, threshold EY, TPEPIPICO; kinematics; branching ratios
	PUT04	686-701	P	TIY, Auger, and AEICO with F^+ , ultrafast fragmentation
CF₄O	IM&87	670-730	E	CF_3OF , low-lying $\sigma^*(\text{O-F})$
CF_8S	IS&05	680-730	P	PEPICO, PIPICO, site-selective fragmentation

C₂FH₃	MC&87	680-730	E	$\sigma^*(C-F)$
C₂F₂H₂	MC&87	680-730	E	(CH ₂ =CF ₂), $\sigma^*(C-F)$
C₂F₂H₂	MC&87	680-730	E	(CHF=CFH), $\sigma^*(C-F)$
C₂F₃H	MC&87	680-730	E	$\sigma^*(C-F)$
C₂F₃H₃	MS&84	606-777	P	ZEKE, mass spectrum at $\sigma^*(C-F)$, site-selective fragmentation
C₂F₃HO₂	RI&88	630-730	E	CF ₃ COOH, perfluoro effect
C₂F₃N	HS90	680-728	E	CF ₃ CN, absolute, comp. to CF ₃ C:::CH
C₂F₄	MC&87	680-730	E	$\sigma^*(C-F)$
C₂F₆	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 ₂) _n by C _{2n} F _{4n+2} , n=1-5
C₂F₆O₂	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.
C₃F₃H	HS90	680-728	E	CF ₃ CCH, absolute, comp. to CF ₃ CN
C₃F₆	IM&88	680-730	E	perfluorocyclopropane, comp. to C ₄ F ₈ , C ₆ F ₁₂ , $\sigma^*(C-F)$ dominated
C₃F₆O	RI&88	680-730	E	(perfluoroacetone), intense $\sigma^*(C-F)$ res., perfluoro effect
C₃F₈	HFM87	680-730	E	comp. of perfluoro-n-alkanes. $\sigma^*(C-F)$
	IM&88	680-730	E	C _x F _{2x+2} series, $\sigma^*(C-F)$ dominated
C₄F₆	MC&87	680-730	E	perfluorobutadiene
C₄F₆	RI&88	680-730	E	CF ₃ C:::CCF ₃
C₄F₈	RI&88	680-730	E	CF ₃ C=FCFCF ₃
C₄F₈	IM&88	680-730	E	perfluorocyclobutane, comp. to C ₃ F ₆ & C ₆ F ₁₂ , $\sigma^*(C-F)$ dominated
C₄F₁₀	HFM87	680-730	E	comp. of perfluoro-n-alkanes. $\sigma^*(C-F)$
	IM&88	680-730	E	C _x F _{2x+2} series, $\sigma^*(C-F)$ dominated
	AC&95	685-710	T	STEX ab initio; absolute; growth of poly-(CF ₂) _n by C _{2n} F _{4n+2} , n=1-5
C₅F₁₀	RI&88	680-730	E	perfluorocyclopentene
C₅F₁₂	RI&88	680-730	E	perfluorocyclopentane
C₅F₁₂	HFM87	680-730	E	comp. of perfluoro-n-alkanes. $\sigma^*(C-F)$
	IM&88	680-730	E	per-F-n-pentane, C _x F _{2x+2} series, $\sigma^*(C-F)$ dominated
C₅F₁₂	IM&88	680-730	E	perfluoro-neo-pentane, comp. to C ₂ F ₆ , additional low-lying $\sigma^*(C-F)$
C₆FH₅	HF&87	680-730	E	weak $\sigma^*(C-F)$
	PY&97	684-700	T	STEX, comp to HF&87
C₆F₂H₄	HF&87	680-730	E	(1,4 = para-difluoro), weak $\sigma^*(C-F)$
C₆F₃H₃	HF&87	680-730	E	(1,3,5-trifluoro), weak $\sigma^*(C-F)$
C₆F₄H₂	HF&87	680-730	E	(1,2,4,5 = para-dihydro), weak $\sigma^*(C-F)$
C₆F₅H	HF&87	680-730	E	weak $\sigma^*(C-F)$
C₆F₆	HF&87	680-730	E	weak $\sigma^*(C-F)$
	D92a	689	P	PEPICO, PEPIPICO at π^* res.; comp. to C 1s
C₆F₁₂	IM&88	680-730	E	perfluoro-cyclohexane, comp. to C ₃ F ₆ , C ₄ F ₈ , $\sigma^*(C-F)$ dominated
C₆F₁₄	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 ₂) _n by C _{2n} F _{4n+2} , n=1-5
C₈F₁₈	AC&95	685-710	T	STEX ab initio; absolute; growth of poly-(CF ₂) _n by C _{2n} F _{4n+2} , n=1-5
C₁₀F₈	RI&88	680-730	E	perfluoronaphthalene, F1s--> π^*
C₁₀F₁₆	HI88a	680-730	E	perfluoroadamantine; absolute
C₁₀F₂₂	AC&95	685-710	T	STEX ab initio; absolute; growth of poly-(CF ₂) _n by C _{2n} F _{4n+2} , n=1-5
C₁₂F₁₀	WC&05	686-708	E,T	biphenyl, absolute, GSCF ₃ , ring-ring-interactions (comp to o,o-dibromo)
ClF₃	BS87	680-730	E	high res.
	SB89	680-730	E	high res., partial bar. effects
FH	DC76	690-700	T	ab initio calc.

	MK&76	690-700	T	ab initio calc., oscillator strengths
	HB81b	680-720	E	comp. to F ₂ spectrum
	B82a	680-720	E,R	comp. to F ₂ 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 ₃ , NH ₂ , 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
F ₂	HB81b	670-720	E	discrete σ^* shape res.
	B82a	670-720	E,R	discrete σ^* shape res., review (HB81b data)
	BD&82	680-720	E,R	review (HB81b data)
	SSH84b	690	T	prediction of σ^* energy from E(Z,R)
	SG&89	680-700	T	σ^* shape res.; pos. & shape as f(R); approx. cyl. well & ab initio
	S92	694	E,R	σ^* position
F ₂ O	IM&87	675-715	E	low-lying $\sigma^*(C-F)$
F ₃ 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 σ^* res., shake-up cont. comp. to XPS satellite
	SSH84a	690	T	σ^* -res./bond length relationship
F ₄ N ₂	HIR89	680-740	E	perfluoro-hydrazine, comp. to N ₂ H ₄
F ₃ P	SB85c	685-760	E	comp. to PX ₃ series
	HBC96	670-740	P	TIY, PIY, PEPIPICO; comp. of PCl ₃ , PF ₃ , CF ₃ PCl ₂
	NJ&98	670-720	P,T	absolute; GSCF3 calc.; LS-state; comp of PX ₃ , YPF ₃ . X=Cl,F, Y=O,S)
F ₃ OP	SB85c	675-775	E	pot. bar. effects
F ₅ P	SB85c	675-775	E	pot. bar. effects
F ₂ OS	BHK92	680-700	T	Δ SCF, comp of all edges
F ₄ S	BH87	680-750	E	comp. to S2p, S2s, S1s
	KBH90	680-700	T	ab initio, comp. to BH87; revised $\sigma^*(S-F)$ assignments
	BHK92	680-700	E,T	Δ SCF, comp of all edges
F ₄ Si	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 ²⁺ yield up x2 in cont.; sel. frag.
F ₅ I	CZB95	670-760	E	centrifugal pot. barrier; I 4f cont. res.; comp. to TeF ₆ , XeF ₄
F ₆ S	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 ($a_{1g}=688.3\text{eV}$)
	GN&83	680-750	P,T	comp. of core & valence cont. shapes
	SB84	688.27(s)	E	calibration standard (a_{1g})

	VA&85	680-730	P,R	comp. to BF_3 , N_2 , NO_3^- ; KPF_6 (s); shape resonances
	KBH90	680-700	T	ab initio, comp. to SF_4 (BH87)
	NMA90	680-750	T	MS-X α calc.; order of res. identified; comp. to expt. (ZV71)
	SB90	680-780	E	comp of TeF_6 , SeF_6 , SF_6 ; Z-dependence of pot. bar.s
	NMA91	680-740	T	absolute; DV-X α ; 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 !; β s; comp. to localized core hole calc; vibronically induced core hole localization
	FM&98	680-900	E	4 keV impact; Auger, no bound SF_6^{++} 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^- , F^- ; anion signals specific to shape resonances
	PU&05	687-689	P	3D ion momentum AEPIPICO, detuning energy creates fragmentation
F ₆ Se	SB90	680-780	E	comp of TeF_6 , SeF_6 , SF_6 ; Z-dependence of potential barriers
F ₆ Te	SB90	680-780	E	comp of TeF_6 , SeF_6 , SF_6 ; Z-dependence of potential barriers

Gadolinium 4d (145 eV)

GdF ₃	CP84	120-190	P	4d->f cont. res., comp. to lineshape of C84, no F-influence
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Gallium 3d (19 eV)

C ₃ H ₉ Ga	NS&89	14-31	P	$\text{Ga}(\text{CH}_3)_3$; 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 ₃ H ₉ Ga	US&90c	90-260	P	$\text{Ga}(\text{CH}_3)_3$, total & partial IYs; PIPICO; H^+ enhanced by sec. proc.
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Gallium 1s (10.37 keV)

AsGa	BF&93	10.3-11.1	P	GaAs; EXAFS; in situ monitor of CVD; fluorescence detection
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Germanium 3d (30 eV)

C ₄ GeH ₁₂	NSK88	28-41	P	$\text{Ge}(\text{Me})_4$, thresh. e-; ionic frag.; comp. of $\text{M}(\text{Me})_4$ M=Ge,Sn,Pb
	NS&90	28-41	P	ZEKE, PI yield, BR, comp. of $\text{M}(\text{Me})_x$ frag. (Bi, Ga, Zn, Ge, Sn, Pb)
	BS&02B	50-450	P, T	GeMe ₄ ; PEPIPICO, PIPICO, partial ion yields; EICVOM calc
Cl ₄ Ge	SN&86	21-42	P	threshold e-; review of apparatus

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

C ₄ GeH ₁₂	BS&02B	50-450	P, T	GeMe ₄ ; PEPIPICO, PIPICO, partial ion yields; EICVOM calc
C ₄ GeH ₁₂	KN&13	125-135	P,T	enhanced resolution, 2d PES to defeat super-Coster-Kornig broaden
C ₁₀ GeH ₂₀ N ₂	LU&99	110-140	E	unsaturated germylene; broad
C ₁₀ GeH ₂₂ N ₂	LU&99	110-140	E	saturated germylene; broad
Cl ₄ Ge	GD&96	100-300	E,T	comp. to Cl 2p, Ge2p/3p of GeCl_4 ; comp. to ETS
GeH ₄	HBK71	120-130	P	two lines at 124.7 & 129.7 eV

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

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

Germanium 1s (11.17 keV)

GeH ₄	G51	11.1-12.0	P	comp. to GeCl ₄ , absence of EXAFS
	NM&81	11.1-11.2	T	X- α (MSM) calc., comp. to experiment (G51)
	BB&88	11.0-11.3	P	EXAFS, expt test of multiple scat. (v.v. weak); σ^* (Ge-Cl)
	GD&96	11.1-11.2	T	ab initio SCF; comp. to 2p, 2s calc; 2p experimental
ClGeH ₃	BB&88	11.0-11.3	P	EXAFS, expt test of multiple scat. (v.v. weak); σ^* (Ge-Cl)
Cl ₄ 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- α ; comp. to experiment (G51, KE75)
	BB&88	11.0-11.3	P	EXAFS, experimental test of mult. scattering (v.v. weak); σ^* (Ge-Cl)
	BM&89b	11.0-11.3	P	EXAFS, experimental test of multiple scattering (v.v. weak)
	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 ₂ , GeCl ₄ , SF ₆
	GD&96	11.1-11.2	T	ab initio, comp. to Cl 2p, Ge2p/3p of GeCl ₄
	FA98	11.0-11.2	P	EXAFS; MSX α ; high precision – 0.1 pm accuracy; comp to ED

Iodine 4d (55 eV)

BrC ₂ H ₄ I	TH&92	50-61	P	CH ₂ Br-CH ₂ I; TEY; TOF-MS & PIPICO; sel. frag.; pref. Br ⁺ , I ⁻ -loss
CH ₃ 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 $\sigma^*(\text{C-I})$ 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 PEPPIPICO and (Auger, ion)
	SL&96	95	P,R	PE3PICO; atomic fragmentation; non-Coulombic mech.; impulsive model
C ₂ H ₃ I	SBK88	45-100	E	high res., comp. to other vinyl halides
C ₆ H ₅ I	HP&78	46-62	E	cont. res.
F ₅ I	CZB95	40-100	E	centrifugal pot. barrier; I 4f cont. res.; comp. to TeF ₆ , XeF ₄
HI	KL86	50-100	T	atomic type d-->f res.; distinguished from molecular shape res.
	MN87	43-58	P	TPES, DES at $\sigma^*(\text{C-I})$ res., no dissociation prior to AI
I ₂	CNS73	45-160	P,T	absolute, gas-solid comp., Rydberg analysis IP (57.25, 58.95)
	MB87	25-130	E	thr. electron impact; I ⁺ -yield follows 4d structure

Iodine 3d (650 eV)

CH ₃ I	HB78a	615-705	E	cont. res.
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F ₅ I	CZB95	610-720	E	centrifugal pot. barrier; I 4f cont. res.; comp. to TeF ₆ , XeF ₄
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Iodine 1s (33.2 keV)

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

Iron 3p (60 eV)

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

Iron 2p, 2s (707,720, 845 eV)

B ₅ C ₁₉ FeH ₁₇ O ₂ P	HLD91	650-760	E	Cp(CO) ₂ FeB ₅ H ₂ P(Ph) ₂
C ₂ FeN ₂ O ₄	DFL92	660-670	T	Fe(CO) ₂ (NO) ₂ ; absolute; ab initio-SCF-CI; comp. of 3d spectra of 5 TM compounds; supports MO-model for edge resonances
C₅FeO₅	MSN89	650-760	P	total, partial ion yields; comp to Fe, Fe ₂ (CO) ₉ ,
	HWR90b	650-760	E	comp. to other Fe-org, Fe2p; ligand effect on metal np
(C ₅ FeO 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 ₇ FeH ₆ O ₃	WRH92	650-760	E	RFe(CO) ₃ , R=butadiene; absolute, organo-irons; ligand interactions
C₉FeH₈O₃	HWR90b	650-760	E	CxFe(CO) ₃ ; comp. to other Fe-org, Fe2p; ligand effect on metal np
	WRH92	650-760	E	absolute, organo-irons; ligand interactions
C₉Fe₂O₉	MSN89	650-760	P	total, partial ion yields; comp to Fe, Fe(CO) ₅
	WRH92	650-760	E	absolute, organo-irons; ligand interactions
C₁₀FeH₁₀	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 ₂ , FeCp ₂
	G94	700-740	R	atomic multiplet calc.; review of 2p spectra of all TM cmpds
	KYN09	704-726	P, T	Fe(Cp [*]) ₂ , double excitations; comp of FeCp ₂ [*] , FeCp ₂ , FeCp ₂ (PF ₆)
C₁₁FeH₈O₃	WRH92	650-760	E	RFe(CO) ₃ , R=COT; absolute, organo-irons; ligand interactions
C₁₂FeH₁₂	WRH92	650-760	E	RCpFeCp R=ethylene; absolute, organo-irons; ligand interactions
C₁₄FeH₁₈	WRH92	650-760	E	RCpFeCp R=butane; absolute, organo-irons; ligand interactions
C ₂₀ FeH ₃₀	KYN09	704-726	P, T	Fe(Cp [*]) ₂ , double excitations; comp of FeCp ₂ [*] , FeCp ₂ , FeCp ₂ (PF ₆)

Iron 1s (7.11 keV)

Fe(CO) ₅	JP58	7.10-7.15	P	gas-solid comp.
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	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) ₂	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 ₂	CK&83	7.10-7.13	T	absolute, energy dependent Dirac calc, spin-dependence
Fe ₂	WRE89b	7.10-7.15	T	DV-X α ; XANES; discrete res.; comp. to Ni ₂ , Ni ₃

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 ₂	UF&08	262	P,T	PEPIPICO, interatomic coulomb decay (ICD); spin conserved processes faster than spin-flip processes; dipole forbidden processes observed
Kr _n	KWR98	89-96	P	TEY; Kr ₂ ⁺ yield as f(<size>); site specific spectral features (surf, bulk)
Kr _n	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 _n	SG&95a	1660-1760	P	gas,cluster comparison, 3d exciton in cluster is 0.5 eV above gas
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Krypton 1s (14.11 keV)

(ArKr) _n	NM&08	14.3-14.4	P	<n>=100; ionic fragmentation; singly charged atomic ions dominate
Kr _n	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
KrF ₂	KE&83	14.3-14.4	P	XANES peak 6 NN contraction; T-dep. used to estimate DW factor
	CK&85	14.3-14.4	T	gas-solid comp., near-edge res. absolute, shape res. at edge

Lanthanum 4d (100 eV)

LaF ₃	CP&80	95-145	P	comp. to gas (R79) & metal La, no fluorine effect
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Lead 5d (20 eV)

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

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

C ₄ H ₁₂ Pb	NS&90	50-200	P	total & partial ion yields, site/core-hole selective frag.
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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 ⁺)
	DYM86	55-70	T	valence bond, ab initio, comp. to Li
Li ₂	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. comp. to N ₂ , Li & N, no Cooper minimum
Li ₂ Cl ₂	RS&76	55-70	P	photographic, gas-solid comp., Z+1 analogy

Manganese 3p (60 eV)

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

Manganese 2p (645, 665 eV)

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

Manganese 1s (6.539 keV)

ClMnO ₃	DF&94	6.52-6.54	T	ab initio CI; relaxed orb.; MO _x X _y (Ti,V,Cr,Mn); coval. increases as Cl->F
FMnO ₃	DF&94	6.52-6.54	T	ab initio CI; relaxed orb.; MO _x X _y (Ti,V,Cr,Mn); coval. increases as Cl->F
Mn ₂	WRE89a	6.52-6.56	T	DVM-Xα; XANES; comp. of Co ₂ , Mn ₂ , Ni ₂

Mercury 2p (12.3, 14.2 keV)

Cl ₂ Hg	YK&96	12.2-13.3	P,T	T-dependent xafs; cumulant analysis, Feff 6.0, force constants, anharmonicity
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Molybdenum 3d (230 eV)

C ₆ MoO ₆	TD&92a	200-280	E	Mo(CO) ₆ ; comp. of 2p and 3d edges
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Molybdenum 2p (2520,2625 eV)

C ₆ O ₆ Mo	TD91	2.50-2.80	P	Mo(CO) ₆ ; 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 ₆ Mo	GH&94 GD&95	2.52-2.63 2.52-2.64	P,T P,T	comp. to crystal field multiplets; other MX ₆ species; L ₃ & L ₂ edges differ TIY; ab initio CI; Mo d,p character of orbitals estimated
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Molybdenum 1s (20,000 eV)

C ₆ O ₆ Mo	GD&95	2.52-2.64	P,T	Mo(CO) ₆ ; TIY; ab initio CI; Mo d,p character of orbitals estimated
F ₆ 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 _n	FB&94 BF&95a KB&97	860-960 860-960 860-920	P	variable cluster size; Rydbergs, XANES and EXAFS EXAFS as f(cluster size); apparatus and beamline performance near edge as f(cluster size)
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Nickel 3p, 3s (78, 100 eV)

B ₁₈ C ₄ H ₂₂ Ni	HLD91	40-180	E	Ni(B ₉ H ₁₁ C ₂) ₂ , Ni bollyl complex (Cp-analog)
C ₄ NiO ₄	CSB90	60-110	E	Ni(CO) ₄ ; comp. to CO
C ₁₀ H ₁₀ Ni	RH89b	50-200	E	Ni(Cp) ₂ ; comp to other metallocenes

Nickel 2p (860,880 eV)

C ₄ NiO ₄	DFL92	855-865	T	Ni(NO) ₄ ; absolute; ab initio-SCF-CI; comp. of 3d spectra of 5 TM compounds; supports MO-model for edge resonances
C ₆ H ₁₀ Ni	FD&93 DFL92	855-865 855-865	T T	LCAO-SCF-CI; comp. of L-edges of organometallics Ni(C ₃ H ₅) ₄ ; absolute; ab initio-SCF-CI; comp. of 3d spectra of 5 TM compounds; supports MO-model for edge resonances
C ₁₀ H ₁₀ Ni	RH93b	845-880	P	Ni(Cp) ₂ ; total ion yield; comp. of NiCp ₂ and FeCp ₂

Nickel 1s (8.333 keV)

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

Nitrogen 1s (410 eV)

