FLUO: Correcting XANES for self-absorption in fluorescence measurements

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Contents

Chapter 1

Introduction

1.1 Abstract

This document describes the computer program FLUO, a tool to correct the XANES region of absorption data measured with the fluorescence technique for self absorption effects. These self absorption effects are most significant when the element of interest is concentrated or a heavy atom embedded in a host of lighter atoms. The consequence of this effect is that the measured fluorescence signal, I_f is no longer proportional to the absorption coefficient of interest. Using tabulated absorption cross-sections and some approximations appropiate for the short energy range of the XANES, FLUO corrects most of this distortion so that the actual (within 10%) absorption coefficient is recovered. If fluorescence corrections are not desired, FLUO can be used for energy alignment of several absorption spectra and to calculate their energy derivatives.

1.2 Acknowledgments

This program was written at the University of Washington as an addition to the UWXAFS suite of programs for data analysis. The derivation of the mathematical formulation was done together with Bruce Ravel and Edward A. Stern. Bruce Ravel also provided very valuable guidance and many useful subroutines during the coding period. Most of the subroutines used in FLUO are part of the UWXAFS library and were mostly written by Matt Newville and Bruce Ravel. Most of the character string manipulation subroutines were written by Steve Zabinsky and Matt Newville.

I would like to thank Guang Zhang who pointed out the need for a

XANES self-absorption correction code as part of the UWXAFS package and who provided very valuable input and beta-testing at the original stage. The sulfate data used throughout the document is Guang's data. I also thank Anatoly Frenkel, Shelly Kelly and Hyde Kim for checking the energy-alignment capability of the code against their data.

Chapter 2

Theoretical background

The notation in this section follows that of Hayes and Boyce [1]. Fig. 1 schematically shows the experimental situation in a fluorescence experiment. Radiation of intensity $I_0(\omega)$ impinges on a sample of total thickness z_s at an angle θ_i from the surface. The fluorescence radiation is detected with a detector subtending a solid angle Ω centered at an angle θ_f with the surface.

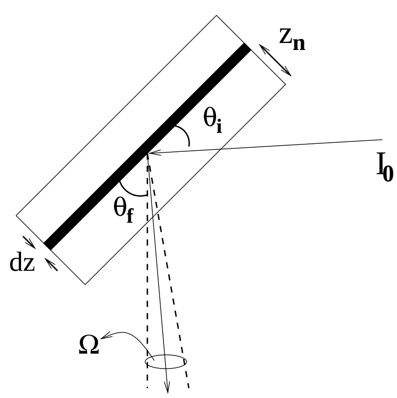

Fig. 1: Schematic representation of fluorescence experimental setup.

The fluorescence intensity I_f due to the edge of interest coming from a slice of sample of width dz at depth z_n is given by

$$I_f(z_n)dz_n = (\frac{\Omega}{4\pi})I_0e^{(-\mu_t(\omega)z_n/\sin\theta_i)}\epsilon_f(\omega)\mu_e(\omega)\frac{dz_n}{\sin\theta_i}e^{-\mu_t(\omega_f)z_n/\sin\theta_f} \tag{2.1}$$

.

Here $\hbar\omega$ is the energy of the incoming photon, $\hbar\omega_f$ is the energy of the fluorescence of the edge of interest, $\mu_t(\omega)$ is the total absorption coefficient which includes contributions from the edge of interest, $\mu_e(\omega)$, and from all other atoms and other edges of the element of interest, which we denote $\mu_b(\omega)$. The fluorescence of interest vanishes below the absorption edge, so the expression above corresponds to experimental data from which the pre-edge background has been subtracted. That background, which includes fluorescence from the sample holder, compton and elastic scattering and fluorescence due to other edges and elements is assumed to be smoothly varying with energy across the absorption edge of interest and therefore fitting a pre-edge line, extrapolating past the edge and subtracting from the data effectively removes the fluoresence background past the edge.

The $I_0e^{(-\mu_t(\omega)z_n/\sin\theta_i)}$ term in eq. 2.1 is the number of incoming photons of energy $\hbar\omega$ which made it to a depth z_n (effective optical path $z_n/\sin\theta_i$). $\epsilon_f(\omega)$ is the probability that the core hole created will decay through a radiative process instead of a non-radiative one (i.e. a photon will be emited instead of the excess energy of the excited state being transfered to electron excitations), $\mu_e(\omega)$ is the absorption coefficient of the edge of interest, $dz_n/\sin\theta_i$ is the effective element of length seen by the photons and assumes that the fluorescent atoms are distributed uniformly over the thickness. The last term, $e^{-\mu_t(\omega_f)z_n/\sin\theta_f}$, measures how much of the fluorescence radiation of constant energy $\hbar\omega_f$ escapes out from a depth z_n.

