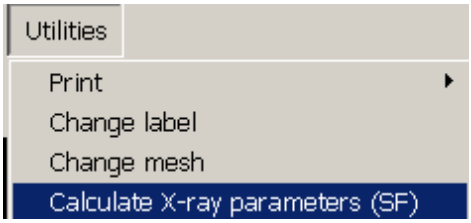
Converting an OD spectrum to an OD1 spectrum

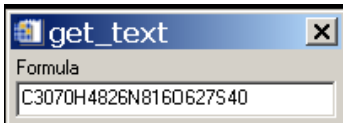
1. Make sure the OD spectrum you are converting is that of a SINGLE species.

2. construct the atomic response from the tabulated elemental constants

Utilities~Calculate X-ray parameters (SF)

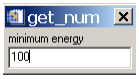


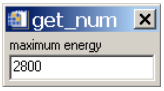
Example: human serum albumin (protein)
Elemental composition is
C3070H4826N816O627S40
(from protein data bank)



* enter **elemental composition** (periodic table (caps/lower case correct)
each element in list ONLY once

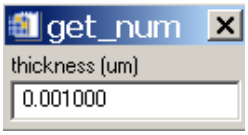
* enter **minimum and max energy** of interest
(here I want S 2p and S 1s)
(data base covers from 30 eV to 10,000 eV)





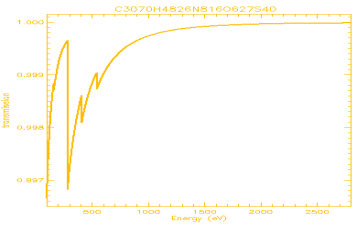
* select type of signal - I use **transmission** . Mass coeff. also works (~10^{-7} relationship) but density cannot be included in the routine as it is written now

* enter standard **density** of bulk material
(if trans. selected) - get from web, etc



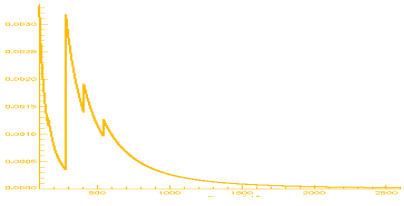
* enter thickness - 0.001 micron = 1 nm

3. convert transmission to OD (computed signal is for white light - I=1 at all E)



Spectra~power~ln

Specrtra~gain~multiply~(-1)

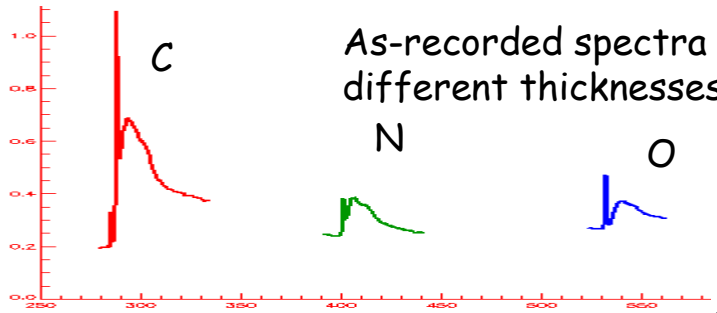


As of Feb-2011 version, transmission is default and the computed transmission for 1 nm is automatically converted to OD1 at end of 'calculate x-ray parameters (SF)'

3. SAVE this ➔ **alb-cnos-sf-od1.txt**

SF (=san francisco ?) was original name of the Fortran program for calculating these signal from CXRO data base