B₃N₃H₆	DG&86 VNP91 SC95	395-445 396-422 399	E E T	(borazine), comp. to Bz & cyclohexane, aromatic, two σ^* res. comp. of benzene, BN(s) and borazine; shape res. MO not R-related ADC local/delocal calc; Jahn-Teller localisation; comp. to B 1s, C ₃ H ₃ ⁺
BrCN	OBI95	380-460	E,T	absolute; 0.1-1 eV fwhm; low lying $\sigma^*(C-Br)$ below $\pi^*(CN)$
CF₃NO	HIR89	390-440	E	absolute
CHN	HB79a	395-435	E	(HCN), cont. res.
	HB79b	395-435	E	cont. res., Z+1 analogy
	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
	LAL91	400-420	T	CNDO, systematic treatment of σ^* energies
	ZZ&92	400-410	T	Δ SCF; core hole localisation; gen. rules for MO shifts in 2nd row
	AC&94	390-430	T	ab initio RPAE-STEX; comp of RCN (R=H,C _n H _{2n-2} , n=1,2,3,5,11); no $\sigma^*(C-C)$ in N 1s; supports building block model

CH₃NO	IH87	390-440	E	HCONH ₂ - formamide, comp. to (HCX, X=OH,F)
CH ₃ NO ₂	VA&92	250-750	P	absolute; analysed as (CH ₃ ⁺ , NO ₂ ⁻); bond length corr.; 0.6 e- in N 2p
CH₄N₂O	UH&95b	390-428	E,T	(NH ₂) ₂ CO, urea; absolute; modelling of polyurethane
CH ₅ N	WB74b	395-435	E	(CH ₃ NH ₂ - methylamine) res. at thresh.
	SSH84a	410	T	σ*-res./bond length relationship
	SB85b	395-445	E	σ* res. at thresh., comp. to (CH ₃) _x NH _{3-x} ,x=0-3
	LAL91	400-420	T	CNDO, systematic treatment of σ* energies
	TD&92b	400-450	P	PIY; charge separation mass spec; decay dynamics
C ₂ Cl ₃ N	IO&99	390-440	P	absolute; selected E mass spec; no site-specific fragmentation
C ₂ D ₃ N	SY&99	395-440	P	CD ₃ CN; relative; TIY, PIY; comp. of D/H; VARTMAN; anisotropic fragmentation at π*
C₂F₃N	HS90	395-455	E	CF ₃ CN, absolute, comp. to other triply bonded species
C ₂ FeN ₂ O ₄	SL&92	390-420	P	PEPIPICO; non-selective, step-wise fragmentation
C₂H₃N	HM&89	390-480	P	(CH ₃ 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 _n H _{2n-2} , 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
C₂H₃N	HTM89	390-440	E	(CH ₃ NC), comp to CH ₃ CN, vibrational ELS
C₂H₃NS	HTM89	390-440	E	(CH ₃ SCN), comp to CH ₃ NCS, vibrational ELS
C₂H₃NS	HTM89	390-440	E	(CH ₃ NCS), comp to CH ₃ SCN, vibrational ELS
C₂H₅NO₂	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 ₃ , gas-solid
	FP&09	398-413	P	comp. of Gly, Gly-gly
	PB&15	398-413	P	comp. of Gly, Gly-gly
C₂H₅N₃O₂	UA&99	390-420	E	biuret; (NH ₂ (CO)NH(CO)NH ₂); absolute
	LC&07	390-420	E,T	malonamide; comp.of di-carbonyls; charge shifts for fingerprinting, GSCF3
C ₂ H ₇ N	SB85b	395-445	E	σ* res. at thresh., comp. of (CH ₃) _x NH _{3-x} ,x=0-3
C ₂ N ₂	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 ₃ H ₃ N	HA&97	395-427	E,T	acrylonitrile; relative; Z+1 calc'n; π* interactions; comp. of CH ₂ =CHCN, C ₂ H ₂ (CN) ₂ , CH ₂ =CHCH ₂ CN
	IC&08	398-401	P,T	vibrational fine structure; rehybridization, local core hole effects. Full potential surface calculation
C ₃ H ₃ NO	IO&00	395-445	P	absolute; E-selected mass spec; low-lying π* _{N=C}
C ₃ H ₃ NS	HH&96	392-427	P	thia-azole; absolute; E-selected mass spec; low-lying π* _{N=C}
C ₃ H ₃ NO ₂	IO&00	395-445	P	methylcayano formate, CH ₃ -0C(O)CN, absolute; E-selected mass spec; comp to C ₄ H ₅ NO ₂ ; size dep..frag.
	TS&05	390-440	P, T	absolute, StoBE-DFT, N 1s and O 1s
C₃H₃N₃	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* ²)
	VG&08	390-440	P,T	relative, transmission, double ion cell, DEMON calc, comp of 5 aza-rings
C₃H₄N₂	AGH93	390-430	E,P	imidazole; absolute; gas-EELS; comp. to sol.-NEXAFS
C ₃ H ₄ N ₂	DH&98	395-420	P	pyrazole, relative, 0.2 eV fwhm, Z+1 HONDO, pyrrole vs. pyrazole

C ₃ H ₅ N	AC&94	390-430	T	C ₂ H ₅ CN, ab initio RPAE-STEX; comp of RCN (R=H,C _n H _{2n-2} , n=1,2,3,5,11); no σ*(C-C) in N 1s; supports building block model
C₃H₆NO₂	GH01	390-420	E	alanine; absolute; comp of amino acids
C ₃ H ₆ NO ₂ S	PC&98	400-430	T	cysteine; (D,L) STEX; comp. of NEXAFS, circ. Dichr. of amino acids
C₃H₆N₂O₂	LC&07	280-320	E,T	malonamide; comp.of di-carbonyls; charge shifts for fingerprinting, GSCF3
C₃H₇NO₂	UH&95b	390-440	E	NH ₂ CO ₂ Et, absolute; modelling of polyurethane PEELS
C ₃ H ₇ NO ₂	PC&98	400-430	T	alanine; (D,L-) STEX; comp. of NEXAFS, circ. Dichr. of amino acids
C ₃ H ₇ NO ₃	PC&98	400-430	T	serine; (D,L-) STEX; comp. of NEXAFS, circ. Dichr. of amino acids
C ₃ H ₉ N	SB85b	395-445	E	N(Me) ₃ ; σ* res. at thresh., comp. of (CH ₃) _x NH _{3-x} ,x=0-3
	LAL91	400-420	T	CNDQ, systematic treatment of σ* energies
	PS&01	390-426	T	STEX, extensive series of C-N compounds
C ₄ H ₂ N ₂	HA&97	395-427	E,T	dicyano-ethylene; relative; Z+1 calc'n; π* interactions; comp. of CH ₂ =CHCN, C ₂ H ₂ (CN) ₂ , CH ₂ =CHCH ₂ CN
C ₄ H ₄ N ₂	PS&01	390-426	T	pyrimidine, STEX, extensive series of C-N compounds
C ₄ H ₄ N ₂	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 ₄ H ₂ N ₂	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 ₄ H ₄ N ₂	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
C₄H₅N	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
(C ₄ H ₅ N cont'd)	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 ₄ H ₅ N	PS&01	390-426	T	(1,3-pyrrole); STEX, extensive series of C-N compounds
C ₄ H ₅ N	HA&97	395-427	E,T	allylcyanide; relative; Z+1 calc'n; π* interactions; comp. of CH ₂ =CHCN, C ₂ H ₂ (CN) ₂ , CH ₂ =CHCH ₂ CN
C ₄ H ₅ NO ₂	IO&99	390-440	P	MeO(CO)CH ₂ CN; absolute; N1s, O1s → π* mass spect; site sel. frag.
	IO&00	395-445	P	absolute; E-selected mass spec; comp to C ₃ H ₃ NO ₂ ; size dep..frag.
	TS&05	390-440	P, T	absolute, StoBE-DFT, N 1s and O 1s
C ₄ H ₇ N	AC&94	390-430	T	C ₃ H ₇ CN, ab initio RPAE-STEX; comp of RCN (R=H,C _n H _{2n-2} , n=1,2,3,5,11); no σ*(C-C) in N 1s; supports building block model
C ₄ H ₇ N	PS&01	390-426	T	(1-pyyroline), STEX, extensive series of C-N compounds
C ₄ H ₇ N	PS&01	390-426	T	(2-pyyroline), STEX, extensive series of C-N compounds
C ₄ H ₇ N	PS&01	390-426	T	(3-pyyroline), STEX, extensive series of C-N compounds
C₄H₇NO₂	LC&07	390-420	E,T	Me(CO)N(CO)Me; di-acetamide; di-carbonyls; charge shifts, GSCF3
C₄H₇NO₄	UH&99	395-435	E,T	ethyl allophanate; absolute; GSCF3; comp. of urethane species
C₄H₈N₂O₄	CG&04	390-420	E	(glycyl-glycine), comp. of Gly, Gly-gly, Gly ₃ , gas-solid
	FP&09	398-413	P	comp. of Gly, Gly-gly
	PB&15	398-413	P	comp. of Gly, Gly-gly
C₄H₈N₂O₃	GC&03	398-420	E,T	absolute, comp Gly, Gly-Gly; tri-gly(s); peptide bonds; GSCF3
C₄H₉N	NIH86	390-440	E	(pyrrolidine), comp. to other heterocyclics
	PS&01	390-426	T	(1-pyyroline), STEX, extensive series of C-N compounds
C₅H₂N₄	AGH93	390-430	E,P	dicyano-imidazole; absolute; gas-EELS; comp. to sol.-NEXAFS
C₅H₅N	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_6H_6 , C_6H_5X
	DR&89	395-420	P	condensed films, comp. to pyrazine & triazene; DES
	ED&90	399	P	DES, dynamic screening effects; comp. of N_2 , N_2O & 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; π^* 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
C_5H_7N	HH&96	390-430	P	N-methyl pyrrole; inductive, mesomeric effects
	PS&01	390-426	T	STEX, extensive series of C-N compounds
C_5H_7N	PS&01	390-426	T	(1,4-dihydropyridine), STEX, extensive series of C-N compounds
C_5H_7N	PS&01	390-426	T	(2,3-dihydropyridine), STEX, extensive series of C-N compounds
$C_5H_7N_5$	PS&01	390-426	T	(2-amino, 4,5-imidazoledicarbonitrile), STEX, extensive C-N compounds
$C_5H_{11}N$	PS&01	390-426	T	(piperidine), STEX, extensive series of C-N compounds
$C_5H_{10}N_2$	HE&01	395-420	E	methyl-carbene; thermal decomposition of tetra-amino ethylene
$C_5H_{11}N$	NIH86	390-440	E	(piperidine)
	PS&01	390-426	T	STEX, extensive series of C-N compounds
$C_5H_{11}NO_2$	PC&98	400-430	T	valine; (D,L-) STEX; comp. of NEXAFS, circ. Dichr. of amino acids
$C_5H_{15}NSi$	UH94b	390-440	E	$Me_3Si(NMe_2)$; comp. of Si-N cmpds; models for SiN_xO_y films
$C_6H_4N_2S$	HD&91	390-430	E	Bz(N-S) ring; comp. of S-N heterocyles, aromaticity
$C_6H_4N_2S_2$	HD&91	390-430	E	Bz(N-S) ring; comp. of S-N heterocyles, aromaticity
$C_6H_4N_2S_3$	HD&91	390-430	E	Bz(N-S) ring; comp. of S-N heterocyles, aromaticity
$C_6H_5NO_2$	TUH96	390-430	E,T	nitrobenzene; absolute, EHMO, comp. to aniline, nitroanilines
$C_6H_6N_2O_2$	TUH96	390-430	E,T	(1,2)-nitroaniline; absolute, EHMO, comp. to aniline, nitrobenzene
$C_6H_6N_2O_2$	TUH96	390-430	E,T	(1,3)-nitroaniline; absolute, EHMO, comp. to aniline, nitrobenzene
$C_6H_6N_2O_2$	TUH96	390-430	E,T	(1,4)-nitroaniline; absolute, EHMO, comp. to aniline, nitrobenzene
C_6H_7N	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 ₂)
	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)
$C_6H_{12}N_2$	RUH95	390-430	E	DABCO; absolute
$C_6H_9N_3O_3$	UA&99	390-430	E	trimethyl-isocyanurate; absolute; polymer model
$C_6H_{12}N_2Si$	UH&94b	390-420	E	bis(dimethylamino)dimethylsilane; exploring Si-N bond
C_7F_5N	IOG97	390-440	P	C_6F_5CN ; absolute; reflectron TOF; π^* split; sym. resolved; comp. of (C_7F_5N , C_6H_5CN , p- $CF_3C_6H_4CN$, p- $CF_3C_6H_4NCO$)
	IO&99	390-430	P	TIY; comp of Cl's, N1s; no site selectivity; mass spec at π^*_{ring}
C_7H_5N	H92a	390-440	E,T	(benzonitrile), absolute; EHMO
	PS&01	390-426	T	STEX, extensive series of C-N compounds
$C_7H_7NO_2$	UH&95b	390-440	E	NH_2CO_2Ph , absolute
$C_7H_8N_2O$	UH&95a	390-430	E	NH_2CO_2Ph ,phenylurea; absolute; comp. to model polyurethanes
	UH&95b	390-440	E	absolute; ureas and urethanes similar at N 1s
$C_7H_8N_2O$	UH&95a	390-420	E	phenylurea; absolute; modelling of polyurethane PEELS
C_7H_9N	UH96	390-430	E	N-methyl aniline; absolute
$C_7H_{15}N$	AC&94	390-430	T	$C_6H_{15}CN$, ab initio RPAE-STEX; comp of RCN (R=H, C_nH_{2n-2} , n=1,2,3,5,11); no $\sigma^*(C-C)$ in N 1s; supports building block model
$C_7H_{18}N_3Si$	UH&94b	390-430	E	tris(dimethylamino)methylsilane; exploring Si-N bond
$C_8F_3H_4NO$	IO&99	390-440	P	p- $CF_3C_6H_4NCO$; TIY; N1s, O1s → π^* frag.; no site selectivity
C_8H_9NO	UH&95b	390-430	E	benzyl carbamate; absolute; modelling polyurethanes