To get the fluorescence signal from the whole sample's thickness we need to evaluate

$$\int_0^{z_s} I_f(z_n)dz_n = I_f(\omega), \tag{2.2}$$

$$I_f(\omega) = \frac{I_0\Omega}{4\pi}\epsilon_f(\omega)\frac{\mu_e(\omega)}{\sin\theta_i}\int_0^{z_s} e^{(-\mu_t(\omega)z_n/\sin\theta_i)}e^{-\mu_t(\omega_f)z_n/\sin\theta_f}dz_n$$

$$= \frac{I_0\Omega}{4\pi}\epsilon_f(\omega)\frac{\mu_e(\omega)}{\sin\theta_i}\frac{e^{-(\frac{\mu_t(\omega)}{\sin\theta_i}+\frac{\mu_t(\omega_f)}{\sin\theta_f})z_n}}{-(\frac{\mu_t(\omega)}{\sin\theta_i}+\frac{\mu_t(\omega_f)}{\sin\theta_f})}\Bigg|_0^{z_s}$$

$$= \frac{I_0(\Omega/4\pi)\epsilon_f(\omega)\mu_e(\omega)}{\mu_t(\omega)+\mu_t(\omega_f)\frac{\sin\theta_i}{\sin\theta_f}}[1-e^{-(\mu_t(\omega)+mu_t(\omega_f)\frac{\sin\theta_i}{\sin\theta_f})\frac{z_s}{\sin\theta_i}}] \quad (2.3)$$

For an "infinitelly" thick sample $\mu_t(\omega) \gg z_s^{-1}$ and therefore $[\mu_t(\omega) + \mu_t(\omega_f)] \gg z_s^{-1}$. Since practically $0 \leq (\theta_{i,f}) \leq 90°$ it follows that

$$[\frac{\mu_s(\omega)}{\sin\theta_i} + \frac{\mu_s(\omega_f)}{\sin\theta_f}] \gg z_s^{-1} \quad (2.4)$$

and then the exponential term in eq. 2.3 can be neglected.
For a thick sample we therefore obtain

$$\frac{I_f(\omega)}{I_0(\omega)} = \epsilon_f(\omega)(\frac{\Omega}{4\pi})[\frac{\mu_e(\omega)}{\mu_t(\omega)+\mu_t(\omega_f)\frac{\sin\theta_i}{\sin\theta_f}}] \quad (2.5)$$

Remembering that the total absorption above the edge includes contributions from the edge of interest and from other atoms and edges of the atom of interest, $\mu_t(\omega) = \mu_e(\omega) + \mu_b(\omega)$, we can immediately see that the measured fluorescence signal I_f/I_0 is not, in principle, proportional to $\mu_e(\omega)$ (the quantity of interest) but has a more complex dependence on it. For example, for the case where the element of interest is concentrated, it dominates the absorption and then $\mu_t(\omega) \approx \mu_e(\omega)$. Since typically $\mu_e(\omega) \gg \mu_e(\omega_f)$ for energies above the edge of interest, the energy dependence of the term in square brackets of eq. 2.5 is washed out (same energy dependence in numerator and denominator) and a nearly constant fluorescence signal is obtained. A similar situation is encountered when the edge of interest corresponds to a heavy atom embedded in a matrix of light atoms since then also $\mu_e(\omega) \gg \mu_b(\omega)$. Configurations that are not as severely affected but still might require significant corrections include those where the edge of interest is that of a dilute atom or a light atom in a heavy matrix.

The fluorescence signal I_f is normalized by the incoming intensity $I_0(w)$. Experimentally, different detectors are used for monitoring $I_{0,f}$ signals. While

I_0 is being detected at different energies ω, I_f is always being detected at the discrete energy ω_f characteristic of the atomic transition that results in the filling of the core hole. The energy dependece in the response of the I_0 detector has to be accounted for to correctly normalize the I_f signal. For quantitative analysis of XAFS which extends over a large energy range this correction can significantly affect the XAFS amplitude. The program *ATOMS* calculates this correction for cases when an ion chamber is used to monitor the I_0 signal based on the fractional volumes of the fill gases. Here we are concerned with correcting the XANES region of the spectra and therefore the energy dependence of the response of the I_0 detector can be approximated by a constant over the ≈ 30 eV of the XANES region.