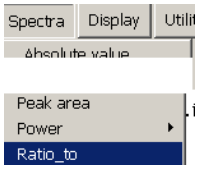
Matching elemental and OD spectra



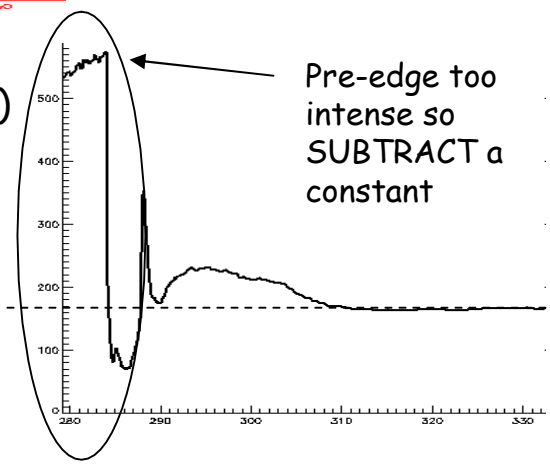
As-recorded spectra on OD scale
different thicknesses used to get better signal

Take EACH spectrum inn turn
* ratio OD to the elemental response ('SF')

Spectra~ratio



$$RATIO = \frac{A*(\text{first Buf})}{B*(\text{second Buf})}$$



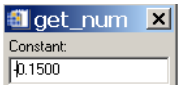
Pre-edge too intense so SUBTRACT a constant

Ideally the pre-edge intensity relative to the continuum is correct, but often (for reasons not easy to understand), this is not the case so be prepared to add/subtract constants

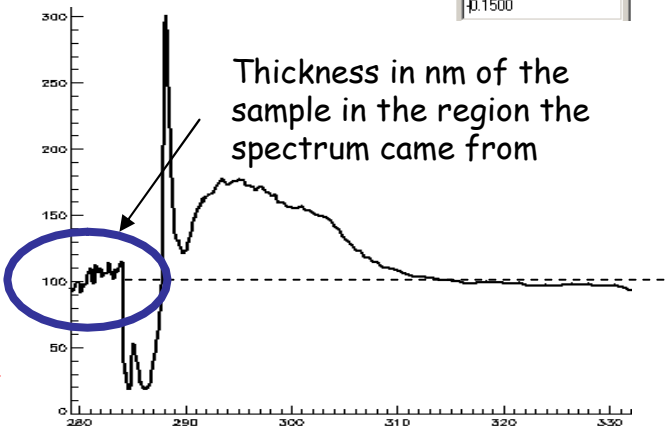
Pre-edge is about 2.5 time too large so remove 70% of it

* goal is to match the scaled OD signal to the SF signal BELOW onset and at high energy in continuum; subtract constants until the ratio is FLAT below and in high energy limit

Spectra~add~constant (1.6)



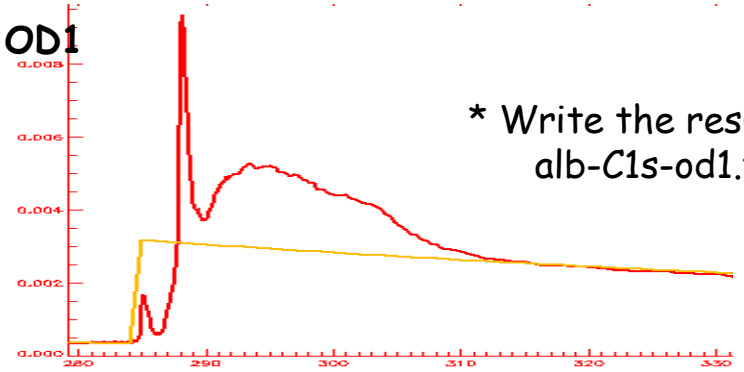
* once ratio is FLAT pre and post NEXAFS, divide the PD spectrum (after any constant subtraction) by the ratio number (which is the thickness)



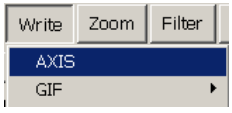
Thickness in nm of the sample in the region the spectrum came from

Spectra~gain~divide (100)