C₈H₉NO₂	GH01	390-430	E	phenylalanine, comp. of amino acids
C₈H₁₁N	HUR93	390-430	E	N,N-dimethylaniline
C₈H₂₄N₄Si	UH94b	390-440	E	Si(NMe ₂) ₄ ; comp. of Si-N cmpds; models for SiN _x O _y films
C₉H₆N₂O₂	UHR99	390-420	E,T	2,4-TDI, absolute; isomeric effect
C₉H₆N₂O₂	UHR99	390-420	E,T	2,6-TDI, absolute; isomeric effect
C₉H₇N	PS&01	390-426	T	(quinoline), STEX, extensive series of C-N compounds
C₉H₇N	PS&01	390-426	T	(isoquinoline), STEX, extensive series of C-N compounds
C₉H₁₁NO₂	UH&95b	390-440	E	Ph-NHCO ₂ Et, absolute; modelling of polyurethane PEELS
C₉H₂₇NSi₃	UH94b	390-440	E	N(SiMe ₃) ₃ ; comp. of Si-N cmpds; models for SiN _x O _y films
C₁₀H₈N₄	PS&01	390-426	T	(2,5-dimethyl-N,N'-dicyanoquinonediimine), STEX, extensive series of C-N compounds
C₁₀H₂₇N	PS&01	390-426	T	N('Bu) ₃ , STEX, extensive series of C-N compounds
C₁₀H₁₉N₂O₂	LC&07	280-320	E,T	comp. of di-carbonyls; charge shifts for fingerprinting, GSCF3
C₁₀H₂₀N₂	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
C₁₀H₂₀N₂Ge	LU&99	396-412	E,T	c-Ge(RNCH=CHNR), comp. cyclic diamino C:, Si:, Ge: ; GSCF3 ab initio
C₁₀H₂₀N₂Si	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
C₁₀H₂₂N₂	LU&99	394-418	E	tBu-NCH ₂ CH ₂ N-tBu; absolute; ligand rel. to cyclic diamino C:,Si:,Ge.
C₁₀H₂₂N₄	HE&01	395-420	E	tetra-amino ethylene; used for thermal decomposition to form carbene
C₁₀H₂₂N₂Ge	LU&99	396-412	E,T	c-Ge(RNCH ₂ CH ₂ NR), comp. cyclic diamino C:, Si:, Ge: ; GSCF3 ab initio
C₁₀H₂₂N₂Si	UH&98	396-412	E,T	c-Si(RNCH ₂ CH ₂ NR), R=tBu, unsat. silylene; absolute;
	LU&99	394-418	E,T	absolute; comparison of cyclic diamino C:, Si:, Ge: ; GSCF3 ab initio
C₁₀H₂₂N₂Ge	LU&99	396-412	E,T	c-H ₂ Ge(RNCH=CHNR), cyc. diamino C:, Si:, Ge: comp ; GSCF3 ab initio
C₁₀H₂₂N₂Si	UH&98	396-412	E,T	c-H ₂ 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
C₁₀H₂₄N₂Ge	LU&99	396-412	E,T	c-H ₂ Ge(RNCH ₂ CH ₂ NR), cyc. diamino C:, Si:, Ge: comp; GSCF3 ab initio
C₁₀H₂₄N₂Si	UH&98	396-412	E,T	c-H ₂ Si(RNCH ₂ CH ₂ NR), R=tBu, unsat. silylene; absolute;
	LU&99	394-418	E,T	absolute; comparison of cyclic diamino C:, Si:, Ge: ; GSCF3 ab initio
C₁₀H₁₃NO₂	UH&95b	390-440	E	Ph-N(CH ₃)-CO ₂ Et, absolute; modelling of polyurethane PEELS
C₁₁H₁₄N₂O₄	UHR99	390-440	E	TDI-bis-methyl urethane; absolute
C₁₁H₂₀N₂	LU&99	396-412	E,T	c-C:(RNCH=CHNR), comparison of cyclic diamino C:, Si:, Ge: ; GSCF3 ab initio; saturated carbene
C₁₁H₂₂N₂	LU&99	396-412	E,T	c-C:(RNCH ₂ CH ₂ NR), comparison of cyclic diamino C:, Si:, Ge: ; GSCF3 ab initio; unsaturated carbene
C₁₁H₂₄N₂	LU&99	396-412	E,T	c-H ₂ C:(RNCH ₂ CH ₂ NR), comparison of cyclic diamino C:, Si:, Ge: ; GSCF3 ab initio; protonated carbene
C₁₂H₁₅N₂O₂Re	HS92	390-440	E	Cπ*Re(CO) ₂ N ₂ ; absolute; split N1s->π* (N _a -N _b chem. shift)
C₁₂H₄N₄	PS&01	390-426	T	(tetracyano-quinodimethane), STEX, extensive series of C-N compounds
C₁₂H₂₃N	AC&94	390-430	T	C ₁₁ H ₂₃ N, ab initio RPAE-STEX; comp of RCN (R=H,C _n H _{2n-2} , n=1,2,3,5,11); no σ*(C-C) in N 1s; supports building block model
C₁₃H₉N	PS&01	390-426	T	(6,7-benzoquinoline), STEX, extensive series of C-N compounds
C₁₃H₉N	PS&01	390-426	T	(acridine), STEX, extensive series of C-N compounds
C₁₃H₁₂N₂O	UH&95b	390-440	E	(Ph-NH) ₂ C=O, absolute; modelling of polyurethane PEELS
	UA&99	390-430	E	tritylisocyanurate; absolute, polymer model
C₂₁H₁₅N₃O₃	UHR92	390-440	E	(Bz-O) ₃ C3N3 (tri-phenoxy-triazine); polyurethane modelling
	UA&99	390-430	E	absolute, polymer model
C₂₄H₂₁N₃O₃	UA&99	390-430	E	tritylisocyanurate; absolute, polymer model
C₃₂H₁₆N₈Ni	RSH93	50-450	E	Ni-phythalocyanine; compared to solid
D₃N	ST&93	400-405	P,T	high res; ab initio; no resolved vib; comp. to NH ₃ (no 3s vibronic); comp of H ₂ O, NH ₃ , CH ₄ re Ryd/val char.
F₃N	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., $1s-\pi^*$ thresh. observed
	SBC84	400-450	E	discrete $\sigma^*(N-F)$, 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_3 , PX_3 1s edges; pot. barr. effects
F₄N₂	HIR89	390-440	E	per-fluorohydrazine, comp to N_2H_4 , NH_3
H ₂ N	CC&82	405-415	T	ab initio calc. (CI)
H ₃ N	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)
	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_2O , CH_4 , 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^+ IY from surface of condensed NH_3 , EY, extra peak at 420eV
	SSH84a	420	T	σ^* -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_3 , N_2 , Ne ; res. effects; atomic 2p resonance
	H90a	395-425	E,R	absolute, comp. of N_2 , NH_3 , N_2H_4 , Ne ; σ^* vs. Ryd
(NH ₃ cont'd)	MR&90	390-440	P	H^+ des. from Ru-adsorbed; comp. to AEY, TEY, gas (WB74b)
	RC&90	390-440	P	comp. of gas, solid; ion yields, H^+ ultrafast diss.
	LAL91	400-420	T	CNDO, systematic treatment of σ^* energies
	S92	395-435	E,R	comp. of NH_3 , N_2H_4 , N_2 ; $\sigma^*(N-N)$
	ST&93	400-405	P,T	high res; ab initio; no resolved vib; comp. to NH_3 (no 3s vibronic); comp of H_2O , NH_3 , CH_4 re Ryd/val char. NH_4
	KNP92	400-408	T	SCF-CI in (Z+1) approx.
	MH&95	420	P	Auger-ion-ion coincidence; KERDs; mapping NH_3^{2+} potential surface; simultaneous vs. sequential bond breaking
	JC01	397-417	P	relative; comparison of NX_3 , PX_3 1s edges; pot. barr. effects
	LG&05	400-405	P	TIY, PEPICO, alignment modelled
	SG&05	400-407	P	TIY, PIY, vibrationally resolved, NH_3^{2+} yield strongly v dependent
	JV&07	399-407	P	partial luminescence yield, Balmer lines (H^*), ultrafast decay
H₄N₂	HIR89	390-440	E	hydrazine, comp to N_2F_4 , NH_3
	H90a	395-425	E,R	absolute, comp. of N_2 , NH_3 , N_2H_4 , Ne ; σ^* vs. Ryd
	S92	395-435	E,R	comp. of NH_3 , N_2H_4 , N_2 ; $\sigma^*(N-N)$
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_2 , NO & O_2 , 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 π^* in N ₂ , NO, N ₂ O, comp. to N ₂ calc. (RO79)
	LT&84	414-440	P	cont. res. shape comp. to calc. (WDD82), β -params
	SSH84a	420	T	σ^* -res./bond length relationship
	LPL85	400-430	T	MS, quantum defect calc, R-dependence of σ^* res.
	RL&85	400-430	P	comp. of multilayer PSID & ISEELS; comp. of CO, N ₂ , NO, N ₂ O
	RO85	400	T	π^* GOS, quadrupole transition, constant for N ₂ ,NO,N ₂ O
	CA&87	400	E	Auger-loss coinc.; vibnl-time interference; cf. ETS boomerang model
	CF&87	400	E	GOS, constant for π^* in N ₂ , NO, N ₂ O, comp. to N ₂ calc (RO79)
	SG&89	410-430	T	σ^* shape res.; pos. & shape as f(R); approx. cyl. well & ab initio
	PV&90	395-422	P	comp. to NO ₂ ⁻ , NO ₃ ⁻ (sol); $\delta(\pi-\sigma)$ correlated with R(NO)
	S90b	398-430	R,P	ionic fragmentation; ion KERD; ion (PIPICO) angular distribution
	MC&91	397-411	P	50 meV fwhm; π^* - 2 vib'l series (2 Σ^- , 2 Δ); Ryd. vib'ns
	SS91	397-423	P	TEY; partial ion yields; KERD at π^* ; β -param.
	CT92	399	E	DES by (e,e); U _{CV} > 0
	H92a	398-402	E	⁴ π -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 ₃ , N ₂ H ₄ , N ₂ ; $\sigma^*(N-N)$; MS-X α ; vibnl struct.; Ryd.
	ZZ&92	400-410	T	Δ SCF; core hole localisation; gen. rules for MO shifts in 2nd row
	MLH93	401-480	P	luminescence spectra; rotational dist. of N ₂ ⁺ at 401, 419, 480; no variation with E; interchannel coupling is origin of N ₂ ⁺ above N 1s IP
	RD&93	396-420	P	74 meV fwhm; vibrational details of 3 π^* 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
(NO cont'd)	FM&96	410-500	E	Auger-ion coincidence; low-lying NO ⁺⁺ states identified
	F97	399	T	de-excitation spectrum of π^* 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 π^* ; C s filtered; separates 2 Δ , 2 Σ^+ 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 π^* ; CIS filtered; separates 2 Δ , 2 Σ^+ states
	YOW01	399-401	T	excitation energies and potential curves for π^* states
	JW&02	412,420	P, T	fixed-in-space PES; COLTRIMS; circular dichroism at shape resonance, MS , RPAE calc
NO ⁻	HA&04	410-425	P,T	multiple-specific shape resonance, PE ang. dist., partial wave analysis
NO ₂	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 ₂ , NaNO ₂ (sol); $\delta(\pi-\sigma)$ correlated with R(NO)
	SCC77	400-412	P,T	photographic, Z+1 analogy calc., cont. shape res.
	SSH84a	420	T	σ^* -res./bond length relationship - inconsistent
	BS87	380-430	E	high res.
	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	Δ SCF; core hole localisation; gen. rules for MO shifts in 2nd row
N ₂	GT&03b	398-426	P	angle resolved ion spectra; high-res; spectral assignments
	M38	350-450	P	photographic; second gas phase XAS
	NS&69	400-412	P	photographic, 0.03A res., Z+1 analogy
	WSB70	390-420	E	ionic fragmentation (N ⁺ , N ²⁺ yields); FIRST ISEELS SPECTRUM
	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
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)
(N ₂ cont' d)			
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 ₂ , NO & O ₂ , 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.; ³ 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 ⁻ ion spectra, DES at 401 eV
GN&83	400-440	P,T	comp. of core & valence cont. shapes
HH&83	395-430	P	N ⁺ yield from solid N ₂ surfaces, comp. to gas, e ⁻ 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 ₂ , NO, N ₂ O, comp. to theory (RO79)
HS&84	385-430	E	apparatus paper for Auger-energy loss coincidence
K84	399-402	E	³ π; comp. to E(³ π- ¹ π) in CO, CO ₂ , 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 $\pi^*(0.055\text{eV FWHM})$
	BS85	400-415	T	absolute; pol.-propogator, allowed, forbidden, double excit.
	MR&85	399,401	E	ang. dist. of ${}^1\pi$ & ${}^3\pi$ elastic res., l=3 demonstrated
	RL&85	400-430	P	comp. of multilayer PSID & ISEELS; comp. of CO, N ₂ , NO, N ₂ O
	RO85	400	T	π^* GOS, quadrupole transition, constant for N ₂ ,NO,N ₂ O
	UT85	401,416	E	autoionization & Auger decay by (e,2e)
	VA&85	400-440	P,R	comp. of BF ₃ , N ₂ , NO ₃ ⁻ , shape resonances
	YPM85	410-436	T	ab initio, complex basis, coupled channels, comp. to (RL77, LM84)
	SS86b	395-435	P	N ⁺ , N ₂ ²⁺ yields, partial spectra as function of ion kinetic energy
	CF&87	400	E	GOS, constant for π^* in N ₂ , NO, N ₂ 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; σ^* due to neighbor, π^* = 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-> π^* OS - 0.21(2)
	AVZ88	398-480	P	absolute; comp. of NH ₃ , N ₂ , Ne re osc. dist of discr/cont.; relates π^* to atomic 2p resonance; f(π^*)=0.12
(N ₂ cont' d)	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 ₂ (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 π^* 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- excit'n
	H89	380-440	E,R	review of electron-beam core excitation spectroscopies (Aussois)
	PK&89	385-435	P	dispersed-FL detn. (CIS); vibnlly-sensitive; σ^* & cont. enhanced
	SG&89	410-430	T	σ^* shape res.; pos. & shape as f(R); approx. cyl. well & ab initio
	SS89b	390-430	P	ion kinetic E; ion β 's; small +ve β value at σ^*
	SS89c	390-430	P	partial ion yield; KE dist'n; analysis of dissoc. paths
	SS&89	401	P	N ⁺ KERD; apparatus (grasshopper mono); π^* β (-0.7)
	YM&89	395-435	P	absolute, total ion yield; ion β ; N ₂ ²⁺ KERD
	BS90	410-500	P,R	satellite X-sections; comp. to CO
	CS90	398-424	P	50 meV fwhm; π^* , Ryd. vib'n; 2e-; Z+1 tested
	DQB90	399-403	E	σ -resonance in ${}^1\pi$ excitation; ${}^3\pi$ - ${}^1\pi$ branching ratio as f(Eo)
	ED&90	399	P	DES, dynamic screening effects; comp. of N ₂ , N ₂ O & azabenzenes
	H90a	395-425	E,R	absolute, comp. of N ₂ , NH ₃ , N ₂ H ₄ , Ne; σ^* vs. Ryd
	HMS90	392-439	P	ZEKE; ZEK-ion coinc.; huge N ₂ ⁺ 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.; β -s; comp. to theory (RO85)
	PV&90	395-415	P,T	XANES-MS calc.; comp. to expt [ZAV87]; $\delta(R)$ of σ^* shape res.
	S90b	398-430	R,P	ionic fragmentation; ion KERDs; ang. dist.
	SU&90c	390-440	P	total ion yield; mol. orient. (N ⁺ +N ²⁺); β : (-1 at π^* , +1 at σ^*)
	BB91	0-1000	E	GOS and sum rules; experimental methods reviewed
	L91	410-430	T	β -param; comp. to expt. [YM&89]; frozen versus relaxed core
	LAL91	400-420	T	CNDO, systematic treatment of σ^* 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-X α of edge; EXAFS of low-Z; comp. to HB80a
	BB92	41-850	E	generalised osc. str.; $f_{\text{opt}}(\pi^*)=0.19$; comp to calc (CF&87, BNH92)
	BNH92	402	T	OOS&GOS - dipole&quad.; $f_{\text{opt}}(\pi^*)=0.20$; GOS comp (CF&87, BB92)
	DM&92	400-403	P	high res. (80 meV); 2nd order
	ER&92	401-410	P	DES of π^* , 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 $^+$ luminescence (excited frags.)
	LD&92	400-440	P	ion yield, N $^+$ 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 $_3$, N $_2$ H $_4$, N $_2$; $\sigma^*(N-N)$; high res.; vibn'l struct.; Ryd.
	SU&92a	395-445	P	total ion; symmetry-resolved states from N $^+$ 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 ($f^{(1)}(E)$)
	M93	400-403	P	50 meV fwhm resolution
	ODF93	400-420	T	many body CI; Δ SCF; comp to NiN $_2$; 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; $120 < \Gamma < 132$ 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
(N $_2$ cont' d)	DRK94	398-402	P,R	SX700 high res. studies; vibrational structure in small molecules
	LB&94b	399-433	P	10^4 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 $_2$ and O $_2$
	S94	802	T	doubly K-excited & K-ionized states predicted; Δ SCF 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 vibrnlly-resolved PEY, PSD of multilayer N $_2$ /Pt(111); desorption dominated by ultrafast, directly repulsive N $_2^+$ states
	MBN95	410	T	core hole localisation is 78%; comp to CO $_2$ (60); C $_2$ H $_4$ (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.; β s; width=103(10) meV; comp. to calc; vibnl 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 $_2^{K^*}$ 6 N + N $^+$ + e ; (Z+1) calc for N $^{K^*}$
	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; comp. of π - σ sep. in CO, C ₂ H ₂ , C ₂ H ₄ , N ₂ , O ₂
STS96	398-420	T	analytical treatment of SR for diatomics (constant chemical potential); bond length determination; N ₂ and O ₂
SCT96	420-440	T	core-valence double ionisation; ¹ π , ³ π states; comp. of CO, H ₂ CO, N ₂
BN97	360-450	T	comparison of N ₂ , quark-N ₂ (+1/3N-N(-1/3)); 1/3 charge shifts ~40 eV
JA&97	400-403	P	relative; 32 meV; E/ Δ E ~ 12500
KA&97a	403-418	P	comp. of gas-sol; pol. dep.; bulk excitons by e- TOF; N ₂ , 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 σ^* resonance; (pf) coherent interfer; comp to CO ₂
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 π^* ; int. coupling; vibronic
PK&99a	400-403	P	CIS at π^* ; vibration resolved; 160 mV total; participator decay
PK&99b	400-403	P,T	relative; high res; π^* AI as f(v); resonant Raman; detuning; vib. interfer.
PV&99	400-415	P	π^* 115(4) & Ryd [3s 113(5), 3p 107(5), 4s 112(5)] lifetime widths
CS&00	410-445	P,T	RPA; $\sigma_g \rightarrow \sigma_u$, $\sigma_u \rightarrow \sigma_g$ coupled; fixed-in-space β ; comp. SA&95c
NK&00	404-420	P,T	Auger partial yield (384 eV); 2e in discrete (406,407); PEY removes Ryd., σ^* , single ioniz.
PF&00	400-403	P,T	resonant Auger; vibrational excitation dependent; bond length effects
PR00	390-440	P,T	relative; molecule, cluster, solid comparison; (N ₂ Ar) _n mixed clusters; claims shape resonance changes in clusters
SH&00	400-402	P	TIY, PIY, PIPICO; lifetime-vibration effects; comp. of CO & N ₂
SP&00	398-425	P	SB7 LURE beamline tests; Δ E/E > 8500
SR&00	400-402	P	TIY; (PES, Auger) coincidence at π^*
YH&00	399-403	P	TEY, resolution test of CSRF-SGM
AD&01	399-401	E,T	threshold ejected electron spectra of ¹ π , ³ π , DW calc.
HK&01	390-445	P	σ_g^{-1} , σ_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
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, π^* 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 ₀ < 1000 eV, 90°; X-sect differ from SK&84, autoionization of ³ 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^+) coinc peak at threshold, polarization dep. Of autoionization electrons
	BF15	903	P,T	double core hole (DCH) PES&Auger; compare CO, CO ₂ , N ₂ , N ₂ O
	PN&15	836,901	P	1-site, 2-site double core hole IP (ts-DCH), SR, not FEL, coincidences
	TKU15	836	T	(XH _m -YH _n) X,Y = C,N,O,F; m,n = 0-3 – 2-site double core hole IPs
(N ₂) _n	R92	390-460	P	PIY,PEPICO, KER; clusters up to n=30; comp. to N ₂ molecule
	FP&01	399-412	P	cluster-gas comparison, small shift in π^* ; Ryd-exciton shift
N ₂ Ni	DCT98	401	T	partial localized core hole; comp to N ₂ /Ni(100) NEXAFS; XPS ang. effects
N ₂ 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-> π^* thresh. observed
	SK&83	390-410	E	dipole forbidden transition
	CF&84a	400	E	GOS, constant for π^* in N ₂ , NO, N ₂ O, comp. to theory (RO79)
	SSH84a	420	T	σ^* -res./bond length relationship - inconsistent with
(N ₂ O cont 'd)	RL&85	400-430	P	comp. of multilayer PSID & ISSELS; comp. of CO, N ₂ , NO, N ₂ O
	RO85	400	T	π^* GOS, quadrupole transition, constant for N ₂ ,NO,N ₂ O
	MN&86	380-460	P	total & partial ion yields, comp to HBW79
	SKR86	395-408	E	high res (65 meV), triplets observed, $E(\pi^*\pi)=0.7,0.9\text{ eV}$
	CF&87	400	E	GOS, constant for π^* in N ₂ , NO, N ₂ O, comp. to N ₂ calc (RO79)
	HK87	397-407	E	triplet states (1s _C =0.98 eV, 1s _T =0.65 eV)
	PL&87	390-430	T	shape-resonance bond length refutation
	GC&88	400-550	P,T	absolute; partials, βs, N1s (C), N1s(T) comp. to expt (main line 420-450); chemical effects on β at σ^* res.
	H89	390-440	E,R	review of electron-beam core excitation spectroscopies (Aussois)
	LE&88	390-400	P,T	DES at (N _T , π^*), (N _C , π^*); spectator & participator lines
	SG&89	410-430	T	σ^* shape res.; pos. & shape as f(R); approx. cyl. well & ab initio
	ED&90	399	P	DES, dynamic screening effects; comp. of N ₂ , N ₂ O & azabenzenes
	H90a	395-425	E,R	absolute, comp. of N ₂ , NH ₃ , N ₂ H ₄ , Ne; σ^* vs. Ryd
	H90b	398-405	P	ionic frag. at N _T ,N _C -> π^* ; comp. to O1s-> π^*
	HB&90	398-435	P	total ion; ZEKE; MS at N _T ,N _C -> π^* and ZEKE peaks (very different)
	HM&90	400	P	M ₂₊ (Auger-selected) multiple ion coinc. (ERAEMKO)
	LLM90	390-450	P	total ion; PIPICO; PEPIPICO; frag. dynamics; 1- vs. 2-step
	LAL91	400-420	T	CNDO, systematic treatment of σ^* energies
	MC&91	399-412	P	50 meV fwhm; Ryd. vib'n; intensities unusual
	PBV91	390-430	T	MS; comp.to expt; dev. from δ(R)
	SK&91	412-460	P,T	absolute; N _C , N _T ; ab initio calc; shape res. in partials
	SL&91b	423	P	multi-coincidence PEPIPICO; 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	ΔSCF; core hole localisation; gen. rules for MO shifts in 2nd row
	BSS93	396-436	P	PEPICO-, PIY-, PIPICO-yield, β; comp. of β for N ₂ , NO, N ₂ O, O ₂
	LL&93	390-450	P	PIY, TIY, PEPIPICO at both π^* ; σ^* diss. dynamics
	ML&93	395-425	P	PE2PICO; frag.of N ₂ O, CO ₂ , Fe(CO) ₂ (NO) ₂

	LH&94	395-445	P	(zeke, Auger) coinc; small threshold signal rel. to 'normal'; chemically sitt selective Auger
	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 ΔSCF-CI; symmetry resolved ion yields; Renner-Teller; Ryd.-val. mixing; σ^* identified; large bending in π^*
	F95	399	T	de-excitation spectrum of π^*
	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 _T ,N _C 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 ⁻ 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
N ₂ O ₂	BF15	902	P,T	double core hole (DCH) PES&Auger; compare CO, CO ₂ , N ₂ , N ₂ O
	PT&95	395-450	P,T	(NO) ₂ ; multilayer NEXAFS; DFT calc; low-lying $\sigma^*(N-N)$ consistent with long bond (2.24 Å); 1.5 eV fwhm resol.
(N ₂ O) _n	R92	390-460	P	PIY,PEPICO, KER; clusters up to n=20; comp. to N ₂ molecule; asymmetric charge fragmentation
	TT&05	401.1	P	PIY, TOF-PIMS, PEPICO, KERdissociation mechanisms, $\langle n \rangle$ up to 16

Oxygen 1s (535 eV)

BHO	EH99	525-560	E,T	absolute; transient from H ₂ S+B+SiO ₂ ; comp of HBO, HBS, H ₃ B ₃ O ₃
	HE&01	525-560	E	absolute; transient ISEELS
B₃H₃O₃	EH99	530-560	E,T	absolute; from H ₂ O+B; comp of HBO, HBS, H ₃ B ₃ O ₃
B ₅ C ₁₉ FeH ₁₇ O ₂ P	HLD91	520-560	E	Cp(CO) ₂ FeB ₅ H ₂ PBz ₂ , phosphaboranes
BrC₅MnO₅	HSW89	525-570	E	Mn(CO) ₅ Br, comp. to Mn(CO) ₁₀
	HWR90	525-560	E	absolute; comp. of TM carbonyls; f(π^*) as f(backbond)
CCl₂O	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); π^* osc. str.; comp. of Cu-CO clusters
CCu ₁₇ O	YA&97	534	T	Cu ₁₇ (CO); π^* osc. str.; comp. of Cu-CO clusters
	PA&96	530-580	T	absolute, STEX; comp. of CO, Cu ₁₇ CO, Cu ₅₀ Co; models of CO/Cu(100)
CCu ₅₀ O	YA&97	534	T	Cu ₅₀ (CO); π^* osc. str.; comp. of Cu-CO clusters
	PA&96	530-580	T	absolute, STEX; comp. of CO, Cu ₁₇ CO, Cu ₅₀ Co; models of CO/Cu(100)
CD ₂ O	RD&92	528-540	P	high res. isotope effects
CDH ₃ O	AM&05	526-542	P	TIY, PIY, state-selective frag, isotope effects
CFHO	IH87	525-575	E	HCOF, formyl fluoride, comp. to HCOOH, HCONH ₂
	RI&88	525-575	E	C-F σ^* res., absolute, perfluoro effect
	SLD95	534	T	absolute, DF-LCAO; OS for C1s, O1s → π^* ; orbital mapping
	HC96	531	T	DFT; ${}^3\pi^{-1}\pi = 0.34$ eV
CF₂O	RI&88	525-575	E	C-F σ^* res., absolute, perfluoro effect
	SLD95	534	T	absolute, DF-LCAO; OS for C1s, O1s → π^* ; orbital mapping
	HC96	531	T	DFT; ${}^3\pi^{-1}\pi = 0.32$ eV
CF₃NO	HIR89	525-575	E	absolute