Back to eq. 2.5, I_f/I_0 corresponds to pre-edge subtracted data; i.e., is zero below the absorption edge of interest. Adding edge-step normalization we obtain a normalized signal N given by

$$N = \frac{\frac{I_f}{I_0}(\omega)}{\frac{I_f}{I_0}(\omega_0^+)} = \left[\frac{\epsilon_f(\omega)\mu_e(\omega)}{\epsilon_f(\omega_0^+)\mu_e(\omega_0^+)}\right]\left[\frac{\mu_t(\omega_f)\frac{\sin\theta_i}{\sin\theta_f} + \mu_b(\omega_0^+) + \mu_e(\omega_0^+)}{\mu_t(\omega_f)\frac{\sin\theta_i}{\sin\theta_f} + \mu_b(\omega) + \mu_e(\omega)}\right] \tag{2.6}$$

where, as before, $\mu_t(\omega) = \mu_e(\omega) + \mu_b(\omega)$ and ω_0^+ indicates an energy above the main absorption edge (the data is actually normalized by the edge-step). Dividing numerator and denominator by $\mu_e(\omega_0^+)$,

$$N = \frac{\mu_e(\omega)}{\mu_e(\omega_0^+)}\frac{\epsilon_f(\omega)}{\epsilon_f(\omega_0^+)}\left[\frac{\frac{\mu_t(\omega_f)}{\mu_e(\omega_0^+)}\frac{\sin\theta_i}{\sin\theta_f} + \frac{\mu_b(\omega_0^+)}{\mu_e(\omega_0^+)} + \frac{\mu_e(\omega_0^+)}{\mu_e(\omega_0^+)}}{\frac{\mu_t(\omega_f)}{\mu_e(\omega_0^+)}\frac{\sin\theta_i}{\sin\theta_f} + \frac{\mu_b(\omega)}{\mu_e(\omega_0^+)} + \frac{\mu_e(\omega)}{\mu_e(\omega_0^+)}}\right]. \tag{2.7}$$

Defining $\beta = \frac{\mu_t(\omega_f)}{\mu_e(\omega_0^+)}$, $\gamma = \frac{\mu_b(\omega)}{\mu_e(\omega_0^+)}$, $\gamma' = \frac{\mu_b(\omega_0^+)}{\mu_e(\omega_0^+)}$ and solving for $\frac{\mu_e(\omega)}{\mu_e(\omega_0^+)}$ we obtain

$$\frac{\mu_e(\omega)}{\mu_e(\omega_0^+)} = \frac{N(\beta\frac{\sin\theta_i}{\sin\theta_f} + \gamma)}{(\beta\frac{\sin\theta_i}{\sin\theta_f} + \gamma' + 1) - N}. \tag{2.8}$$

Since we are concerned with the small energy interval of the XANES region, we made the approximation that $\frac{\epsilon_f(\omega)}{\epsilon_f(\omega_0^+)} \approx 1$ in deriving eq. 2.8. In this small energy range $\mu_b(\omega) \approx \mu_b(\omega_0^+)$ and therefore $\gamma \approx \gamma'$.

FLUO does a pre-edge subtraction and edge-step normalization to the experimentally measured I_f/I_0 to obtain N and uses the tabulated cross sections of McMaster [2] to calculate β and γ to yield the desired corrected, edge-step normalized absorption coefficient $\mu_e(\omega)/\mu_e(\omega_0^+)$ as per eq. 2.8.

Chapter 3

Using the code

3.1 A typical example

FLUO reads an input file *fluo.inp* containing the names of the files needing corrections (and/or files you want to check whether a correction is needed) plus some additional information needed for the calculation such as the element and edge whose XANES is being measured, the relative amounts of atoms in the sample, incident and fluorescent angles, etc. The usage of FLUO can best be described through an example. Assume you have fluorescence data (I_f/I_0) for a concentrated water solution of $(NH_4)_2SO_4$ whose Sulfur K-edge XANES has been measured. *fluo.inp* will then look something like this:

```
% fluo.inp file for 0.94M sulfate solution
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
    e0=2481.15              % e0 to be used for normalization
    central =S  edge=K      % Central atom and edge type
    out=sul094M             % output filename
    atmwei = true           % atomic fractions in weight perc.
    atoms
     S  2.82
     N  2.47
     O  84.18
     H  10.53
    files
       sul094stenor.001  * 0.94M solution  % data + comment
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

%# Input-mode Time-stamp: <99/05/24 17:48:47 haskel>
```

Example *fluo.inp* file corresponding to a 0.94 Molar water solution of $(NH_4)_2SO_4$ at room temperature.