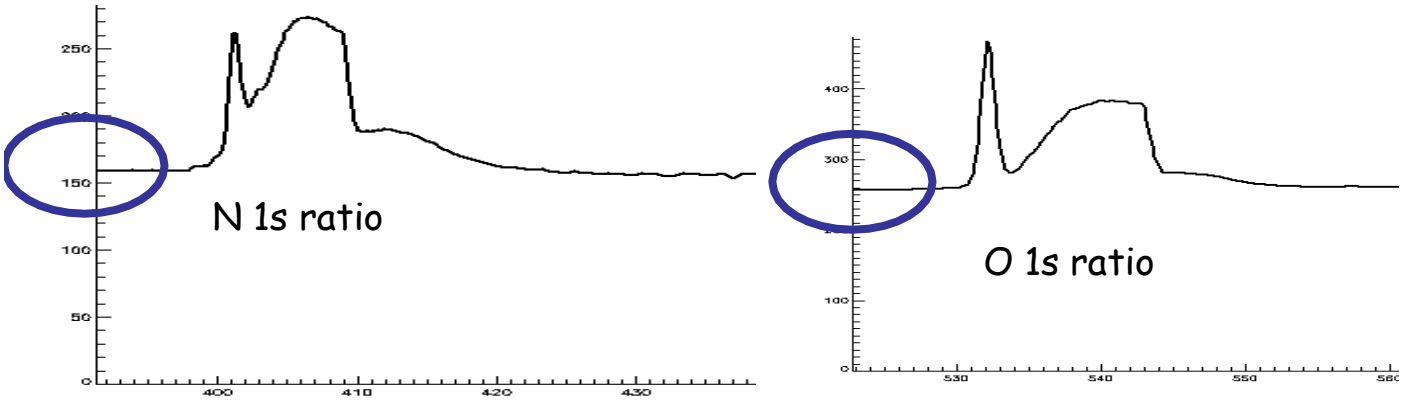
* check your result by overplotting the OD1 reference spectrum and the SF spectrum