	PV&93	530-550	T	quasi-atomic calc; short-range order (bond length) correlation
CF₄O	IM&87	525-575	E	absolute OS low-lying $\sigma^*(O-F)$
CH ₂ O	HB80b	525-565	E	formaldehyde; cont. res., Z+1 analogy
	SSH84a	540	T	σ^* -res./bond length relationship
	RI&88	525-575	E	C-F σ^* res., absolute, perfluoro effect
	SBT88	529-537	T	absolute, ab initio, weak Ryd., comp to HB80b
	SG&89	535-550	T	σ^* shape res.; pos. & shape as f(R); approx. cyl. well & ab initio
	LAL91	530-550	T	CNDO, systematic treatment of σ^* energies
	RD&92	528-540	P	high res. isotope effects
	S92	530-570	E,T,R	MS-X α ; comp. of CO, H ₂ CO, CH ₃ 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 ₂ CO, N ₂
	YA&96	520-560	T	absolute; STEX; comp. of R ₂ CO; comp. to expt.
	YA&97	520-560	T	absolute; STEX; comp. of R ₂ CO; comp. to expt.
	TPA98	525-570	T	absolute; DFT vs. STEX, compares CO and R ₂ 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
CH ₂ O ₂	IH87	525-575	E	(formic acid), $\sigma^*(C-O)$
CH ₃ NO	IH87	525-575	E	HCONH ₂ , formamide, comp. to HCOOH, HCOF
CH ₃ NO ₂	VA&92	280-750	P	absolute; analysed as (CH ₃ ⁺ , NO ₂ ⁻); bond length corr.
	PV&93	530-550	T	quasi-atomic calc; short-range order (bond length) correlation
CH₄N₂O	UH&95b	528-550	E,T	(NH ₂) ₂ CO, urea; absolute; EHMO; modelling of polyurethane
CH ₄ O	WB74b	525-570	E	(CH ₃ OH - methanol) res. at thresh.
	SSH84a	540	T	σ^* -res./bond length relationship
	YKS87	500-950	P	EXAFS; comp. of CO, CO ₂ , COS, Me ₂ CO, CH ₃ OH, EtOEt, furan, C ₈ H ₈ O ₂
	IH88	525-570	E	absolute OS, used to test spectral additivity in methyl formate
	LAL91	530-550	T	CNDO, systematic treatment of σ^* energies
	S92	530-570	E,T,R	MS-X α ; comp. of CO, H ₂ CO, CH ₃ 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 ⁻ 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
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(π^*)=0.13
	SLD95	534	T	absolute, DF-LCAO; OS for C1s, O1s $\rightarrow \pi^*$; orbital mapping
CO	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 π^*)
	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
	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, π^*) comp. to expt (HB80a)
	TS&83	540-630	P	absolute, cont. cross-sections, β values
	UT83	530-540	E	search for triplet (1s, π^*), not seen at $E_0=650\text{eV}$
	ZMP83	520-580	E	appearance pot.s, π^* at 536.2
	AA84	530-555	T	ab initio, CI, all one & two-electron transitions, osc.str.
	JH&84	529-539	P	e^- 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 (π^*)
	SSH84a	540	T	σ^* -res./bond length relationship
	TL&84	535-690	P	Auger, PES X-sections, β 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--> π^* , comp. to IPES, NiCO, sensitive to R(Ni-C)
(CO cont'd)	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 σ^* , comp to val, C1s ionization
	CT89	534	E	DES by (e,2e); CO, CO ₂ & COS similar O K-hole decay; atomic?
	SG&89	535-550	T	σ^* 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) ₄
	DX&90	532-543	P	85 meV fwhm; π^* vib'n (weak but there !!)
	HWR90	525-560	E	absolute; comp. to TM carbonyls; f(π^*) 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 ₂
	LAL91	530-550	T	CNDO, systematic treatment of σ^* 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 π^* vibrational structure; SX-700(II)
	RS&92a	530-560	P	clusters; PIPICO and TIY spectra
	S92	530-570	E,T,R	MS-X α ; comp. of CO, H ₂ CO, CH ₃ OH; $\sigma^*(C-O)$
	SK&92a	536-560	P	absolute cross-sections and β from PES
	ZZ&92	530-540	T	Δ 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(π^*)=0.13
	SH&93	525-555	P,T	symmetry resolved spectra using ion ang. dist.
	BSS94	530-560	P,T	ion- β ; -0.8 at π^* , +0.5 at σ^* ; 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
	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 σ^* 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 ₁₇ CO, Cu ₅₀ Co; models of CO/Cu(100)
	SCT96	550-570	T	core-valence double ionisation; $^1\pi$, $^3\pi$ states; comp. of CO, H ₂ CO, N ₂
	YA&96	520-560	T	absolute; STEX; comp. of R ₂ 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; π^* vibrations – 10% ; 2 nd 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 ₂ CO; comp. to expt.
	ZZL97	534-557	T	MS-SCF; comp. to DV-X α using Z+1 and g.s. approaches
	GTM98	534	P,T	Auger resonant Raman; time domain; detuning effects
(CO cont'd)	TPA98	525-570	T	absolute; DFT vs. STEX, compares CO and R ₂ CO, R = H, Me
	BW&99	534	P	PEPICO; Auger-ion coinc; 2-step (C ⁺ ,O ⁺) at π^* ; wall coll. & KERD
	PD&99	532-543	P,T	65 meV fwhm; R(π^*) = 129.1 pm (8 pm longer); MC calc
	PV&99	530-540	P	π^* 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 ⁺⁺ PE curves
	HS&02	541-545	P	anion yield at threshold, high-res – vib'l effects; PCI
	GM&04	525-575	P	TIY, PIPICO, PEPICO, absolute, partial ion & ion pair yields
	MTU04	542-557	P	vibrationally resolved PI X-sections – bond length dependence of SR
	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 ⁻ 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
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
	NH&88	530-560	R	comp. of all edges, ETS, (WB74e), σ^* locations suggested
	CT89	534	E	DES by (e,2e); CO, 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 CO ₂ , COS & 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

CO ₂	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 σ^*
	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 α
	GA&05b	542-570	P, T	AR-PEPICO, comp of S2p, C1s, O1s at selected energies, MS-X α
	WB74a	530-575	E	cont. res.
	L75b	525-560	P	absolute, distorted cont. shape
	VA&75	525-560	P	comp. to O ₂ , C ₂ H ₅ 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, π^*), comp. to expt (WB74a)
	ZMP83	520-580	E	appearance pot.s, π^* at 539.0
	SA&84	520-950	P	absolute, 0.5eV FWHM, compared to WB74a, Z+1 analogy
	SSH84a	540	T	σ^* -res./bond length relationship - anomalous
	TL&84	535-690	P	Auger, PES X-sections, β 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
(CO ₂ cont'd)	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	σ^*_g , σ^*_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, CS ₂ re σ^* locations
	CT89	535	E	DES by (e,2e); CO, 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 CO ₂ , COS & CS ₂ - all edges
	SG&89	535-550	T	σ^* 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 σ^* energies
	VBA91	500-900	T	CI effect on EXAFS; HF-SCF; comp. to (YKS87); forward foc. MS
	S92	530-570	T,R	MS-X α , comp to W74a; $\sigma^*(C-O)$
	SK&92a	536-570	P	absolute cross sections and β '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)
	L94	530,540	T	X-ray emission at π^* , σ^* ; compared to resonant AI
	BM&95	530-540	P	HERMON at SRC; 1e5 resolving power
	BSS95	530-580	P	total and partial ion yields, β 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; β 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 π^* energies (-2 eV detune); vibrinic coupling in SLOW, not-FAST non-resonant processes
	YA&96	520-560	T	absolute; STEX; comp. of R_2CO ; comp. to expt.
	CG&97	530-560	P,T	RIXS, symmetry breaking at π^* 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_2CO ; π^* OS; initial & final state effects
	GG&98a	530-565	P,T	use of X-ray emission as $f(\theta)$ to assign XAS; 541 eV peak is $\sigma(s)$
	MK&98b	530-590	P	absolute; Beers' law absorption; vibn'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 σ^* 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 π^* , Ryd; MC-GMS calc ; strong quadrupole GOS
	SU&00	534-538	P	C^+/O^+ yield; $3s\sigma_g$ enhanced in O^+ ; asymmetry; KERD, RT coupling
	TE&01b	520-580	E,T	GOS at π^* , Ryd; MC-GMS calc indicate strong quadrupole GOS
(CO ₂ cont'd)	K02	530-560	P,T,R	symmetry resolved, high resolution; review
	OS&02	533-570	P	relative, Anion, cation PIY; only O^- at ($C1s^{-1}, \pi^*$); O^- , C^- 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 ($1s^{-1}$, π^*)
	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
	HK&07	530-560	P	relative, O^- 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^+ , O^+ emitters dominate
	KAR12	542	P	XES – PI coincidence at O 1s edge
	SS&12	540	P	Auger-ion-ion coincidence, [Auger, metastable CO_2^{2+}] coinc
	BF15	1173	P,T	double core hole (DCH) PES&Auger; compare CO, CO_2 , N ₂ , N ₂ O.
C ₂ DH ₅ O	AM&05	526-542	P	(CH ₃ CH ₂ OD), TIY, PIY, state-selective frag, isotope effects
C ₂ D ₃ H ₃ O	AM&05	526-542	P	(CD ₃ CH ₂ OH), TIY, PIY, state-selective frag, isotope effects
C ₂ F ₃ HO ₂	RI&88	525-575	E	CF ₃ COOH, absolute, comp. to acetic acid, perfluor effect
C ₂ F ₆ O ₂	H86b	525-575	E	CF ₃ OOCF ₃ , 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)
	RH91	525-560	E	absolute; comp. of peroxides and H ₂ O; low-lying $\sigma^*(O-O)$
C ₂ H ₄ O	HB80b	525-565	E	(CH ₃ CHO - acetaldehyde) cont. res.
	SSH84a	540	T	σ^* -res./bond length relationship
	YA&96	520-560	T	absolute; STEX; comp. of R_2CO ; comp. to expt.
	YA&97	520-560	T	absolute; STEX; comp. of R_2CO ; π^* OS; initial & final state effects
	TJ&99	525-565	P	relative; TIY; participator decay; 2 states in π^*
C ₂ H ₄ O	SB91a	530-555	E	ethylene oxide
C ₂ H ₄ O ₂	IH88	525-575	E	CH ₃ COOH (acetic acid); absolute
	DF&08	525-575	E,T	valence-Rydberg mixed states; vibrational structure; ab initio, Z+1
C ₂ H ₄ O ₂	IH88	525-575	E	HCOOCH ₃ , methyl formate
	JT94b	520-565	P,T	ISEELS as f(resolution); DES by (e,2e); differs from DES of other R-CO
C ₂ H ₅ NO ₂	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

C₂H₅N₃O₂	CG&04	525-555	E	comp. of Gly, Gly-gly, Gly ₃ , gas-solid
	UA&99	520-560	E	biuret; (NH ₂ (CO)NH(CO)NH ₂); absolute
	LC&07	525-565	E,T	comp.of di-carbonyls; charge shifts for fingerprinting, GSCF3
C ₂ H ₆ O	WB74b	530-570	E	(CH ₃ OCH ₃ - dimethyl ether) res. at thresh.
	SSH84a	540	T	σ*-res./bond length relationship
	LAL91	530-550	T	CNDO, systematic treatment of σ* energies
C₂H₆O	VA&75	525-560	P	(CH ₃ CH ₂ 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 ₃ CH ₂ OH), TIY, PIY, state-selective frag, isotope effects
(C ₂ H ₆ O) _n	TY&05	533-545	P	ethanol clusters TIY, PIY
C ₂ H ₆ OS	TB&88	525-555	E	(CH ₃) ₂ S=O, DMSO, comp. to S1s
C₂H₆O₂	HUR92	525-570	E	(CH ₃ O) ₂ CO methyl carbonate; comp. to polymer EELS
C ₂ H ₆ O ₂	EUH98	525-565	E	ethylene glycol; (CH ₂ OH-CH ₂ OH); absolute; comp to PEO
C ₂ H ₈ O ₂	IH07	530-544	T	methanol dimer, relative, Gaussian augmented plane wave (GAPW) - DFT; (-5 to +3 eV errors on 14 small molecules
C ₃ ClH ₅ O	LDN07	528-548	P	epichlorohyrin – CH ₃ (CH-O-CH ₂); TIY, PEPICO, site selective
C₃F₆O	RI&88	525-575	E	(perfluoroacetone), C-F σ* res., absolute, perfluoro effect
C₃H₂O₂	IH88	525-575	E	propionic acid, comp. to solid, absolute, group analysis
C ₃ H ₃ NO ₂	IO&00	525-560	P	absolute; E-selected mass spec; comp to C ₄ H ₅ NO ₂ ; size dep..frag.
	TS&05	520-570	P, T	absolute, StoBE-DFT, N 1s and O 1s
C ₃ H ₄ O	IH88	525-575	E	propionic alcohol, comp. to solid, absolute, group analysis
C ₃ H ₄ O	DF&03	520-560	E	CH ₂ =CH-CHO, acrolein; π* delocalisation; ab initio GAMES
C₃H₄O₂	IH88	525-575	E	acrylic acid, comp. to solid, absolute, group analysis
C₃H₆NO₂	GH01	525-565	E	alanine; absolute; comp of amino acids
C ₃ H ₆ NO ₂ S	PC&98	530-560	T	cysteine; (D-,L-) STEX; comp. of NEXAFS, circ. dichr. of amino acids
C₃H₆N₂O₂	LC&07	525-565	E,T	malonamide; comp.of di-carbonyls; charge shifts for fingerprinting, GSCF3
C₃H₆O	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 ₂ CO; π* OS; initial & final state effects
	TPA98	525-570	T	absolute; DFT vs. STEX, compares CO and R ₂ CO, R = H, Me
	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 ₃ H ₆ O	YA&96	520-560	T	ethylaldehyde; absolute; STEX; comp. of R ₂ CO; comp. to expt.
	YA&97	520-560	T	absolute; STEX; R ₂ 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 ₃ H ₆ O	PL&07	528-542	P, T	methyloxirane CH ₃ -[CHOCH ₂]; TIY; XPS
C₃H₆O	IH88	525-575	E	acrylic alcohol, comp. to solid, absolute, group analysis
C ₃ H ₆ O ₂	IH88	525-575	E	propanoic acid, comp. to solid, absolute, group analysis
C₃H₆O₃	HW&91	525-570	E	dimethylcarbonate; absolute
C₃H₆O₃	H01	525-565	E	lactic acid; Me(CHOH(COOH); absolute
C₃H₇NO₂	UH&95b	525-575	E	NH ₂ CO ₂ Et, absolute; modelling of polyurethane PEELS
C ₃ H ₇ NO ₂	PC&98	530-560	T	alanine; (D-,L-); STEX; comp. of NEXAFS, circ. Dichr. of amino acids
C ₃ H ₇ NO ₃	PC&98	530-560	T	serine; (D-,L-); STEX; comp. of NEXAFS, circ. Dichr. of amino acids
C₃H₈O	IH88	525-575	E	n-propanol, absolute, group analysis

	TH&98	532-543	P	threshold e-; TIY; TPEPICO; triple coinc; isomer study
C ₃ H ₈ O	TH&98	532-543	P	(isoproponol); threshold e-; TIY; TPEPICO; triple coinc; isomer study
C ₃ H ₈ O ₂	EUH98	525-565	E	1,2-propane diol; absolute; comp to PPO
C ₄ H ₄ O	NIH86	525-575	E	(furan)
C ₄ H ₅ NO ₂	IO&99	525-575	P	MeO(CO)CH ₂ CN; absolute; N1s, O1s → π* mass spect; site sel. frag.
	IO&00	525-560	P	absolute; E-selected mass spec; comp to C ₃ H ₃ NO ₂ ; size dep..frag.
	TS&05	520-570	P, T	absolute, StoBE-DFT, N 1s and O 1s
C ₄ H ₆ O ₃	LC&07	525-565	E,T	acetic anhydride; di-carbonyls; charge shifts for fingerprinting, GSCF3
C ₄ H ₆ O ₅	LC&07	525-565	E,T	MeO(CO)O(CO)OMe; di-carbonyls; charge shifts, GSCF3
C ₄ H ₇ NO ₂	LC&07	525-565	E,T	Me(CO)N(CO)Me; di-acetamide; di-carbonyls; charge shifts, GSCF3
C ₄ H ₇ NO ₂	UA&99	525-565	E	ethyl allophanate (NH ₂ (CO)O(CO)OEt); absolute; polymer model
	UH&99	525-565	E,T	ethyl allophanate; absolute; GSCF3; comp. of urethane species
C ₄ H ₈ N ₂ O ₃	GC&03	520-540	E,T	absolute, comp Gly, Gly-Gly; tri-gly(s); peptide bonds; GSCF3
C ₄ H ₈ N ₂ O ₄	CG&04	525-555	E	(glycyl-glycine), comp. of Gly, Gly-gly, Gly ₃ , gas-solid
C ₄ H ₈ O	NIH86	525-575	E	(tetrahydrofuran)
	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 ₄ H ₈ O	YA&96	520-560	T	propaldehyde; absolute; STEX; comp. of R ₂ CO; comp. to expt.
	YA&97	520-560	T	absolute; STEX; R ₂ CO comp; π* OS; initial,final state effects
C ₄ H ₈ O ₂	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 ₄ H ₉ F ₃ O ₃ SSi	UH94a	525-560	E	Me ₃ SiOSO ₂ CF ₃ ; comp of SI-O-X species re inductive, resonance effects
C ₄ H ₁₀ O	IM&87	525-575	E	t-butanol, absolute, comp. to t-butyl peroxide
C ₄ H ₁₀ O	YKS87	500-900	P	(C ₂ H ₅ OC ₂ H ₅ , 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
C ₄ H ₁₂ OSi	UH94a	525-560	E	Me ₃ Si(OMe); comp of SI-O-X species re inductive, resonance effects
C ₄ NiO ₄	CSB90a	525-580	E	Ni(CO) ₄ ; comp. to CO
	HWR90	525-560	E	absolute; comp. of TM carbonyls; f(π*) as f(backbond)
C ₅ FeO ₅	SLD95	534	T	absolute, DF-LCAO; OS for C1s, O1s → π*; orbital mapping
	MSN89	500-650	P	total, partial ion yields; comp to CO, Fe ₂ (CO) ₉
	HWR90	525-560	E	absolute; comp. of TM carbonyls; f(π*) as f(backbond)
	WRH92	525-570	E	absolute, comp. of organo-iron complexes, ligand interaction effects
C ₅ HMnO ₅	SLD95	534	T	absolute, DF-LCAO; OS for C1s, O1s → π*; orbital mapping
	RH89	525-560	E	HMn(CO) ₅
	SLD95	534	T	absolute, DF-LCAO; OS for C1s, O1s → π*; orbital mapping
C ₅ H ₈ O ₂	LC&07	525-565	E,T	Me(CO)Me(CO)Me; di-carbonyls; charge shifts, GSCF3
C ₅ H ₈ O ₄	LC&07	525-565	E,T	MeO(CO)Me(CO)OMe; di-carbonyls; charge shifts, GSCF3
C ₅ H ₈ O	HI88	525-575	E	(1,3-dihydropyran)
C ₅ H ₈ O ₂	CH98	534	T	malonaldehyde (CH ₃ COC=C(OH)CH ₃); DFT; 0.2 eV keto-enol π* shift
C ₅ H ₈ O ₂	CH98	534	T	acetylacetone (CH ₃ COCH ₂ (CO)CH ₃); DFT; 0.2 eV keto-enol π* shift
	YY&99	510-570	P	TIY, PIY, site slective fragmentation; enhanced Me ⁺ , MeCO ⁺
C ₅ H ₁₀ O	LC&07	525-565	E,T	absolute, GSCF3, comp of dicarbonyls
	NIH86	525-575	E	(tetrahydropyran)
	YA&96	520-560	T	diethylketone; absolute; STEX; comp. of R ₂ CO; comp. to expt.
	YA&97	520-560	T	absolute; STEX; R ₂ CO comp; π* OS; initial,final state effects
C ₅ H ₁₁ NO ₂	PC&98	520-560	T	valine; (D-,L-) STEX; comp. of NEXAFS, circ. Dichr. of amino acids
C ₅ H ₁₄ O	UHR95	520-560	E	sec-butyl ethyl ether; absolute
C ₅ H ₁₄ OSi	TC&02	525-565	E	Me ₃ SiOEt; absolute; comp. to vinyl silanes
C ₆ CrO ₆	CSB90	525-575	E	comp. of M(CO) ₆ , M=Cr,Mo,W
	SLD95	534	T	absolute, DF-LCAO; OS for C1s, O1s → π*; orbital mapping
C ₆ H ₄ O ₂	FH92	520-570	E,T	benzoquinone, absolute, EHMO; quinoid effect