In the same spirit as the other UWXAFS programs, the input file structure is not very rigid in the sense that you can have several keywords and their associated values in the same line or in any order. However, there are two strict rules: The keyword "atoms" indicates the beginning of the atoms list and must be in its own line followed by the list of elements and their relative amounts. The keyword "files" must also be in its own line and indicates the end of the atom list and the beginning of the file list.

When FLUO is run (by typing *fluo* at the command line) with the above input file, the following running message will be displayed to the screen:

```
=================================================================
Fluo --0.02 Correcting for self absorption.      by Daniel Haskel
=================================================================
Atom list given ...
 Mcfluo calculating corrections ...
 Normalizing and correcting data from "sul094stenor.001"
  >>> Wrote ascii output to "sul094M.001"
 fluo is done. Have a nice day
=================================================================
```

Running message written to the screen by FLUO while processing the input file above.

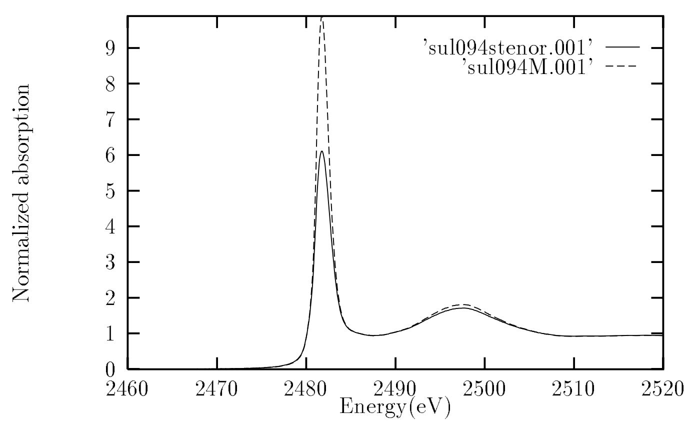

Fig. 2: Fluorescence data of 0.94 Molar water solution of $(NH_4)_2SO_4$ at room temperature before and after self absorption corrections by FLUO

The fluorescence data before and after self-absorption corrections is shown in Fig. 2. Let's look at the input file with more detail. A value of e0 is given and it will be used for edge-step normalization of the measured data. If not given, e0 will be found by FLUO somewhere in the main absorption edge. If the value given is outside the data range FLUO will find its own value. When more than one files are listed in the "files" list, FLUO will energy-align consecutive files relative to the first one for easy comparison of files after correction.

The central atom (the chemical symbol of Sulfur, S) is specified by the keyword "central" (case insensitive). The absorption edge (K-edge) is specified by the keyword "edge" (case insensitive). The output filename is specified by the keyword "out". Since the input/output format is not specified, FLUO will figure out that the input file is in ascii format and then use the same format for the output file. Since there could be several files in the "files" list, FLUO appends an increasing index (001 and up) for the corresponding output files. In the case above the output is written to *sul094M.001*. Since FLUO uses energy derivatives to align different data sets in the "files" list, the energy-derivatives of the uncorrected data are also written out; here to *sul094M_der.001*.

The relative amounts of atomic elements in the sample can be given in atomic percent, their stoichiometric relation in the formula unit or in atomic weight percent. Only if atomic weight percent is used the keyword "atmwei" must be specified and set equal to true. The keyword "atoms" is in its own line, followed by all elements and (in the example here) their relative amounts in atomic weight percent. The keyword "files" is in its own line, followed by the one file (or files) being corrected. The "*" character next to the file indicates a comment line associated with the file and will be appended to the beginning of the output file. Additional information appended to the output file are the edge step and pre-edge line used for data normalization. The value of the maximum derivative and its energy are appended to the derivative output file.

As already mentioned, another use of FLUO is energy alignment of several data scans (transmission or fluorescence). FLUO will attempt to correct the raw data for self absorption only if the keyword "atoms" is found in *fluo.inp* and there is at least one element in the atom list (the central atom). FLUO will stop if something does not make sense (for example "atoms" is found but the central atom is not on the list or you mistyped an element symbol). Hopefully you will also get a meaninfull error message that will help you correct your input file. If "atoms" is not found, *FLUO* will normalize and align the different data scans in the "files" list.