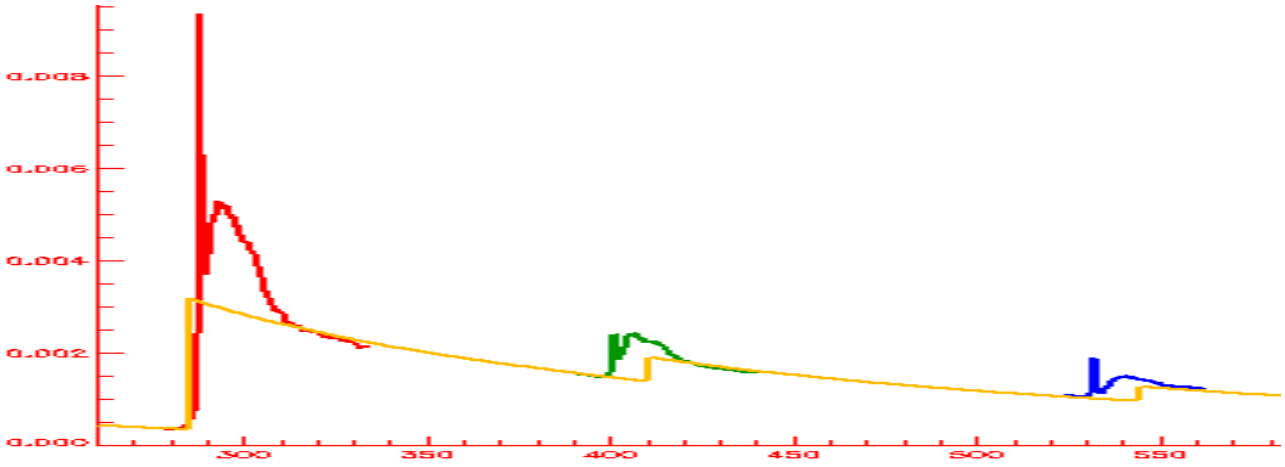


* Write the result to disk
alb-C1s-od1.txt **Write~axis**



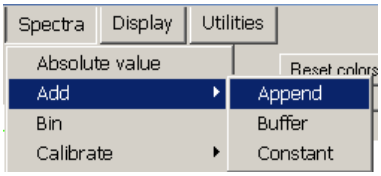
Final result for HSA

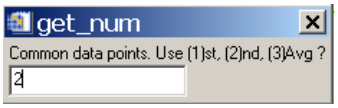


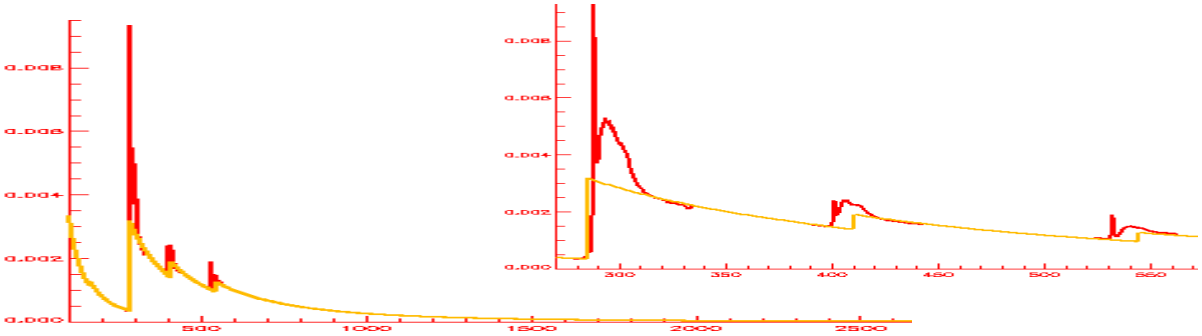


Sometimes I combine multiple edges in 1 reference spectrum and 'fill in' the missing parts using the elemental response

Spectra~add~append
Put priority to the SPECTRUM so it determined the signal, not the SF values







Dialog with Zoe Pettifer (Finders U, Adelaide)

•At 12:18 AM 3/2/2016, you wrote:
Hi Adam,

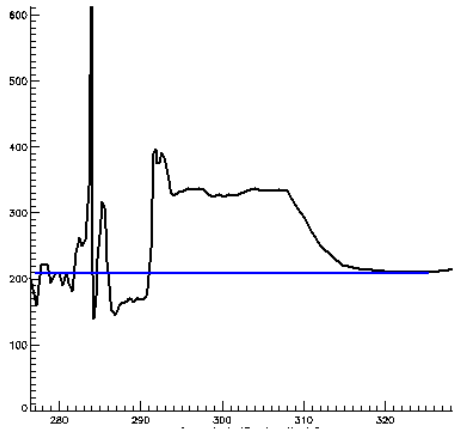
I have a few questions about the "Converting and OD spectrum to an OD1 spectrum" instructions you provided.

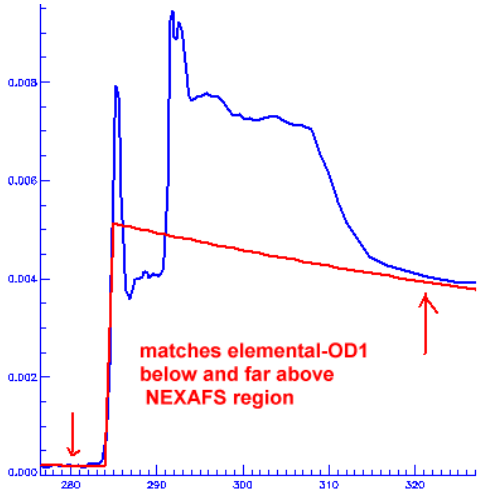
Firstly, I would like to double check that I am making the "SF" spectrum correctly, and that I should be using a thickness of 1 nm. When this file is created a pop up box asks me if I would like to convert to OD, which I say "yes" to. Does this mean I don't have to do anything further to this spectrum?
The alternative to 'yes' (ie if you do not click on yes) is to compute the response function as transmission.