C₆H₅NO₂	TUH96	525-565	E	nitrobenzene; absolute; EHMO, comp. to nitroanilines
C₆H₆N₂O₂	TUH96	525-565	E,T	(1,2)-nitroaniline; absolute, EHMO, comp. to aniline, nitrobenzene
C₆H₆N₂O₂	TUH96	525-565	E,T	(1,3)-nitroaniline; absolute, EHMO, comp. to aniline, nitrobenzene
C₆H₆N₂O₂	TUH96	525-565	E,T	(1,4)-nitroaniline; absolute, EHMO, comp. to aniline, nitrobenzene
C₆H₆O	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 ₂)
	PP&00	285	T	MC-SCF Z+1 calc; vibrational structure, XPS better than NEXAFS
C₆H₆O₂	FH92	520-570	E,T	hydroquinone, absolute, EHMO; quinoid effect
C₆H₈O	UHR99	520-570	E	2-cyclohexene-1-one; absolute; conjugation test
C₆H₈O₂	FH94	520-570	E,T	1,2-cyclohexanedione, absolute, conjugation of $\pi^*(CO)$
C₆H₈O₂	FH94	520-570	E,T	1,3-cyclohexanedione, absolute, conjugation of $\pi^*(CO)$
C₆H₈O₂	FH94	520-570	E,T	1,4-cyclohexanedione, absolute, conjugation of $\pi^*(CO)$
C₆H₉N₃O₃	UA&99	520-570	E	trimethyl-isocyanurate; absolute; polymer model
C₆H₁₀O	FH94	520-570	E,T	(cyclohexanone); absolute; comp. to o,m,p-cyclohexanenedione
C₆H₁₀O	UHR99	520-570	E	4-hexene-3-one; absolute; conjugation test
C₆H₁₄O	UH&95a	525-575	E	i-Pr-ether; absolute; model for poly-ol of polyurethanes
	UH&95b	525-575	E	absolute; comp. to diethylether
C₆H₁₆OSi	UH94a	525-560	E	Et ₃ SiOH; comp of SI-O-X species re inductive, resonance effects
C₆H₁₈OSi₂	UH94a	525-560	E	Me ₃ SiOSiMe ₃ ; comp of SI-O-X species re inductive, resonance effects
C₆H₁₈O₃Si₃	UH94a	525-560	E	c-(SiMe ₂ O) ₃ ; comp of SI-O-X species re inductive, resonance effects
C₆MoO₆	CSB90	525-575	E	comp. of M(CO) ₆ , M=Cr,Mo,W
	SLD95	534	T	DF-LCAO; absolute osc. str for C1s, O1s → π^* ; orbital mapping
C₆O₆V	TD&92	525-575	P,E	V(CO) ₆ , absolute
C₆O₆W	CSB90	525-575	E	comp. of M(CO) ₆ , M=Cr,Mo,W
C₇CoH₅O₂	HWR90	525-560	E	CoCp(CO) ₂ ; absolute; comp. of TM carbonyls; f(π^*) as f(backbond)
	RWH91	520-700	E	absolute; comp. to other mixed-Cp, CO species
C₇FeH₆O₃	WRH92	525-570	E	RFe(CO) ₃ , R=butadiene; absol; organo-irons; ligand interactions
C₇H₆O	HUR92	525-570	E	benzaldehyde; comp. to polymer EELS
	RY&92	520-560	E	comp. of small mol. analogs with PET polymer
C₇H₇NO₂	UH&95b	525-575	E	NH ₂ CO ₂ Ph, absolute; modelling of polyurethane PEELS
C₇H₈O	HU97	530-560	E	anisole (Ph-OMe); absolute
C₇H₈O	AM&05	526-542	P	(CD ₃ CH ₂ OH), TIY, PIY, state-selective frag, isotope effects
C₇H₈N₂O	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
C₇H₁₂O₂	LUH97	525-560	E	butyl acrylate; absolute; polymer model
C₇H₁₄O	YA&96	520-560	T	dipropylketone; absolute; STEX; comp. of R ₂ CO; comp. to expt.
	YA&97	520-560	T	absolute; STEX; R ₂ CO comp; π^* OS; initial,final state
C₈Cl₂H₄O₂	HUR92	525-570	E	terphthalyl chloride; comp. to polymer EELS
	RY&92	520-560	E	comp. of small mol. analogs with PET polymer
C₈Co₂O₈	HWR90	525-560	E	Co ₂ (CO) ₈ ; absolute; comp. of TM carbonyls; f(π^*) as f(backbond)
	RWH91	520-700	E	absolute; comp. to mixed-Cp, CO species
C₈F₃C₆H₄NO	IO&99	520-565	P	p-CF ₃ C ₆ H ₄ NCO; TIY; N1s, O1s → π^* frag.; no site selectivity
C₈H₆O₂	HUR92	525-570	E	terphthaldehyde; comp. to polymer EELS
	RY&92	520-560	E	comp. of small mol. analogs with PET polymer
C₈H₉NO	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
C₈H₉NO₂	GH01	520-560	E	phenylalanine, comp. of amino acids
C₈H₁₂O₃Si	TC&02	520-560	E	(CH ₂ =CH)Si(OAc) ₃ ; absolute; vinyl silanes
C₈H₁₈O₃Si	TC&02	280-320	E	(CH ₂ =CH)Si(OEt) ₃ ; absolute
C₈H₁₆O	UHR92	525-575	E	sec-But-ether, absolute; modelling of polyurethane PEELS
C₈H₁₈O₂	IM&87	525-575	E	t-Bu-O-O-t-Bu, absolute, low lying $\sigma^*(O-O)$
	RH91	525-560	E	absolute; comp. of peroxides and H ₂ O; low-lying $\sigma^*(O-O)$

C₈H₂₄O₄Si₄	UH94a	525-560	E	c-(SiMe ₂ O) ₄ ; comp of SI-O-X species re inductive, resonance effects
C ₉ CrH ₆ O ₃	W92	520-560	E	BzCr(CO) ₃ , absolute
	WHR92	520-560	E	BzCr(CO) ₃ , absolute
C₉FeH₈O₃	WRH92	520-560	E	CxFe(CO) ₃ ; comp. of Fe(CO) ₅ , RFe(CO) ₃ , Fe(Cp) ₂ ; mix. lig. effect
C₉Fe₂O₉	MSN89	500-650	P	total, partial ion yields; comp to CO, Fe(CO) ₅
	WRH92	520-560	E	CxFe(CO) ₃ ; comp. of Fe(CO) ₅ , RFe(CO) ₃ , Fe(Cp) ₂ ; mix. lig. effect
C ₉ H ₅ O ₄ V	WHR92	525-550	E	cyclopentadienyl vanadium tetracarbonyl
C₉H₆N₂O₂	UHR99	520-560	E,T	2,4-TDI, absolute; isomeric effect
C₉H₆N₂O₂	UHR99	520-560	E,T	2,6-TDI, absolute; isomeric effect
C₉H₇MnO₃	W92	520-560	E	Me-CpMn(CO) ₃ , absolute
C ₉ H ₈ O ₂	LUH97	520-560	E	vinyl benzoate; absolute; model for PET X-ray damage
C₉H₁₀O₂	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
C₉H₁₁NO₂	UH&95b	525-575	E	Ph-NHCO ₂ Et, absolute; modelling of polyurethane PEELS
C₁₀ClCo₃O₉	HM&93	525-560	E,P	Cl-C-[Co(CO) ₃] ₃ , abs.; gas(E,P-ions), sol(P); PIPICO, TOF-MS
C ₁₀ CrH ₈ O ₃	W92	520-560	E	CH ₃ -BzCr(CO) ₃ , absolute
	WHR92	520-560	E	absolute
C₁₀H₁₀O₄	UH&96	525-545	E,T	p-dimethylphthalate (MeO ₂ C-C ₆ H ₄ -CO ₂ 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
C₁₀H₁₀O₄	UH&96	525-545	E,T	o-dimethylphthalate (MeO ₂ C-C ₆ H ₄ -CO ₂ 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
C₁₀H₁₀O₄	UH&96	525-545	E,T	m-dimethylphthalate (MeO ₂ C-C ₆ H ₄ -CO ₂ 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
C₁₀H₁₃NO₂	UH&95b	525-575	E	Ph-N(CH ₃)-CO ₂ Et, absolute; modelling of polyurethane PEELS
C₁₀H₁₉O₄	LC&07	525-565	E,T	'BuO(CO)NH(CO)O'Bu; di-carbonyls; charge shifts, GSCF3
C₁₀Mn₂O₁₀	HSW89	525-570	E	Mn ₂ (CO) ₁₀ , absolute, comp to CO, Mn(CO) ₅ Br
C₁₁Co₃H₃O₁₀	HM&93	525-560	E,P	CH ₃ O-C-[Co(CO) ₃] ₃ , abs.; gas(E), sol(P)
C₁₁FeH₈O₃	WRH92	525-570	E	RFe(CO) ₃ , R=COT; absolute, organo-irons; ligand interactions
C₁₁H₁₄N₂O₄	UHR99	525-570	E	TDI-bis-methyl urethane; absolute
C₁₂H₁₀O₃	HUR92	525-570	E	(BzO) ₂ CO phenyl carbonate; comp. to polymer EELS
C ₁₂ H ₁₈ O	LL&14	530-545	T	diphenylether, TIY, TD-DFT (Q-CHEM-4.1)
C₁₂H₁₅N₂O₂Re	HS92	520-560	E	Cp*Re(CO) ₂ N ₂ , absolute
C ₁₂ O ₁₂ Ru ₃	SF&90	520-560	P	relative, TEY; comp. to free CO; relaxation d(R) effects
C₁₃H₁₂N₂O	UH&95b	525-575	E	Ph-NH ₂ C=O; absolute; modelling of polyurethane PEELS
C ₁₃ H ₁₅ MnO ₃	WRH89	520-570	E	Cp*Mn(CO) ₃ ; absolute
C ₁₄ H ₁₀ O ₃	LUH97	520-560	E	benzoic anhydride; absolute; polymer model
C₁₅H₂₄O	LUH97	520-560	E	butylated hydroxy toluene; absolute; polymer model
C ₁₈ H ₁₄ O ₂	LL&14	530-550	P,T	1,3-diphenoxylbenzene, TIY, TD-DFT (Q-CHEM-4.1)
C₁₈H₁₆OSi	UT&97	520-560	E	triphenylsilanol; absolute; Si-Si, Si-O-R systems
C₂₁H₁₅N₃O₃	UHR92	520-560	E	(Bz-O)C ₃ N ₃ , triphenoxyl-triazine; polyurethane modelling
	UA&99	520-560	E	tritylisocyanurate; absolute, polymer model
C₂₄H₂₁N₃O₃	UA&99	520-560	E	tritylisocyanurate; absolute, polymer model
Cl ₃ OP	SB85d	525-600	E	pot. barr. effects
ClO ₂	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 ₂ O	RR&83	525-575	P	D ⁺ yields from sol; gas, solid, EY comp; extra peak at 560eV

F₂O	KP94b	530-540	T	ab initio DSCF-CI; vibrational analysis; comp. of H ₂ O/D ₂ O
F ₃ OP	IM&87	530-570	E	absolute; comp. to H ₂ O; conj. val.- Ryd. obsv'd; strong σ*(O-O)
HO	SB85d	525-600	E	pot. barr. Effects
H₂O	SRA02	525-528	P	high res.; comp. of vib'n & Ryd of OH,OD; v. low E (526eV)
	WB74b	530-575	E	weak cont. features
	WB74g	530-540	E	Z+1 analogy (H ₂ 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 ₃ ,CH ₄ ,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 ₂ O, H ₂ O) (s), comp. to gas (WB74b), O Auger yield,, residual Rydbergs, EXAFS, O ⁺ yield follows O _K -cont.
(H ₂ O cont'd)	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 ₂ 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 ⁺
	MR&90	520-570	P	ion desorption (H ⁺); comp. to AEY, gas EELS (WB74b)
	RC&90	520-570	P	comp. of gas, solid; ion yields, H ⁺ ultrafast diss.
	LAL91	530-550	T	CNDO, systematic treatment of σ* energies
	RH91	525-560	E	absolute; comp. of peroxides and H ₂ 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 ⁺ , OH ⁺ , O ⁺ , O ⁺⁺); comp. to PSID of 10 L H ₂ O/Si(100)
	M93	532-542	P	partial ion yields (H ⁺ , OH ⁺ , O ⁺ , O ⁺⁺)
	ST&93	533-540	P,T	(120 mV); ab initio SCF(ADC); no resolved vib; comp of H ₂ O, NH ₃ , CH ₄ re Ryd/val char.NH ₄ ; ultrafast dissociation; abs. osc. str. calc.
	KP94b	530-540	T	ab initio DSCF-CI; vibn=l analysis; comp. of H ₂ O/D ₂ 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 ⁺ , O ²⁺ , O ³⁺); comp. to PSID for H ₂ O/Si(100); no ultrafast H ⁺ ; first PIPICO at a surface (O ⁺ ,H ⁺)
	HP&98	532-534	P	reosnant Auger coinc. with OH ⁺ , H ₂ O ⁺ , ultrafast decay
	PH&99	531-542	P	TIY, PIY, PE3PICO; H ²⁺ from 2b ₂ ; H ^o at 4a ₁ ; ultrafast; 170 meV
	PK&99c	532-540	P	reosnant Auger; non-linear dispersion; potential curves; no ultrafast
	RB99	530-534	T	absolute; GOS; 4a ₁ 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 ₂ ⁺ formation at 2b ₂ ; (from PH&99)
	SS&03	528-550	P	TIY, partial ion yields, O ⁻ yield; deduce O [*] H ⁻ decays radiatively
	KC&06	533-542	P	TIY, Lyman-α 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

(H ₂ O) _n	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)
H₂O₂	RH91	525-560	E	absolute; comp. of peroxides and H ₂ O; low-lying σ*(O-O)
	TV93	530-540	T	ab initio-SCF-EICVOM; pre-edge res. (π^* , σ^*_{O-O} , σ^*_{S-S}); comp. RH91
H ₄ O ₂	IH07	530-544	T	water dimer, acceptor & donor, relative, Gaussian augmented plane wave (GAPW) - DFT; (-5 to +3 eV errors on 14 small molecules
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 ₂ , NO & O ₂ , 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 ₂ , NaNO ₂ (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 ₃ ⁻ , NO ₂ ⁻ , 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)
(NO cont'd)	SS91	526-556	P	TEY; partial ion yields; KER at π^* ; ion b-param
	CT92	532	E	DES by (e,2e); U _{C,V} 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-CI; 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
	YHA05	520	P, R	ion angular dist; fixed-molecule PAD spectra, review
NO ₂	SCC77	530-541	P,T	photographic, Z+1 analogy calc.
	SSH84a	540	T	σ*-res./bond length relationship, anomalous
	BS87	530-570	E	high res.
	JC02	525-555	P,T	relative, Gaussian94 calc (Z+1)
	GT&03b	525-555	P	angle resolved ion spectra; high-res; spectral assignments
N ₂ 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	σ*-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	σ* shape res.; pos. & shape as f(R); approx. cyl. well & ab initio
	H90b	535	P	ionic frag. comp to N _T , N _C -> π^*
	PBV91	520-560	T	MS; comp.to expt; dev. from d(R)
	SK&91	540-600	P,T	absolute; comp to N _C , N _T ; ab initio; O 1s like N _C ; E(σ*) 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 ₂ , NO, N ₂ O, O ₂
	PV&93	530-550	T	quasi-atomic calc; short-range order (bond length) correlation
	L94	530,540	T	X-ray emission at π^* , σ^* ; comp. to resonant AI
	AK&95a	530-570	P,T	ab-initio DSCF-CI; symmetry resolved ion yields; Renner-Teller; Ryd.-val. mixing; σ^* 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 ₂ , CH ₄ 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
N ₂ O ₂	PT&95	525-570	P,T	(NO) ₂ ; multilayer NEXAFS; DFT calc; low-lying $\sigma^*(N-N)$ consistent with long bond (2.24 Å); 1.5 eV fwhm resol.
O₂				
	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 ₂ , C ₂ H ₅ 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 ₂ , NO & O ₂ , 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	σ^* -res./bond length relationship
	YKS85b	500-1000	P	EXAFS, non-standard phase shifts indicated
	THY86	546	P	luminescence from O ₂ ²⁺ (K*)
	YKS86	500-950	P	EXAFS, corrected for second order radiation
	YKS87	500-550	P	EXAFS; comp. of CO,CO ₂ ,COS,Me ₂ CO,CH ₃ OH,EtOEt;furan,C ₈ H ₈ O ₂
	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	σ^* shape res.; pos. & shape as f(R); approx. cyl. well & ab initio
	SS89a	520-560	P	electron yield; O ⁺ ,O ²⁺ yields; ion b's ($\pi^* = -1$; 3p Ryd = 1.2)
	SS89d	520-560	P	partial IY; ion KERDs; diss. pathways; π^* 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 π^* , σ^* , cont.
	LL&90b	490-590	P	total ion yield; DES at π^* , σ^* and continuum (AI and Auger)
	S90b	525-570	R,P	ionic frag; KERD; ang. dist.
	SS90	531	P	KERD in (O ⁺ ,O ⁺); PIPICO
	SU&90c	520-560	P	total ion yield; mol. orientation param. (-0.8 at π^* ; 1 at both σ^*)
	JJ&91	530-800	T	MS calc; NEXAFS and EXAFS; CO and O ₂
	MC&91	525-560	P	50 meV; Ryd. structure resolved on "exchange split" σ^*
	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 ₋ Auger,ion) coinc.; multi-det; intermediate state ident.
	K92	530-550	R	survey of numerical XANES
	KA&92b	531	P	ion ang. dist. at π^* ; 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 ⁺ , O ⁻ attributed to decay of O ₂ ^{K+}
	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 ₂ on Pt, Ag
	YS92	525-565	P	sym. resolved by ion yield; BOTH features are σ^* ; high res (84 meV)
	HF&93	520-560	E,T	absolute; comp. of ¹ D- ³ S; DSCF-CI calc; magnetic splitting in ³ D
	NR&93	530-545	P	autoionization (DES) used as selective detector of σ^* ; exchange split only 0.6 eV (both σ^* in B)
(O ₂ cont'd)	RAZ93	540-1000	P,T	comp. of MS-Feff with expt.; reproduces σ^* & EXAFS if >13 legs
	SC&93	520-560	P	Auger, autoionization at π^* (530.9), 540 (σ^*), 542 (σ^*), 552 (1s ⁻¹); atomic O ^K decay detected (ultrafast decay)
	NR&94	529-532	P,T	DES at π^* ; lifetime-vib'n interference strong in partials; comp. to CO, N ₂
	YND94	538-570	T	absolute; ab initio Z+1; multi-excitation; comp to (BB&79); strong (1s ⁻¹ ,p ⁻¹ ,p ⁴) 2e- state at 539 eV in σ^* 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; σ^* identified; large bending in π^*
	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 ₂ O (78%), CO ₂ (60), C ₂ H ₄ (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.
	AL&96	529-545	T	STEX; ² S channel only one with exchange split of σ^* ; ⁴ 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 ₂ H ₂ , C ₂ H ₄ , N ₂ , O ₂
	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 ₂ , 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 ¹ 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; ($1\pi_g$) and ($1\pi_u$) participator decay plots; σ^* , $^4\Sigma$, $^2\Sigma$ 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; DCl, HCl-Cl2p; H ₂ S - S2p, O ₂ -O1s)
	GT&03b	536-546	P	high resolution Ryd- σ^* ; BL4B UVSOR-II commissioning
(O ₂) _n	RS&92b	520-560	P	PIY, TIY, TEY of cluster versus molecular O ₂
O ₂ S	AVZ82c	525-555	P	comp. to S2p (VZ71b) & S1s (MB&72) spectra of SO ₂
	TKM82	525-540	T	X-alpha (MSM), comp. to expt (K77)
	B85	525-545	E	high res. (0.09eV FWHM)
(SO ₂ cont'd)	SB&87	525-545	E	high res., comp. to MCQD calc & other edges
	PK&93	500-900	P	EXAFS; comp to SO ₂ (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
O ₃	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 ₂ ; spectral stripped; $2\pi^*$ @ 529.1,535.4 eV; GSCF3
	OK02	530	T	ab initio CI calc, geometry dependence; TDM not aligned aling O-O bonds
	MM&07	528-548	P	relative, TIY, PEPEPICO; PIY; dissociative mechanisms at π^*

Palladium 2p (31.7, 33.3 keV)

C ₆ H ₁₀ Pd	DFL92	3.16-3.17	T	Pd(C ₃ H ₅) ₂ ; absolute; ab initio-SCF-CI; comp. of 3d spectra of 5 TM compounds; supports MO model of edge structure
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Phosphorous 2p (140 eV)

B ₅ C ₁₂ H ₁₈ P	HLD91	130-220	E	Ph ₂ PB ₅ H ₈
B ₅ C ₁₉ FeH ₁₇ O ₂ P	HLD91	130-220	E	Cp(CO) ₂ FeB ₅ H ₂ P(Ph) ₂
Br ₃ P	II&87	130-270	P	PBr ₃ ; absolute, high res. (0.03-0.07 eV)
CCl ₂ F ₃ P	HBC96	130-170	P	CF ₃ PCl ₂ ; absolute; ab initio; TIY,PIY,PIPICO; comp. to PF ₃ ,PCl ₃
	NJ&98	120-170	P,T	absolute; GSCF3 calc.; LS-state; comp of PX ₃ , YPF ₃ . X=Cl,F, Y=O,S)
	NH&03	130-200	P	absolute; TIY, PIY, quantitative fragmentation; comp to (e, e+ion)
C ₃ H ₉ P	SB85c	130-210	E	P(CH ₃) ₃ ; strong cont. res.
	LC&90	125-210	P,T	high res.; MS-Xa; Ryd.; pot. barr. shape res.; PX ₃ (X=H,F,CH ₃)
	HH&98	128-150	E	absolute; comp. of (t-Bu) ₂ PCl, PCl ₃ , PMe ₃
C ₈ ClH ₁₈ P	HH&98	128-150	E	(t-Bu) ₂ Cl; absolute; comp. of (t-Bu) ₂ PCl, PCl ₃ , PMe ₃
Cl ₃ 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 ₅ , POCL ₃ , POF ₃ ; cont. res.
Cl ₃ P	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 _x , SO _x , ClO _x)
	HBC96	130-170	P	absolute; ab initio; TIY, PIY, PIPICO; PE2PICO; PF ₃ , PCl ₃ , CF ₃ PCl ₂ 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 ₃ ⁺ yield; LS-states; GSCF3 ab initio
	HH&98	128-150	E	absolute; comp. of (t-Bu) ₂ PCl, PCl ₃ , PMe ₃
	NJ&98	120-170	P,T	absolute; GSCF3 calc.; LS-state; comp of PX ₃ , YPF ₃ . X=Cl,F, Y=O,S)
	NH&03	130-200	P	absolute; TIY, PIY, quantitative fragmentation; comp to (e, e+ion)
Cl ₃ PS	TKM82	133-143	T	X-alpha (MSM), comp. to expt (K77)
F ₃ P	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 ₃ (X=H,F,CH ₃)	
(PF ₃ cont'd)	VK&92	130-150	P	TEY; res. Auger/AI differ; participator vs. spectator; ultrafast decay
	N95	130-170	T	DVXa; absolute; comp to II&87; bond length corr. (also PO _x , SO _x , ClO _x)
	HBC96	130-170	P,T	absolute; ab initio; TIY, PIY, PIPICO; PF ₃ , PCl ₃ , CF ₃ PCl ₂ comp.
	KB&96	130-150	P,T	TIY vs PF ₃ ⁺ ; ab initio; (LS) state at 136.4 eV - only 2p _{1/2} 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 ₂ ⁺ as well; improved timing
	NJ&98	120-170	P,T	absolute; GSCF3 calc.; LS-state; comp of PX ₃ , YPF ₃ . 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
	KI00	134-140	T	ab initio; spin-orbital Breit-Pauli; molecular field; comp. of SO ₂ , COS, PF ₃
	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 ₃ OP	SB85d	130-210	E	strong cont. res.
	LC&92a	130-180	P,T	relative, high res. (200 meV); comp. of PF ₅ , POCL ₃ , POF ₃ ; cont. res.
	JKC99	134-160	P,T	relative, GSCF3; comp. to NSF ₃
F ₃ 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 ₅ 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 ₅ , POCL ₃ , POF ₃ ; cont. res.
H ₃ 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 ₃ (X=H,F,CH ₃)
	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 _n (X=Si,P,S,Cl)
	U98	131-132	P,R	resonant Auger; ultrafast dissociation