It is worth mentioning that the same theoretical self-absorption correction will be applied to all the data files in the "files" list. This is appropiate for cases where you have different scans of the same sample or scans of the same sample at different temperatures. However, if you have samples of different concentrations you will have to run each file at a time. Of course if you only want energy alignment you can align whatever you want.

Before giving several more examples to illustrate other usage options in the next section, I show in Fig. 3 the raw data for three different solutions of $(NH_4)_2SO_4$ in water before and after self absorption corrections. Assuming that the local environment of the Sulfur atoms doesn't change with concentration and that identical experimental conditions were used in collecting the data, the differences between pre-edge subtracted, edge-step normalized data scans are totally due to self absorption. As seen in Fig. 3, *FLUO* does reasonably well in bringing them close to each other, but by no means is perfect. The correction should be considered good to within about 10%. The limited accuracy in correcting this particular data may suffer from the fact that both K_α and K_β lines of Sulfur were detected in the experiment (only 156 eV apart). However several experimental unknowns will affect the accuracy of the correction in any case. For example, whereas the *mean* incident and fluorescent angles can be taken into account in eq. 2.8, the actual fluorescence photons are collected with a large solid angle and their geometrical absorption paths in the sample will vary significantly across the angular range determined by the large solid angle typically used in fluorescence measurements. Correcting for this effect requires very accurate information on experimental geometries.

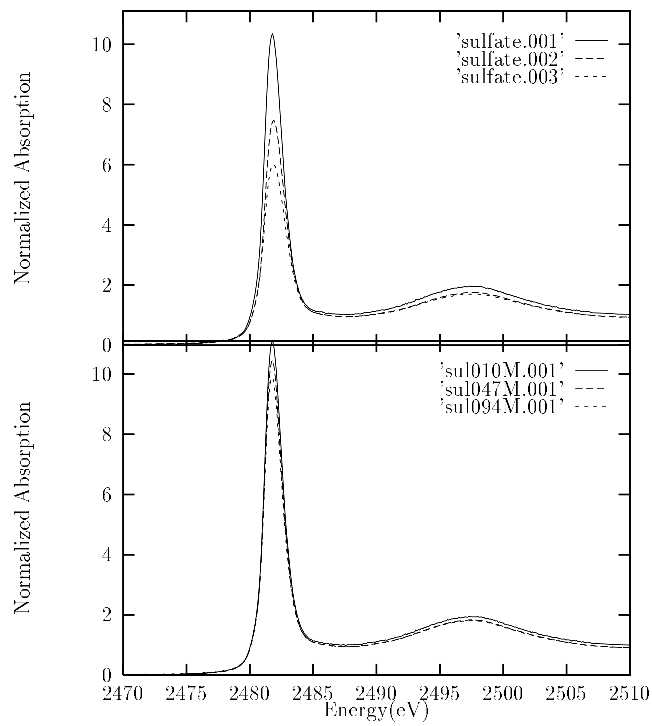

Fig. 3: Upper panel: fluorescence raw data for three different concentrations of $(NH_4)_2SO_4$ in water (0.1 Molar, 0.47M and 0.94M). Lower panel: fluorescence data corrected by FLUO.

3.2 Keywords used by FLUO

This is a list of all the relevant keywords with their meaning used to input information in FLUO:

e0: Value of e0 to be used for pre-edge subtraction and edge step normalization. If not specified it will be found by FLUO. If specified but is outside data range, FLUO will find its own value for e0 (and report it). The edge step used to normalize the data as well as the pre-edge line will be written in the header of the output file.

pre(1,2): Energy boundaries for pre-edge fitting. Values are in eV and relative to e0. Default values are pre1=-200.0, pre2=-50.0. FLUO checks for unreasonable values (e.g. outside data range) and resets value if necessary.

nor(1,2): Energy boundaries for post-edge fitting. Values in eV and relative to e0. Default values are nor1=100.0, nor2=500.0. FLUO checks for unreasonable values and resets if necessary.

out: Name of output filename. If not specified, FLUO will figure out one which is related to the input file name. Usually it will append a file extension ".nor" if the output is uwexafs format or ".00#" if ascii.

formin: Data format of input file(s). Either uwxafs or ascii. It is not required as FLUO knows how to figure that out. Note that you can have both ascii and uwxafs files in your list and the format will be deduced correctly.

formout: Data format of output file(s). Either ascii or uwxafs. Not required. If not specified, FLUO uses the same format of the input file to write the output file(s).

format: For input and output file(s) that have the same data format (uwxafs or ascii). Not required.