Since you want to end up in "OD-space", yes is the right answer. After you say 'yes' it will display a default header, which in the most recent version of aXis, summarizes the information you provided
e.g.
C d(g/cc) = 1.00 t(nm) = 1.0 SF OD1
(composition, density, thickness)
You can of course change that default header as you wish - for example to start it with the name of the material whose elemental response you are computing.
When you hit 'enter' to finalize the header, aXis2000 then displays the OD1 response function for the set of parameters you calculated in the buffer you happen to have aXis2000 pointed at. Lets call that spectrum the 'elemental-OD1'.
This is exactly the spectrum you will be using to scale your experimental OD spectrum such that it matches outside of the NEXAFS region to the elemental-OD1.

I am having trouble following most of the instructions on the second page. I have taken the ratio of my spectrum to the elemental response "SF" spectrum, and I believe I am doing this correctly.

•click on buffer with your experimental-OD spectrum
~spectra~ratio to ; select a factor (1) then click on buffer with the elemental-OD1. aXis2000 displays the ratio in buffer 0.



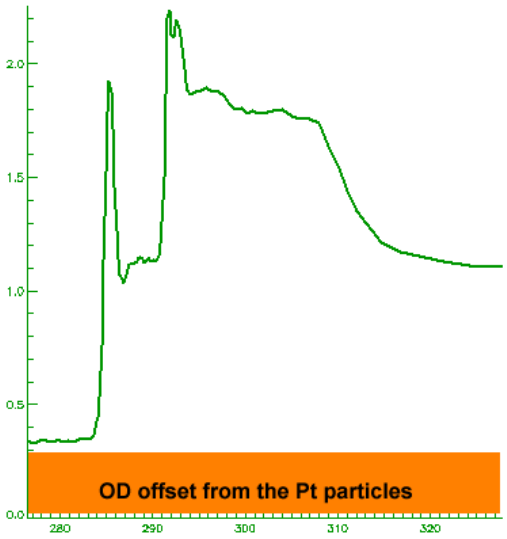


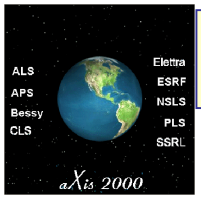
Dialog with Zoe Pettifer (Finders U, Adelaide)

I then don't understand how you are correcting the pre edge in the example you give. My understanding is that when you subtract a constant, it is simply going to shift the y axis, but not change the shape of the spectrum at all. Could you please clarify how you have corrected the pre-edge?
So, ideally, if you have got the correct experimental-OD spectrum, and your elemental formula, and density are right, you get the situation above. However, there are reasons that this does not work properly, even though elemental formula, and density are right. One of the most common is that the Io you used to generate the experimental-OD spectrum was wrong (e.g. time difference from when I was run; change in slits, change in dwell, phase of the moon, ring operator is not paying attention and has let the beam drift; whatever). In those cases, the Io is typically wrong by a multiplicative scale factor (typical if dwell's are not matched) If you work through Lambert-Beer formula, a multiplicative factor, a, in -ln(I/a*Io) ends up giving you a constant offset.

OD = -ln(I/a*Io) = - ln(I/Io) + ln(a) where -ln(I/Io) is the correct value and ln(a) is a constant offset.

Another situation is where the region you took the experimental-OD spectrum from was the correct material, but it was sitting on some other material(e.g. a window, or substrate, or ...) which may not contribute to spectral shape but provide a slowly varying background.
This is what the part that is confusing you is about.





Dialog with Zoe Pettifer (Finders U, Adelaide)

So I subtract 5/6 of 0.35 = 0.30 and I end up with good agreement of pre- and post-NEXAFS region ratios

Once this is done (or if it isn't required), you then say to divide the OD spectrum by the ratio number.

Yes. The way to think of this is that number is the thickness in nm of the region we're the elemental spectrum was measurer - WHY ? because the elemental-OD1 is computed for 1 nm of the material in its standard density

From the document I am lead to believe that this number is the intensity level of the pre-edge area of the OD spectrum?
No, it is what I say above. But that is only after you have got good agreement of pre- and post-NEXAFS region ratios

I do not understand how dividing by this number will produce a reference spectrum that overlaps with the SF spectrum. In the example you give it also appears as though the shape of the reference spectrum has changed again.
The SHAPE of the experimental spectrum should not change - only its intensity