Phosphorus 1s (2155 eV)

Br₃P CJ99 2.14-2.15 P chemical shifts of P1s→1e^{*}; correlation to XPS, Auger

CCl ₂ H ₃ P	CJ99	2.14-2.15	P	chemical shifts of P1s→1e [*] ; correlation to XPS, Auger
CCl ₂ H ₃ OP	CJ99	2.14-2.15	P	chemical shifts of P1s→1e [*] ; correlation to XPS, Auger
CCl ₂ H ₃ OP	CJ99	2.14-2.15	P	chemical shifts of P1s→1e [*] ; correlation to XPS, Auger
CCl ₂ H ₃ PS	CJ99	2.14-2.15	P	chemical shifts of P1s→1e [*] ; correlation to XPS, Auger
C ₂ ClH ₆ PO ₂ S	CJ99	2.14-2.15	P	chemical shifts of P1s→1e [*] ; correlation to XPS, Auger
C ₃ H ₉ P	CJ99	2.14-2.15	P	chemical shifts of P1s→1e [*] ; correlation to XPS, Auger
C ₃ H ₉ O ₄ P	CJ99	2.14-2.15	P	chemical shifts of P1s→1e [*] ; correlation to XPS, Auger
C ₃ H ₉ O ₃ P	CJ99	2.14-2.15	P	chemical shifts of P1s→1e [*] ; correlation to XPS, Auger
C ₃ H ₉ O ₃ PS	CJ99	2.14-2.15	P	chemical shifts of P1s→1e [*] ; correlation to XPS, Auger
C ₆ H ₁₅ P	CJ99	2.14-2.15	P	chemical shifts of P1s→1e [*] ; correlation to XPS, Auger
C ₁₈ H ₁₅ PO ₃	KC&92	2.14-2.19	P,T	(C ₆ H ₅ O) ₃ P; relative, MS-Xa of PO ₃ ³⁻ clusters
C ₁₈ H ₁₅ PO ₄	KC&92	2.14-2.19	P,T	(C ₆ H ₅ O) ₃ PO; relative, MS-Xa of PO ₄ ⁴⁻ clusters
Cl ₃ OP	CJ99	2.14-2.15	P	chemical shifts of P1s→1e [*] ; correlation to XPS, Auger
Cl ₃ P	GDT97	2.14-2.20	P,T	relative; TIY, MS-Xa; pot. barr.; AsCl ₃ , PCl ₃ , GeCl ₄ , SnCl ₄ comp.
	CJ99	2.14-2.15	P	chemical shifts of P1s→1e [*] ; correlation to XPS, Auger
Cl ₃ PS	CJ99	2.14-2.15	P	chemical shifts of P1s→1e [*] ; correlation to XPS, Auger
F ₃ P	CJ99	2.14-2.15	P	chemical shifts of P1s→1e [*] ; 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 ₃ , PX ₃ 1s edges; pot. barr. effects
F ₃ PS	CJ99	2.14-2.15	P	chemical shifts of P1s→1e [*] ; 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 ₃ OP	CJ99	2.13-2.18	P	chemical shifts of P1s→1e [*] ; correlation to XPS, Auger
	NT&99B	2.12-2.20	P	TIY, PIY; PEPIPICO; pol. dep.; selective frag.; cascade processes
F ₅ P	CJ99	2.14-2.15	P	chemical shifts of P1s→1e [*] ; correlation to XPS, Auger
H ₃ P	CJ99	2.14-2.15	P	chemical shifts of P1s→1e [*] ; correlation to XPS, Auger
	JC01	2.14-2.18	P	relative; comparison of NX ₃ , PX ₃ 1s edges; pot. barr. effects
H ₄ P	KNP91	2.14-2.19	T	PH ₄ , SCF-CI in (Z+1); comp. of CH ₄ , SiH ₄ , PH ₄ , NH ₄ K-shell spectra
NiP ₂	DCT98	2.15	T	partial localization of core hole
O ₆ P ₄	KC&92	2.14-2.16	P,T	relative, EXAFS; MS-Xa of PO ₃ ³⁻ ; bond length corr.
	EK&97d	2.13-21.8	P,T	relative; ioniz. yield; comp. of PO _n X cage compounds; DFT
O ₆ P ₄ S	EK&97d	2.13-21.8	P,T	relative; ioniz. yield; comp. of PO _n X cage compounds; DFT
O ₆ P ₄ Se	EK&97d	2.13-21.8	P,T	relative; ioniz. yield; comp. of PO _n X cage compounds; DFT
O ₇ P ₄	EK&97d	2.13-21.8	P,T	relative; ioniz. yield; comp. of PO _n X cage compounds; DFT
O ₁₀ P ₄	KC&92	2.14-2.16	P,T	relative, EXAFS; MS-Xa of PO ₄ ⁴⁻ ; 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) _n	TW&99	3.59-3.66	P	cluster spectra s f(<n>) n = 2 – 18; comp. to KF, solid

Rhenium 4f (42 eV)

C ₁₂ H ₁₅ N ₂ O ₂ Re	30-280	HS92	E	Cπ*Re(CO) ₂ N ₂
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Selenium 3d (60 eV)

C ₄ H ₄ Se	HTB89	50-160	E	(selenophene), comp. to solid
C ₅ H ₆ Se	HTB89	50-160	E	(3-methylselenophene), comp. to solid

SeF ₆	SB90	60-160	E	comp of TeF ₆ , SeF ₆ , SF ₆ ; Z-dependence of pot. barr.s
Se ₂	CM77b	50-160	P	photographic, double excitation, comp. to solid Se

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

SeF ₆	AT&86b	160-210	P	absolute, comp. to SF ₆ , SF ₅ Cl, weak Se 4d cont. res.
	SB90	160-270	E	comp of TeF ₆ , SeF ₆ , SF ₆ ; Z-dependence of pot. barr.s
C₄H₄Se	HTB89	160-210	E	(selenophene), comp. to solid
C ₅ H ₆ Se	HTB89	160-210	E	(3-methylselenophene), comp. to solid

Selenium 1s (12660 eV)

Se ₂	NY&02	12.3-13.9	P	TIY, PEPICO; cluster-size selective EXAFS through PIY; R _{Se-Se} = 2.17
Se ₅	NY&02	12.3-13.9	P	TIY, PEPICO; cluster-size selective EXAFS through PIY
Se ₆	NY&02	12.3-13.9	P	TIY, PEPICO; cluster-size selective EXAFS through PIY; R _{Se-Se} = 2.35
Se ₇	NY&02	12.3-13.9	P	TIY, PEPICO; cluster-size selective EXAFS through PIY

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

Br ₄ Si	PV&79	100-140	T	X-alpha (MSM) calc. of cont. shape
	PDK97	90-120	P	high res.; vibrational structure -> excited geom, SiX ₄ , X=H,D,F,Cl,Br
	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
CCl ₃ H ₃ Si	BL&98	50-450	P,T	relative, TIY, PIY
	FZ&70	102-112	P	MeSiCl ₃ ; pot. barr. effects
	BNZ72	102-112	T	semi-empirical calc., comp. to expt. (FZ&70)
CF ₃ H ₃ Si	BBT90	100-200	P,T	MeSiF ₃ ; 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
	NMK97	100-180	P,R	site-specific fragmentation; comp. to SiMe ₄ ; surface desorption
C ₂ Cl ₂ H ₆ Si	NF&02	1001-20	P	site-specific fragmentation; comp. of X ₃ Si-y-SiMe ₃ , X=F,Cl, y = (C _x H _y) Me ₂ SiCl ₂ ; pot. barr. effects
	FZ&70	102-112	P	semi-empirical calc., comp. to expt. (FZ&70)
	BNZ72	102-112	T	60 meV; comp. to solid; valence/Rydberg char.
	CL&97	102-104	P	SiMe ₂ Cl ₂ , luminescence yield, Si*, Si ⁺ , CH*, H*, excited diatomic
C ₂ F ₂ H ₆ Si	CL&05	103-117	P	Me ₂ SiF ₂ ; relative, 0.15 eV fwhm; Xa; res. incr. with more F
	BBT90	100-200	P,T	relative; TEY, TIY, PA compared; quadrupole-MS PIMS; CH ₃ more labile than F; CH ₃ ⁺ enhanced in discrete res.; F 1s mass spec
	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 ₃ ClH ₉ Si	FZ&70	102-112	P	Me ₃ SiCl; pot. barr. effects
	BNZ72	102-112	T	semi-empirical calc., comp. to expt. (FZ&70)
C ₃ Cl ₃ H ₉ Si ₂	NO&93	100-112	P	Me ₃ Si-SiCl ₃ ; site-specific ionic. fragm.; PEPICO, PIPICO resonant Auger; comp. of SiMe ₄ , SiCl ₄ ; Si ₂ Me ₆ and Cl ₃ Si-SiMe ₃
	NF&02	100-120	P	site-specific fragmentation; comp. of X ₃ Si-y-SiMe ₃ , X=F,Cl, y = (C _x H _y)
C ₃ FH ₉ Si	NE&14	100-120	P	Auger and resonant-PES, electronic basis for site-specific fragmentation
	BBT90	100-200	P,T	Me ₃ 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 ₃ more labile than F; CH ₃ ⁺ enhanced in discrete res.; F 1s mass spec
C ₃ F ₃ H ₉ Si ₂	NF&02	1001-20	P	site-specific fragmentation; comp. of X ₃ Si-y-SiMe ₃ , X=F,Cl, y = (C _x H _y) c-(SiMe) ₃ ; cyclo-polysilanes; ab initio EICVOM calc.
C ₃ H ₆ Si	TWM95	93-100	T	Me ₃ SiOSO ₂ CF ₃ ; comp of SI-O-X species re inductive, resonance effects
C ₄ F ₃ H ₉ O ₃ SSi	UH94a	100-200	E	F ₃ Si(CH ₂)SiMe ₃ ; site-specific frag.; comp. to SiMe ₄ ; surface desorption
C ₄ F ₃ H ₁₁ Si ₂	NMK97	100-180	P,R	site-specific fragmentation; comp. of X ₃ Si-y-SiMe ₃ , X=F,Cl, y = (C _x H _y)
	NF&02	1001-20	P	

C₄F₃H₁₄Si₂	NO&95	100-120	P	CF ₃ SiCH ₂ SiMe ₃ , ionic fragmentation; site specific (SiF ₃ vs. SiMe ₃) partial yields identify chemical shift undetected in absorption
C₄H₈Si	TWM95	93-100	T	c-(SiMe) ₄ ; cyclo-polysilanes; ab initio EICVOM calc.
C₄H₁₂OSi	SK&93b	90-190	P,T	Me ₃ Si(OMe); 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
	UH94a	100-200	E	comp of Si-O-X species re inductive, resonance effects
	WMT94b	95-140	E,T	EICVOM SCF (gamess) calc.; Ryd.-val mix; Me _x Si(OMe) _{4-x} , x=0-4 absolute; Si-Si & Si-O-R
C₄H₁₂O₂Si	UT&97	90-110	P	
	SK&93b	90-190	P,T	Me ₂ Si(OMe) ₂ ; 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
	WMT94b	95-140	E,T	EICVOM SCF (gamess) calc.; Ryd.-val mix; Me _x Si(OMe) _{4-x} , x=0-4
C₄H₁₂O₃Si	SK&93b	90-190	P,T	MeSi(OMe) ₃ ; 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
	WMT94b	95-140	E,T	EICVOM SCF (gamess) calc.; Ryd.-val mix; Me _x Si(OMe) _{4-x} , x=0-4
C₄H₁₂O₄Si	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
	WMT94b	95-140	E,T	EICVOM SCF (gamess) calc.; Ryd.-val mix; Me _x Si(OMe) _{4-x} , x=0-4
C₄H₁₂Si	FZ&70	102-112	P	Me ₄ Si; 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 ₄ Si; 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
	W92	100-150	E	comp. of SiMe ₄ , Si ₂ Me ₆ , Si ₆ Me ₁₂ ; σ*(Si-Si)
	NO&93	100-112	P	site-specific ionic. fragm.; PEPICO, PIPICO resonant Auger; comp. of SiMe ₄ , SiCl ₄ ; Si ₂ Me ₆ and Cl ₃ Si-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 (gamess) calc.; Ryd.-val mix; Me _x Si(OMe) _{4-x} , x=0-4
C₅Cl₃H₉Si₂	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 ₃ Si-y-SiMe ₃ , X=F,Cl, y = (C _x H _y)
	NO99	95-120	P	Cl ₃ SiC:::CsMe ₃ ; TIY, PIY; site specific fragmentaiton
	NF&02	1001-20	P	site-specific fragmentation; comp. of X ₃ Si-y-SiMe ₃ , X=F,Cl, y = (C _x H _y)
C₅F₃H₉Si₂	NF&02	1001-20	P	site-specific fragmentation; comp. of X ₃ Si-y-SiMe ₃ , X=F,Cl, y = (C _x H _y)
C₅F₃H₁₁Si₂	NF&02	1001-20	P	site-specific fragmentation; comp. of X ₃ Si-y-SiMe ₃ , X=F,Cl, y = (C _x H _y)
C₅F₃H₁₃Si	NMK97	100-180	P,R	F ₃ Si(CH ₂) ₂ SiMe ₃ ; site-specific frag.; comp. to SiMe ₄ ; surface desorption
	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 ₃ Si-y-SiMe ₃ , X=F,Cl, y = (C _x H _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
C₅H₁₀Si	TWM95	93-100	E,T	c-(SiMe) ₅ ; cyclo-polysilanes; ab initio EICVOM calc.; expt. comp. to ETS
C₅H₁₄OSi	TC&02	85-220	E	Me ₃ SiOEt; absolute; comp. to vinyl silanes

C₅H₁₅NSi	UH94b	90-200	E	Me ₃ Si(NMe ₂) ₂ ; comp. of Si-N cmpds; models for SiN _x O _y films
C ₆ F ₃ H ₁₅ Si ₂	NF&02	1001-20	P	site-specific fragmentation; comp. of X ₃ Si-y-SiMe ₃ , X=F,Cl, y = (C _x H _y)
C ₆ H ₆ OSi	UT&97	90-110	P	Ph ₃ SiOH; absolute; Si-Si & Si-O-R
C ₆ H ₁₂ Si	TWM95	93-100	E,T	c-(SiMe) ₆ ; cyclo-polysilanes; ab initio EICVOM calc.; expt. comp. to ETS
C ₆ H ₁₆ OSi	UH94a	100-200	E	Et ₂ SiOH; comp of SI-O-X species re inductive, resonance effects
C₆H₁₈Si₂	W92	100-150	E	Me ₃ Si-SiMe ₃ ; comp. of SiMe ₄ , Si ₂ Me ₆ , Si ₆ Me ₁₂ ; σ*(Si-Si)
	NO&93	100-112	P	site-specific ionic. fragm.; PEPICO, PIPICO resonant Auger; comp. of SiMe ₄ , SiCl ₄ ; Si ₂ Me ₆ and Cl ₃ Si-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
C₆H₁₈OSi₂	UH94a	100-200	E	Me ₃ SiOSiMe ₃ ; comp of SI-O-X species re inductive, resonance effects
C ₆ H ₁₈ O ₃ Si ₃	UH94a	100-200	E	c-(SiMe ₂ O) ₃ ; comp of SI-O-X species re inductive, resonance effects
C ₆ H ₁₈ OSi ₂	UT&97	90-110	P	Me ₃ Si-O-SiMe ₃ ; absolute; Si-Si & Si-O-R
C ₆ H ₁₈ Si ₂	UT&97	90-110	P	Me ₃ Si-SiMe ₃ ; absolute; Si-Si & Si-O-R
C ₇ H ₈ N ₂ O	UH&95a	100-160	E	phenylurea; absolute; modelling of polyurethane PEELS
C₈H₁₂Si	HS90	90-140	E	HC/C-CH ₂ -C/C-SiMe ₃ ; absolute; comp. to other :::-bonded species
C₈H₁₂O₃Si	TC&02	90-200	E	(CH ₂ =CH)Si(OAc) ₃ ; absolute; vinyl silanes
C₈H₁₈O₃Si	TC&02	90-200	E	(CH ₂ =CH)Si(OEt) ₃ ; absolute
C ₈ H ₂₄ N ₄ Si	UH94b	90-200	E	Si(NMe ₂) ₄ ; comp. of Si-N cmpds; models for SiN _x O _y films
C₈H₂₄O₄Si₄	UH94a	100-200	E	c-(SiMe ₂ O) ₄ ; comp of SI-O-X species re inductive, resonance effects
C ₉ H ₂₇ NSi ₃	UH94b	90-200	E	N(SiMe ₃) ₃ ; comp. of Si-N cmpds; models for SiN _x O _y films
C ₉ H ₂₈ Si ₄	UX&94	90-170	P	HSi(SiMe ₃) ₃ ; Xa; search for σ*(Si-Si)
C₁₀H₂₀N₂Si	UH&98	95-170	E,T	c-Si(RNCH=CHNR), R=tBu, silylene; absolute; delocal. in Si-N-C=C
C₁₀H₂₂N₂Si	UH&98	95-170	E,T	c-Si(RNCH ₂ CH ₂ NR), R=tBu, unsat. silylene; absolute;
C₁₀H₂₂N₂Si	UH&98	95-170	E,T	c-H ₂ Si(RNCH=CHNR), R=tBu, silylene; absolute; no delocal.
C₁₀H₂₄N₂Si	UH&98	95-170	E,T	c-H ₂ Si(RNCH ₂ CH ₂ NR), R=tBu, unsat. silylene; absolute
C ₁₁ H ₂₁ NOSi ₂	NF&96	100-130	P,T	Me(SiMe ₃ N)=COSiMe ₃ ; PEPICO; ion yields; PIPICO; no Si site select.; gs. calc of MeCF ₃ , SiH ₃ CF ₃ , MeSiF ₃ , SiH ₃ SiF ₃ ; LUMO of SiH ₃ SiF ₃ is p Si[Si(CH ₃) ₃] ₄
C₁₂H₃₆Si₅	W92	90-140	E	comp. of edges of Si-Si compounds
	UX&94	90-170	E	MS-Xa calc of Si 2p and Si 1s
	XJ&95	90-130	P,T	c-Si ₆ Me ₁₂ ; comp. of SiMe ₄ , Si ₂ Me ₆ , Si ₆ Me ₁₂ ; σ*(Si-Si)
C ₁₂ H ₃₆ Si ₆	W92	100-150	E	comp. of edges of Si-Si compounds; σ*(Si-Si)
	UX&94	90-170	E	triphenylsilanol, comp. of Si-O-X species
C₁₈H₁₆OSi	UT&97	100-145	E,T	Bz ₃ Si-SiBz ₃ ; absolute; Si-Si & Si-O-R
C ₃₀ H ₃₀ Si ₂	UT&97	90-110	P	Bz ₃ Si-O-SiBz ₃ ; absolute; Si-Si & Si-O-R
C ₃₀ H ₃₀ Si ₂ O	UT&97	90-110	P	comp. of ETS, ISEELS; orb. order; {SiH _x Cl _{4-x} (x=0-4),SiF ₄ } SE 6.1eV
ClH ₃ Si	WM&89	100-110	T	comp. of ETS, ISEELS; orb. order; {SiH _x Cl _{4-x} (x=0-4), SE 6.1 eV
	WM&91	100-110	T	comp. of ISEELS TV and ²⁹ Si nmr shielding; {SiH _x Cl _{4-x} (x=0-4)}
	T94	100-120	T	ab initio; ISEELS vs. ETS; questions 'constancy of stabilization energy'-(TV-EA); comp. of SiH _x Cl _{4-x} , x= 0-3
	WMT94a	100-140	E,T	comp. of ETS, ISEELS; orb. order; {SiH _x Cl _{4-x} (x=0-4),SiF ₄ } SE 6.1eV
Cl ₂ H ₂ Si	WM&89	100-110	T	comp. of ETS, ISEELS; orb. order; {SiH _x Cl _{4-x} (x=0-4), SE 6.1 eV
	WM&91	100-110	T	comp. of ISEELS TV and ²⁹ Si nmr shielding; {SiH _x Cl _{4-x} (x=0-4)}
	T94	100-120	T	ab initio; ISEELS vs. ETS; questions 'constancy of stabilization energy'-(TV-EA); comp. of SiH _x Cl _{4-x} , x= 0-3
	WMT94a	100-140	E,T	comp. of ETS, ISEELS; orb. order; {SiH _x Cl _{4-x} (x=0-4),SiF ₄ } SE 6.1eV
Cl ₃ HSi	WM&89	100-110	T	comp. of ETS, ISEELS; orb. order; {SiH _x Cl _{4-x} (x=0-4), SE 6.1 eV
	WM&91	100-110	T	comp. of ISEELS TV and ²⁹ Si nmr shielding; {SiH _x Cl _{4-x} (x=0-4)}
	T94	100-120	T	ab initio; ISEELS vs. ETS; questions 'constancy of stabilization energy'-(TV-EA); comp. of SiH _x Cl _{4-x} , x= 0-3
	WMT94a	100-140	E,T	comp. of ETS, ISEELS; orb. order; {SiH _x Cl _{4-x} (x=0-4),SiF ₄ } SE 6.1eV

Cl₄Si	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 ₂ 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
	CM&88b	100-113	P	DES, weak non-spectator (participator) obs; 2p<--7t ₂ strongest
(SiCl ₄ cont'd)	TL&89	90-140	T	absolute, X-alpha calc.; cont. & discrete; Rydbergs
	WM&89	100-110	T	comp. of ETS, ISEELS; orb. order; {SiH _x Cl _{4-x} (x=0-4, SiF ₄) SE 6.1 eV
	RW&90a	102-112	P	TEY, fluoresc. (SiCl ₄ ⁺ , Si) yields; comp. to abs (YL&89); enhanced FI at val. & Rydbergs
	RW&90b	100-140	P	wavelength-res. lum.; comp. of FY and PA
	IF&91	100-170	T	DV-Xa; comp. to exp: SiX ₄ , X=H,Cl,F; Virt. val. MOs dominate
	RF91	102-112	P	comp. of TEY sol and gas PA (BT&87); distinguish val & Ryd.
	WM&91	100-110	T	comp. of ETS, ISEELS; orb. order; {SiH _x Cl _{4-x} (x=0-4), SE 6.1 eV
	D92a	100-140	P,R	fluorescence from core hole decay; comp. of SiF ₄ , SiCl ₄
	W92	100-150	E	comp of SiCl ₄ , Si ₂ Cl ₆
	NO&93	100-112	P	Me ₃ Si-SiCl ₃ ; site-specific ionic. fragm.; PEPICO, PIPICO resonant Auger;
				comp. of SiMe ₄ , SiCl ₄ ; Si ₂ Me ₆ and Cl ₃ Si-SiMe ₃ , C ₆ H ₁₈ Si ₂
	T94	100-120	T	comp. of ISEELS TV and ²⁹ Si nmr shielding; {SiH _x Cl _{4-x} (x=0-4)}
	WMT94a	100-140	E,T	ab initio; ISEELS vs. ETS; questions 'constancy of stabilization energy'- (TV-EA); comp. of SiH _x Cl _{4-x} , x= 0-3
	CK&95	102-115	P	ion yields; compared TEY and CL ⁺ 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 ₄ , X=H,D,F,Cl,Br
	MG&98	102-125	P	resonant Auger; strong participator; comp. of SiF ₄ , SiCl24
	PDK97	90-120	P	high res.; vibrational structure -> excited geom, SiX ₄ , X=H,D,F,Cl,Br
	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
	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 ₁ obs. & calc (vibronic)
Cl₆Si₂	W92	100-150	E	comp of SiCl ₄ , Si ₂ Cl ₆
D₄Si	SB&92	101-108	P	high res. (50 meV); vib's in Rydberg; analysed rel. to PES; isotope effect
	SL&94	101-109	P	high resolution; vibrationally-resolved Rydbergs; comp. of SiH ₄ , SiD ₄ ,
	PDK97	90-120	P	high res.; vibrational structure -> excited geom, SiX ₄ , X=H,D,F,Cl,Br
Si₂H₆	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 ₄ , X=H,D,F,Cl,Br,Me; Z+1 tests; Franck-Condon analysis; G of 40-85 meV
F₂Si	ZV72	100-150	P,R	pot. barr. Effects
F₄Si	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), $\text{SiF}_6^{2-}(\text{sol})$
	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 $\sigma^*(\text{a}_1)$, 4s & 3d, comp. to normal Auger
(SiF_4 cont'd)	BA&86	116-150	P,T	absolute, MS-Xalpha, t_2 res., bs
	R86	100-170	P	comp. of F^+ , e-, PSID of cond. MLs with gas abs.; F^+ 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; $\{\text{SiH}_x\text{Cl}_{4-x}(x=0-4, \text{SiF}_4)\}$ 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_3 more labile than F; CH_3^+ 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_4 , 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_3 more labile than F; CH_3^+ enhanced in discrete res.; F 1s mass spec
	D92a	100-140	P,R	fluorescence from core hole decay; comp. of SiF_4 , SiCl_4
	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); vib'n'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_4 , X=H,D,F,Cl,Br
	MG&98	102-125	P	resonant Auger; strong participator; comp. of SiF_4 , SiCl_4 ; continuum Auger signal ascribed to nuclear motion (ultrafast decay precursor)
	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
	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 ₄ 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 $\sigma^*(\text{Si-H})$
	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 103 (σ^*) & 120 eV; proposes 30% fluorescence yield at σ^*
(SiH ₄ cont'd)	WM&89	100-110	T	ETS, ISEELS comp.; orb. order; {SiH _x Cl _{4-x} (x=0-4, SiF ₄)}, SE 6.1 eV
	IF&91	100-170	T	DV-Xa; comp. to exp: SiX ₄ , X=H, Cl, F; Virt. val. MOs dominate
	WM&91	100-110	T	comp. of ETS, ISEELS; orb. order; {SiH _x Cl _{4-x} (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 ₄ , SiD ₄ , Si ₂ H ₆
	T94	100-120	T	comp. of ISEELS TV and ²⁹ Si nmr shielding; {SiH _x Cl _{4-x} (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 _n (X=Si, P, S, Cl)
	ISN97	90-150	P	mass spectra & abs.; filtered white light to enhance SiH ₄ -> 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 ₄ , 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 ₄ , X=H, D, F, Cl, Br, Me; Z+1 tests; Franck-Condon analysis; G of 40-85 meV
H ₆ Si ₂	SB&92	101-108	P	SiH ₃ -SiH ₃ ; 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 ₄ , SiD ₄ , Si ₂ H ₆ ; low-lying $\sigma^*(\text{Si-Si})$
H ₈ Si ₃	SB&92	101-108	P	SiH ₃ -SiH ₂ -SiH ₃ ; high res. (50 meV); vibrational structure in Rydberg; analysed rel. to PES; isotope effect

Silicon 1s (1850 eV)

Br ₄ 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 ₃ H ₃ Si	HC&87a	1.84-1.90	P	shape res.
	FBN90	1.83-1.90	P	discrete & cont. shape res.; double excitation
C ₂ Cl ₂ H ₂ Si	HC&87a	1.84-1.90	P	shape res.
	FBN90	1.80-2.35	P	discrete & cont. shape res.; KL double excitation
C ₃ ClH ₃ Si	HC&87a	1.84-1.90	P	shape res.
	FBN90	1.83-1.90	P	discrete & cont. shape res.; double excitation
C ₃ Cl ₃ H ₉ Si ₂	SE&13	1.83-1.87	P	TIY, site dependent, KLL resonant Auger
C ₄ H ₁₀ OSi	UT&97	1.83-1.87	P	trimethylsilanol; absolute; Si-Si & Si-O-R
C ₄ H ₁₂ O ₄ Si	BMN90	1.80-2.15	P,T	(OMe) ₄ Si; rel.; chem. comp.; KL, KV 2e- excit; Ryd-val mix; CI calc
C ₄ H ₂₀ O ₄ Si	BMN90	1.80-2.15	P,T	(OEt) ₄ Si; rel.; chem. comp.; KL, KV 2e- excit; Ryd-val mix; CI calc
C ₄ H ₁₂ Si	BN86	1.83-1.88	P	Si(Me) ₄ ; relative, comp. to SiX ₄ , X=F, Cl, H, CH ₃
	BNM86	1.84-1.88	P,T	comp. to SiX ₄ , X=F, Cl, H, CH ₃ , 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 ₄ , Si(GeMe ₃) ₄ , Si(SiMe ₃) ₄ , Ge(SiMe ₃) ₄ ; Si-Ge ALS
	SK&93b	1.83-1.89	P,T	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
	UX&94	1.82-1.90	P	comp. of edges of Si-Si compounds; search for $\sigma^*(\text{Si-Si})$
	XJ&96b	1.83-2.60	P	xanes, xafs; comp. of SiMe ₄ , Si(SiMe ₃) ₄ , Si(GeMe ₃) ₄ , Ge(SiMe ₃) ₄
	SK&11	1.83-1.86	P	resonant Auger
C ₄ H ₁₂ SiO	SK&93b	1.83-1.89	P,T	Me ₃ Si(OMe); 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
	UT&97	1.83-1.87	P	absolute; Si-Si & Si-O-R
C ₄ H ₁₂ SiO ₂	SK&93b	1.83-1.89	P,T	Me ₂ Si(OMe) ₂ ; 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 ₄ H ₁₂ SiO ₃	SK&93b	1.83-1.89	P,T	MeSi(OMe) ₃ ; 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 ₄ H ₁₂ SiO ₄	SK&93b	1.83-1.89	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 ₅ H ₁₅ NSi	UH&94b	1.82-2.20	P	Me ₃ Si(NMe ₂); comp. of Si-N cmpds; models for SiN _x O _y films
C ₅ F ₃ H ₁₃ Si ₂	SN&09	1.84-1.87	P, T	F ₃ Si(CH ₂) ₂ Si(CH ₃) ₃ ; site selective fragmentation, TIY, STOBE-DEMON
	NT&08	1990	P	AEPPIPICO, site selective fragmentation, Si 2p & Si 1s compared
C ₆ H ₈ Si	UT&97	1.83-1.87	T	phenylsilane; ab initio; EHMO; comp to Ph ₃ Si-X
C ₆ H ₁₈ N ₂ Si	UH&94b	1.82-2.20	P	Me ₂ Si(NMe ₂) ₂ ; comp. of Si-N cmpds; models for SiN _x O _y films
C ₆ H ₁₈ N ₃ Si	UH&94b	1.82-2.20	P	HSi(NMe ₂) ₃ ; comp. of Si-N cmpds; models for SiN _x O _y films
C ₆ H ₁₈ OSi ₂	UT&97	1.83-1.87	P	Me ₃ Si-OSiMe ₃ ; absolute; Si-Si & Si-O-R
C ₆ H ₁₈ O ₃ Si ₃	UH94a	1.82-2.20	P	c-(SiMe ₂ O) ₃ ; comp of SI-O-X species re inductive, resonance effects
C ₆ H ₁₈ Si ₂	UX&94	1.82-1.90	P	Me ₃ Si-SiMe ₃ ; comp. of edges of Si-Si compounds; search for $\sigma^*(\text{Si-Si})$
	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 ₄ , Si(SiMe ₃) ₄ , Si(GeMe ₃) ₄ , Ge(SiMe ₃) ₄
	UT&97	1.83-1.87	P	triphenylsilanol; absolute; Si-Si & Si-O-R
C ₇ H ₂₁ N ₃ Si	UH94b	1.82-2.20	P	MeSi(NMe ₂) ₂ ; comp. of Si-N cmpds; models for SiN _x O _y films
C ₈ H ₂₀ O ₄ Si	UH94a	1.82-2.20	P	Si(OEt) ₄ ; comp of SI-O-X species re inductive, resonance effects
C ₈ H ₂₀ Si	BMN90	1.80-2.15	P,T	(Et) ₄ Si; rel.; chem. comp.; KL, KV 2e- excit; Ryd-val mix; CI calc
C ₈ H ₂₄ N ₄ Si	UH94b	1.80-2.20	P	Si(NMe ₂) ₄ ; comp. of Si-N cmpds; models for SiN _x O _y films
C ₈ H ₂₄ O ₄ Si ₄	UH94a	1.80-2.20	P	c-(SiMe ₂ O) ₄ ; comp of SI-O-X species re inductive, resonance effects
C ₉ H ₁₄ Si	UT&97	1.83-1.87	P	trimethylphenylsilane; a initio; EHMO
C ₉ H ₂₇ NSi ₃	UH94b	1.80-2.20	P	N(SiMe ₃) ₃ ; comp. of Si-N cmpds; models for SiN _x O _y films
C ₁₀ H ₂₀ N ₂ Si	UH&98	1.83-1.86	P,T	c-Si(RNCH=CHNR), R=tBu, silylene; absolute; delocal. in Si-N-C=C
C ₁₀ H ₂₂ N ₂ Si	UH&98	1.83-1.86	P,T	c-Si(RNCH ₂ CH ₂ NR), R=tBu, unsat. silylene; absolute;
C ₁₀ H ₂₂ N ₂ Si	UH&98	1.83-1.86	P,T	c-H ₂ Si(RNCH=CHNR), R=tBu, silylene; absolute; no delocal.
C ₁₀ H ₂₄ N ₂ Si	UH&98	1.83-1.86	P,T	c-H ₂ Si(RNCH ₂ CH ₂ NR), R=tBu, unsat. silylene; absolute;
C ₁₂ GeH ₃₆ Si ₄	HT&93	1.82-1.86	P	comp. of SiMe ₄ , Si(GeMe ₃) ₄ , Si(SiMe ₃) ₄ , Ge(SiMe ₃) ₄ ; Si-Ge ALS
	XJ&96b	1.83-2.60	P	xanes, xafs; comp. of SiMe ₄ , Si(SiMe ₃) ₄ , Si(GeMe ₃) ₄ , Ge(SiMe ₃) ₄
C ₁₂ Ge ₄ H ₃₆ Si	HT&93	1.82-1.86	P	comp. of SiMe ₄ , Si(GeMe ₃) ₄ , Si(SiMe ₃) ₄ , Ge(SiMe ₃) ₄ ; Si-Ge ALS
	XJ&96b	1.83-2.60	P	xanes, xafs; comp. of SiMe ₄ , Si(SiMe ₃) ₄ , Si(GeMe ₃) ₄ , Ge(SiMe ₃) ₄
C ₁₂ H ₃₆ Si ₅	HT&93	1.82-1.86	P	comp. of SiMe ₄ , Si(GeMe ₃) ₄ , Si(SiMe ₃) ₄ , Ge(SiMe ₃) ₄ ; Si-Ge ALS
	UX&94	1.82-1.90	P	comp. of edges of Si-Si compounds; search for $\sigma^*(\text{Si-Si})$
	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 ₄ , Si(SiMe ₃) ₄ , Si(GeMe ₃) ₄ , Ge(SiMe ₃) ₄
C ₁₂ H ₃₆ Si ₆	UX&94	1.82-1.90	P	c-(SiMe ₂) ₆ ; comp. of edges of Si-Si compounds; search for $\sigma^*(\text{Si-Si})$
C ₁₈ H ₁₆ OSi	UT&97	1.83-1.87	P	triphenylsilanol; absolute; Si-Si & Si-O-R
C ₃₀ H ₃₀ Si ₂	UT&97	1.83-1.87	P	Bz ₃ Si-SiBz ₃ ; absolute; Si-Si & Si-O-R
Cl ₄ Si	M66	1.83-2.13	P	extended fine structure (EXAFS)
	BN86	1.83-1.88	P	relative, comp. to SiX ₄ , X=F,Cl,H,CH ₃
	BNM86	1.84-1.88	P,T	comp. to SiX ₄ , X=F,Cl,H,CH ₃ , 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
	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
D ₄ Si	BMN90	1.80-2.15	P,T	relative, chem. comp.; KL, KV 2e- excit; Ryd-val mix; CI calc
FH ₃ Si	KP92b	1.84-1.85	T	SCF-CI; comp. to SiH ₄
F ₂ H ₂ Si	KP93	1.84-1.85	T	ab initio; MRD-CI; dipole & quadrupole; comp. to FH ₃ Si and SiH ₄
F ₄ Si	BN86	1.83-1.88	P	relative, comp. to SiX ₄ , X=F,Cl,H,CH ₃
	BNM86	1.84-1.88	P,T	comp. to SiX ₄ , X=F,Cl,H,CH ₃ , 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
H ₄ Si	BN86	1.83-1.88	P	relative, comp. to SiX ₄ , X=F,Cl,H,CH ₃
	BNM86	1.84-1.88	P,T	comp. to SiX ₄ , X=F,Cl,H,CH ₃ , 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
	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 ₃ 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 ₄ Na	YS&02	190-230	T	relative; MS-Xα plus DFT; geometry dependence
Na ₂	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 ⁻ 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 ₄ Na ₄ (ClNa) _n	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)

BHS	EH99	160-240	E,T	absolute; transient from H ₂ S+B+SiO ₂ ; comp of HBO, HBS, H ₃ B ₃ O ₃
	H00	160-250	E,R	transient ISEELS; comp of HBO,HBS, H ₂ S
	HE&01	160-240	E	absolute; transient ISEELS
CF₈S	KA&10	168-210	PT,	absolute, comp. to SF ₆ , DFT calculation
CH₄S	DTH90	150-290	E	CH ₃ SH, absolute; comp. to S1s, other RSH
COS	WB74e	155-200	E	weak cont. feature
	KGM77	162-174	P	Rydberg analysis IP (170.49)
(COS cont'd)	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 ₂ , COS, CS ₂ re location of σ*; decay of core states
	MH&89	140-280	E,T	absolute, ab initio, comp. of CO ₂ , COS & CS ₂ - all edges
	AEB97b	160-180	P	TIY,PIY; charge state mapping
	EK&97a	163-183	P	TIY, PEPICO; b ; high res.(35 meV); PEPIPICO; bs
	EK&97b	162-172	P	TIY, PEPICO; fragmentation mechanisms; S ³⁺ 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&989	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 ₂ , COS, PF ₃
	MA&03	170-205	P	luminescence (300-650 nm) yield, spectroscopy
	FE&04	163-168	P,T	long lived atomic S ^{L*} 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
	IIS12	166-172	P	resonant Auger, NEXAFS maps, participator Auger after π* excitation
CS₂	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 ₂ , COS, CS ₂ re location of σ*; decay of core states
	MH&89	140-280	E,T	absolute, ab initio, comp. of CO ₂ , COS & CS ₂ - 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 ₂ ⁺ 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. ⁻¹ , MP-CI calc
C₂H₃NS	HTM89	150-285	E	(CH ₃ SCN), comp to CH ₃ NCS, vibrational ELS
C₂H₃NS	HTM89	150-285	E	(CH ₃ NCS), comp to CH ₃ SCN, vibrational ELS
C₂H₆OS	TB&88	160-280	E	(CH ₃) ₂ S=O, DMSO, comp. to S1s
C₂H₆S	BS&12	160-190	P, T	(CH ₃) ₂ S dimethyl sulfide, TIY, PIY; IS-CASSCF calc.
C₂H₆S₂	BS&12	160-190	P, T	(CH ₃) ₂ S dimethyl di-sulfide, TIY, PIY; IS-CASSCF calc.
C₄H₄S	H86b	160-195	E,R	comp. to thiolane
	HHS86	160-255	E,P	(thiophene), S2p, S2s, S1s; comp. to sol. ml; MS-Xa calc; σ*(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 _{Auger} ,ion) coinc.; mass spectra at C1s, S2p with Auger
C ₄ H ₈ S	H86b	160-195	E,R	comp. to thiophene
	HHS86	160-255	E,P	(thiolane), S2p, S2s, S1s; σ*(C-S)
	HE91	(white)	P	(hv;e _{Auger} ,ion) coinc.; mass spectra at C1s, S2p with Auger
C ₅ H ₆ S	HT&90	150-285	E	absolute, 3-alkyl-thiophenes; no mod. of π* (cf. polymer cond.)
C₆H₄N₂S	HD&91	160-280	E	c-BzN ₂ S fused ring; comp. of S-N heterocycles, aromaticity
C₆H₄N₂S₂	HD&91	160-280	E	c-BzN ₂ S ₂ fused ring; comp. of S-N heterocycles, aromaticity
C₆H₄N₂S₃	HD&91	160-280	E	c-BzN ₂ S ₃ fused ring; comp. of S-N heterocycles, aromaticity
C₆H₉S	HT&90	150-285	E	absolute, 3-alkyl-thiophenes; no mod. of π* (cf. polymer cond.)
C₈H₁₃S	HT&90	150-285	E	absolute, 3-alkyl-thiophenes; no mod. of π* (cf. polymer cond.)
C₁₀H₁₇S	HT&90	150-285	E	absolute, 3-alkyl-thiophenes; no mod. of π* (cf. polymer cond.)
C₁₂H₂₁S	HT&90	150-285	E	absolute, 3-alkyl-thiophenes; no mod. of π* (cf. polymer cond.)
C ₁₄ H ₂₄ S	HT&90	150-285	E	absolute, 3-alkyl-thiophenes; no mod. of π* (cf. polymer cond.)
ClF ₅ S	AT&86b	165-215	P	absolute, comp. to SF ₆ & SeF ₆ (Se3p)
Cl ₃ PS	TKM82	162-173	P	X-alpha (MSM) calc., comp. to expt (K77)
	NS&98	150-240	P	absolute; PIY, TIY, PEPICO
D ₂ S	HS&94	160-240	P	30 meV fwhm; comp. of H ₂ S/D ₂ S; vibn'l struct.; val-Ryd. identified
F ₂ 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 ₂ O ₂ S	T91	160-172	T	SCF, EICVOM; orbital char, comp. to expt & Diss. Att.
F ₃ NS	JKC99	164-194	P,T	relative; GSCF3; ion current; two LS-coupled states; comp. to OPF ₃
F ₃ OS	NS&98	150-240	P	absolute; PIY, TIY, PEPICO
F₄S	BZ&67	140-188	P	relative, large background comp. to SF ₆ S 2p
	BH87	160-250	E	S2p, S2s, S1s & F1s comp.
	KBH90	160-180	T	ab initio, comp. to BH87; revised σ*(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 ₄ OS	T91	160-172	T	SCF, EICVOM; orbital char, comp. to expt & Diss. Att.
F₆S	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.
	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 ₃ , N ₂ , NO ₃ ⁻ ; KPF ₆ (s); shape resonances

	AT&86b	165-215	P	absolute, comp. to SF ₅ Cl & SeF ₆ (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 _g , no effect of t _{2g} res. on b, combined 1-e ⁻ /multi-e ⁻ model
(SF ₆ cont'd)	AT&89	160-270	P,T	relative, comp. to valence partial X-sect, SeF ₆ , "F ₆ "; X-alpha calc.
	KBH90	160-180	T	ab initio, comp. to SF ₄ (BH87)
	NMA90	160-260	T	MSXa calc; order of res. identified; comp. to expt. (ZV71)
	SB90	160-240	E	comp of TeF ₆ , SeF ₆ , SF ₆ ; Z-dependence of pot. barr's
	NMA91	160-210	T	absolute; DVXa calc; comp. to expt. (ZV71); H ₂ 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 _{lu} ?) 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 _{2g} /e _g 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 _{lu} (K ² _{max} ~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 ₆ ⁺⁺ 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→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 ₂ ²⁺) observed, spectator resonant below IP, decay of t _{2g} and e _g 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 ⁻¹
	PS&05	170-210	P	relative, TIY, PIY, all +ves and S ⁻ , F ⁻ ; anion signals specific to shape resonances
	KA&10	168-210	PT,	absolute, comp. to SF ₅ CF ₃ , DFT calculation
(SF ₆) _n	PB&08	180-186	T	position and line shape in cluster vs. molecule
F ₁₀ S ₂	T91	160-172	T	SCF, EICVOM; orbital char, comp. to expt & Diss. Att.
H₂S	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 ₂ , CS ₂ & SF ₆ , 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, Stieltjes 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 ₂ , HCl, H ₂ S
	HS&94	160-240	P	30 meV fwhm; comp. of H ₂ S/D ₂ S; vibn'l struct.; val-Ryd. identified
	LB&95	160-220	T	MS-Xa; comp. of XH _n (X=Si,P,S,Cl)
(H ₂ S cont'd)	SA&95a	173-180	P	ultrafast decay of LM 2e excited state detected by HS ^{L*} 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 ($3s_{1/2}-1p_{3/2} = 90$ 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 ₂ S+B+SiO ₂ ; comp of HBO, HBS, H ₃ B ₃ O ₃
	FCB99	50-270	E	absolute; sum rule normalized
	H00	160-250	E,R	transient ISEELS; comp of HBO,HBS, H ₂ 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 Lyma & Balmer lines, ultrafast
	VM&07	162-173	P	TIY, TFY, pFY, excited H detected from Lyma & Balmer lines, ultrafast
	MM12	68-72	P,R	ultra-fast decay (HBr-Br3d; DCl, HCl-Cl2p; H ₂ S - S2p, O ₂ -O1s)
O ₂ 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
	DH&89	165-185	P	negative (O ⁻) & positive (O ⁺ , O ₂ ⁺) yields from S2p (=>SO ²⁺ + O ⁻)?
	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; $\Delta E_{SO} = 1.20$; O _h =0.095eV
	FT&99	163-180	P	TIY, TPES; TPEPICO; TPE2PICO; relative cross sections; PCI; Anisotropic ion ang. distribution; fragmentation; KERD; site-specific
	KI00	172-178	T	ab initio; spin-orbital Breit-Pauli; molecular field; comp. of SO ₂ , COS, PF ₃
	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 _n	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

Sulfur 1s (2470 eV)

CCuHOS ₂	TV93	2.47-2.48	T	CuS ₂ COH; ab initio-SCF-EICVOM; pre-edge res. (π^* , $\sigma^*_{O-O}, \sigma^*_{S-S}$)
CF ₈ S	LD72	2.47-2.51	P	CF ₃ SF ₅ ; pot. barr. Effects
	IS&05	2.46-2.49	P	PEPICO, PIPICO, site-selective fragmentation
CH ₂ S ₂	TV93	2.47-2.48	T	thio-formic acid; ab initio-SCF-EICVOM; pre-edge res. ($\pi^*, \sigma^*_{O-O}, \sigma^*_{S-S}$)
CH ₄ S	BE85	2.46-2.49	P	CH ₃ 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

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 ₂ , COS & CS ₂ ; σ^* loc.; hole decay
	MH&89	2.45-2.55	P,T	absolute, ab initio, comp. of CO ₂ , COS & CS ₂ - all edges
(COS cont'd)	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; β s; Renner-Teller π^* ; 10 σ^* 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 ₂	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 ₂ , COS & CS ₂ ; σ^* loc.; hole decay
	MH&89	2.45-2.55	P,T	absolute, ab initio, comp. of CO ₂ , COS & CS ₂ - 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 ₂
	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 ₂ H ₃ NS	DTM91	2.46-2.49	P	CH ₃ SCN; comp. to ETS; $\sigma^*(S-C)$ bond length correl.
C ₂ H ₃ NS	DTM91	2.46-2.49	P	CH ₃ SNC; comp. to ETS; $\sigma^*(S-C)$ bond length correl.
C ₂ H ₆ OS	TB&88	2.46-2.51	P	(CH ₃) ₂ S=O, DMSO, comp. to S2p,O1s,C1s
C ₂ H ₆ S	HBT89	2.46-2.51	P	(CH ₃) ₂ S, comp. to (CH ₃) ₂ S ₂ , $\sigma^*(S-S)$
	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 ₂ H ₆ S	DTM91	2.46-2.49	P	C ₂ H ₅ SH; comp. to ETS; $\sigma^*(S-C)$ bond length correl.
C ₂ H ₆ S ₂	HBT89	2.46-2.51	P	(CH ₃) ₂ S ₂ , comp. to (CH ₃) ₂ 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) _n -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 ₂ H ₆ S ₃	DB&98	2.46-2.49	P	Me-S ₃ -Me; ioniz. yield; low-lying $\sigma^*(Si-Si)$ level; correl. with ETS
C₄H₄S	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.; π^* , σ^*_{Si-C} components in main res. identified; supports HHS86
	K02	2.46-2.49	P,TR	symmetry resolved, π^* below σ^* , review
C ₄ H ₈ S	H86b	2.47-2.50	P,R	(thiolane); comp. to thiophene
	HHS86	2.47-2.50	P	S2p, S2s, S1s; $\sigma^*(C-S)$
C ₄ H ₁₀ 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 ₆ H ₄ N ₂ S	HD&91	2.46-2.51	P	BzN ₂ S fused ring; absolute; comp. to other edges; matches S2s
C ₆ H ₄ N ₂ S ₂	HD&91	2.46-2.51	P	BzN ₂ S ₂ fused ring; absolute; comp. to other edges; matches S2s
C ₆ H ₄ N ₂ S ₃	HD&91	2.46-2.51	P	BzN ₂ S ₃ fused ring; absolute; comp. to other edges; matches S2s
C ₆ H ₆ S	DTH90	2.46-2.51	P	C ₆ H ₅ 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

C ₆ H ₁₄ S ₂	CH&97	2.46-2.49	P	R(S-S) _n -R, R= iPr; dependence of $\sigma^*(S-S)$, $\sigma^*(S-C)$ on R, n
C ₇ H ₈ S	DTH90	2.46-2.51	P	C ₆ H ₅ SCH ₃ , 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 ₈ H ₁₄ S ₂	CH&97	2.46-2.49	P	R(S-S) _n -R, R=2-butenyl; dependence of $\sigma^*(S-S)$, $\sigma^*(S-C)$ on R, n
C ₈ H ₁₄ S ₃	CH&97	2.46-2.49	P	R(S-S) _n -R, R=2-butenyl; dependence of $\sigma^*(S-S)$, $\sigma^*(S-C)$ on R, n
C ₈ H ₁₈ S ₂	CH&97	2.46-2.49	P	R(S-S) _n -R, R=n-butyl; dependence of $\sigma^*(S-S)$, $\sigma^*(S-C)$ on R, n
C ₈ H ₁₈ S ₃	CH&97	2.46-2.49	P	R(S-S) _n -R, R=n-butyl; dependence of $\sigma^*(S-S)$, $\sigma^*(S-C)$ on R, n
C ₈ H ₁₈ S ₄	CH&97	2.46-2.49	P	R(S-S) _n -R, R=n-butyl; dependence of $\sigma^*(S-S)$, $\sigma^*(S-C)$ on R, n
C ₈ H ₁₈ S ₂	CH&97	2.46-2.49	P	R(S-S) _n -R, R=t-butyl; dependence of $\sigma^*(S-S)$, $\sigma^*(S-C)$ on R, n
C ₈ H ₁₈ S ₃	CH&97	2.46-2.49	P	R(S-S) _n -R, R=t-butyl; dependence of $\sigma^*(S-S)$, $\sigma^*(S-C)$ on R, n
C ₈ H ₁₈ S ₄	CH&97	2.46-2.49	P	R(S-S) _n -R, R=t-butyl; dependence of $\sigma^*(S-S)$, $\sigma^*(S-C)$ on R, n
C ₁₂ H ₁₀ S ₂	CH&97	2.46-2.49	P	R(S-S) _n -R, R=phenyl; dependence of $\sigma^*(S-S)$, $\sigma^*(S-C)$ on R, n
C ₁₂ H ₂₂ S ₂	CH&97	2.46-2.49	P	R(S-S) _n -R, R=Me ₂ C=CMeCH ₂ -; depend. of $\sigma^*(S-S)$, $\sigma^*(S-C)$ on R, n
C ₁₂ H ₂₂ S ₃	CH&97	2.46-2.49	P	R(S-S) _n -R, R=Me ₂ C=CMeCH ₂ -; depend. of $\sigma^*(S-S)$, $\sigma^*(S-C)$ on R, n
C ₁₂ H ₂₂ S ₄	CH&97	2.46-2.49	P	R(S-S) _n -R, R=Me ₂ C=CMeCH ₂ -; depend. of $\sigma^*(S-S)$, $\sigma^*(S-C)$ on R, n
C ₁₄ H ₁₄ S ₂	CH&97	2.46-2.49	P	R(S-S) _n -R, R=C ₆ H ₅ CH ₂ -; dependence of $\sigma^*(S-S)$, $\sigma^*(S-C)$ on R, n
ClFO ₂ S	HBT89	2.46-2.51	P	ionization yield, comp of SO ₂ Cl ₂ , SO ₂ FCI & SO ₂ F ₂
	HT88	2.46-2.56	P	ionization yield, comp to SO ₂ Cl ₂ , SO ₂ FCI
ClF ₅ S	RB&92	2.4-3.1	P,T	relative; comp. to SF ₆ & SCF-CI calc; EXAFS no S 3d participation
	BR&92	2.4-2.8	P	double core vacancy state (1s,2p); comp. of SF ₅ Cl, SF ₆
	NM96	2.4-2.8	P,R	EXAFS; KL double excitation; compared to SF ₆
Cl ₂ OS	HBT87	2.46-2.51	P	comp. to other S,Cl,O compounds, $\sigma^*(S-X)$
Cl ₂ O ₂ 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 ₂ Cl ₂ , SO ₂ FCI
	HBT89	2.46-2.51	P	ionization yield, comp of SO ₂ Cl ₂ , SO ₂ FCI & SO ₂ F ₂
Cl ₂ 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 ₂ Cl ₂ , SO ₂ FCI
Cl ₂ S ₂	HBT87	2.46-2.51	P	comp. to other S,Cl,O compounds, $\sigma^*(S-X)$
D ₂ 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; β for fragmentation
F ₂ OS	LD72	2.47-2.50	P	SF ₂ 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 ₄)
F ₂ O ₂ S	LD72	2.47-2.50	P	SF ₂ O ₂ ; pot. barr. effects
	BK74	2.48-2.50	P	pot. barr. effects
	HBT89	2.46-2.51	P	ionization yield, comp of SO ₂ Cl ₂ , SO ₂ FCI & SO ₂ F ₂
	HT88	2.46-2.56	P	ionization yield, comp to SO ₂ Cl ₂ , SO ₂ FCI
	HBT89	2.46-2.51	P	ionization yield, comp of SO ₂ Cl ₂ , SO ₂ FCI & SO ₂ F ₂
F ₃ 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 ₄ S	BH87	2.48-2.50	P	SF ₄ ; pot. barr. effects
	KBH90	2.48-2.50	T	ab initio, comp. to SF ₆ & 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 ₄ OS	T91	2.46-2.48	T	SCF, EICVOM; orbital char, comp. to expt & Diss. Att.
F ₆ 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

(SF ₆ cont'd)	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 ₄ , $\sigma^*(S-F)$
	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 ₆ vs. H ₂ S & SO ₂ at discrete a _{1g} 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 ₄ (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 ₅ Cl, SF ₆
	RB&92	2.45-2.80	P,T	1-e- & 2-e- excitation; ab initio calc; comp. of SF ₆ & SF ₅ 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 ₂ , GeCl ₄ , SF ₆
	BR&95	2.48-2.55	P	laser generated (3ps) continuum; laser photodissociation
	RW&95	2.45-2.58	P	500 fs pump-probe; bleaching of t _{1u} resonance in first 10 ps; fast diss.
	NM96	2.4-2.8	P,R	EXAFS; KL double excitation; compared to SF ₅ Cl
	RG&96a	2.67-2.69	P,T	KL 2- exc.; CAS-MCSCF calc; (Z+2) interp.; comp. of H ₂ S, SO ₂ , SF ₆
	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; summary of sub-ns XAS
	NL99	2.50-2.63	T	σ resonances in ionization continuum; l = 9 at 2550 eV
	T91	2.46-2.48	T	SCF, EICVOM; orbital char, comp. to expt & Diss. Att.
F ₁₀ S ₂	LD66	2.47-2.50	P	absolute
H ₂ S	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 ₂ resonance
	AHB96	1-15	P	triple coinc. (Auger,ion,ion) PEPIPOCO; triple ioniz.
	AT&96a	2.46-1.51	P	relative; TIY; angle resolved; 3b ₂ /6a ₂ $\Delta E \sim 0.15$ 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 ₂ S, SO ₂ , SF ₆
	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; β for fragmentation
	HA&98c	2.46-2.49	P	relative; PIT, TIY; photofragmentation asymmetry
H ₂ S ₂	TV93	2.47-2.48	T	ab initio-SCF-EICVOM; pre-edge res. (π^* , σ^*_{O-O} , σ^*_{S-S})
O ₂ 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 ₂ in p-hydroquinone clathrate, sharper peaks, Z+1 analysis, comp.to ETS

(SO ₂ cont'd)	BE85	2.46-2.52	P	equivalent core analogy, comp. to ETS res.
	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; π^* 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 ₂ S, SO ₂ , SF ₆
	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 ₂
	K02	2.46-2.49	P,T,R	symmetry resolved, Renner-Teller; GSCF3; review
S ₂	DO&96	2.46-2.50	P	relative; comp. of gas, sol. polymer - S ₈ vs. S _n ⁻ chain; comp. to O ₂ (³ S _g ⁻ g.s.); bond-length correlation

Tellurium 4d (40 eV)

Te ₂	STZ73	37-130	P	photographic
TeF ₄	BST80	40-55	P,T	relative, Z+1 analogy used to predict valence spectrum of IF ₄
TeF ₆	SB90	40-90	E	comp of TeF ₆ , SeF ₆ , SF ₆ ; 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 ₆	SB90	100-190	E	comp of TeF ₆ , SeF ₆ , SF ₆ ; Z-dependence of pot. barr.s
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Tellurium 3d (600 eV)

TeF ₆	SB90	580-680	E	comp of TeF ₆ , SeF ₆ , SF ₆ ; Z-dependence of pot. barr.s
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Tellurium 3p (830 eV)

TeF ₆	SB90	810-870	E	comp of TeF ₆ , SeF ₆ , SF ₆ ; Z-dependence of pot. barr.s
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Thorium 5d (110 eV)

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

Tin 4p,4s (85,135)

C ₄ H ₁₂ Sn	US&90b	60-260	P	partial ion yields, PIPICO
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Tin 3d (510 eV)

C ₄ H ₁₂ 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 ₄ Sn	GDT97	3.90-4.30	P,T	relative; TIY, MS-Xa; pot. barr.; AsCl ₃ , PCl ₃ , GeCl ₄ , SnCl ₄ comp.; σ*(X-Cl) bond length correlation
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Titanium 2p (460 eV)

Br ₄ Ti	DF&94	450-470	T	ab initio CI; relaxed hole; comp. of TiX ₄ , X=F,Cl,Br
C ₅ Cl ₃ H ₅ Ti	W92	450-490	E,T	CpTiCl ₃ ; comnp. to TiCl ₄ ; EHMO
	WH93	450-490	E,T	abs.; comp. of Cp _x TiCl _{4-x} , x=0-2; diff '10Dq' at each edge
C ₁₀ Cl ₂ H ₁₀ Ti	WH93	450-490	E	Cp ₂ TiCl ₂ ; abs.; comp. of Cp _x TiCl _{4-x} , x=0-2; diff '10Dq' at each edge
Cl ₄ Ti	W92	450-490	E,T	TiCl ₄ ; absolute; EHMO; comp. to at.mult.-ligand field calc.
	WH93	450-490	E,T	abs.; comp. of Cp _x TiCl _{4-x} , x=0-2; diff '10Dq' at each edge
	DF&94	450-470	T	ab initio CI; relaxed hole; comp. of TiX ₄ , X=F,Cl,Br; comp. to WH93; t ₂ < e; strong CI mixing
	HT&00	450-470	P	resonant X-ray emission; comp to WH93; high P – absorption saturated ?
F ₄ Ti	DF&94	450-470	T	ab initio CI; relaxed hole; comp. of TiX ₄ , X=F,Cl,Br

Titanium 1s (4966 eV)

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

Uranium 5d (120 eV)

UF ₄	CM&80	70-145	P	photographic, comp. to U solid, shape res. -cont.? (see PC83)
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Uranium 4d (3560 eV)

UCl ₄	GE&89	3.53-3.62	P,T	absolute, comp. to UO ₂ (calc.); MS-calc. of res.
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Uranium 4p (4304 eV)

UCl ₄	GE&89	4.28-4.37	P,T	absolute, comp. to UO ₂ (calc.); MS-calc. of res.
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Vanadium 2p,2s (520,630 eV)

C ₆ O ₆ V	TD&92a	500-660	P,E	V(CO) ₆ , absolute
Cl ₃ OV	DF&94	510-530	T	ab initio CI; relaxed orb.; MO _x X _y (Ti,V,Cr,Mn); more coval. as Cl ÷ F
F ₃ OV	DF&94	510-530	T	ab initio CI; relaxed orb.; MO _x X _y (Ti,V,Cr,Mn); more coval. as Cl ÷ F

Vanadium 1s (5465 eV)

Cl ₃ OV	DF&94	5.46-5.48	T	ab initio CI; relaxed orb.; MO _x X _y (Ti,V,Cr,Mn); more coval. as Cl ÷ F
F ₃ OV	DF&94	5.46-5.48	T	ab initio CI; relaxed orb.; MO _x X _y (Ti,V,Cr,Mn); more coval. as Cl ÷ F

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

XeC ₆₀	PN93	60-140	P	absolute; comp. of atom and Xe in C ₆₀ cage; EXAFS
XeF ₂	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 ₄	CH&73	50-160	P	absolute, gas-solid comp., ligand field core level splitting
XeF ₆	NHS74	50-170	P	absolute, evidence for octahedral symmetry

Zinc 3d (14 eV)

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