angin: Angle (in degrees) between the incident beam and the surface of the sample exposed to the beam. Needed for fluorescence corrections . If not specified, the default is 45 degrees.

angout: Angle (in degrees) between the outgoing radiation (determined by the detector position) and the surface of the sample. Needed for fluorescence corrections. Default is 45 degrees.

cent: Element symbol for central atom. Case insensitive. Needed for fluorescence corrections if atom list is given.

edge: Absorption edge of interest. Can be either K, L1, L2 or L3. Case insensitive. Needed for fluorescence corrections if atom list is given.

atmwei: If set to true indicates that the relative amounts of elements in the atom list are given in atomic weight percent and these will be divided by the respective atomic weight to calculate the cross section. If not specified, default is false.

atoms: Indicates the beginning of the elements' list and their relative amounts. Must be specified for fluorescence corrections to be done. Must be in its own line. The relative amounts of elements can be given in atomic percentage or using the stoichiometry of the formula unit. For example for $BaFe_{12}O_{19}$ one can say;

```
atoms
     ba  1
     fe  12
     o   19
```

If the keyword "atmwei" is used the relative amounts should be given in atomic weight percent.

atoms: Indicates the beginning of file(s) list. Must be in its own line. Following lines contain file(s) names and user supplied comments. Files can be either in ascii or uwexafs format. Comments to be included in the output file header must follow a "*" charachter in the same line of the file name. It looks like this:

```
files
     myfile.xmu,1  * uwxafs format, nkey=1
     myfile.xmu 2  * uwxafs format, nkey=2
     ascii.dat     * this is an ascii file
```

Note that uwexafs files require an "nkey" or "skey" also, separated from the file name by at least one blank space or a comma. If fluorescence corrections are requested, the same corrections will be applied to all the files in the list. The same material at different temperatures or different scans of the same sample need the same corrections. Samples with different concentrations need different corrections and the program needs to be run separately for each.

3.3 Some more examples

This section contains a few more examples to illustrate the use of FLUO.

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%% Example1 fo fluo.inp
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
    central =ba edge=k
    angin=60    angout=10  out =bafile
    atoms
        ba    1
        fe    12
        o     19
    files
         bafeo_amor.xmu 1   * ba edge amorphous 36 K
         bafeo_amor.xmu 3   * ba edge amorphous 300 K

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
```

In example 1 *e0* is not specified so it is find by *FLUO*. The second file will be aligned in energy relative to the first one. The incident and fluorescence angles (relative to the sample's surface) are specified using the keywords *angin* and *angout*. The relative amounts of atom types are given using the stoichiometric relation in $BaFe_{12}O_{19}$. Since input data files are in uwxafs format (nkey given) and, since *formout* is not specified, output files will be written using uwxafs format also (in this example to four records in *bafile*; two records containing the corrected xmu and two records containing the energy derivatives of the uncorrected data used for alignment).

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%% Example 2 for fluo.inp
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
    e0 =37444.4
    central =ba  edge=k
    pre1=-100 pre2=-30 nor1=100 nor2=350
    atmwei = true   formin=uwexafs  formout=uwexafs
    atoms
        ba    137.33
        fe    670.16
        o     304.0
    files
         bafeo_amor.xmu 1   * ba edge amorphous 36 K
         bafeo_amor.xmu 3   * ba edge * amorphous 300 K

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
```

In example 2 the given *e0* value will be used for pre-edge removal and edge-step normalization. Regions for pre-edge and post-edge fitting (relative to *e0*) are specified by keywords pre1, pre2, nor1, nor2. Relative amounts in atom list given in total atomic weight per formula unit. Keyword *atmwei* set to true indicates to FLUO that these quantities need to be divided by the corresponding atom type atomic weight. This is because FLUO calculates cross sections in units of barns/atom. Output files will be in uwxafs format. Since output file name is not specified, the default value will be *bafeo_amor.nor* for the data and *bafeo_amor_der.nor* for the derivatives.

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%% Example 3 for fluo.inp
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
        out=tipt
        format=ascii
    files
        15k.dat        * Ti K-edge in PbTiO3, T=15K
        300k.dat       * Ti K-edge in PbTiO3, T=300K
        600k.dat       * Ti K-edge in PbTiO3, T=600K

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
```

This is a typical example for the use of FLUO as an energy alignment program. Nothing is specified but the files that need energy alignment. FLUO will find *e0* and align all the files relative to the first one. Output is pre-edge subtracted, edge-step normalized data. Output files (data and energy derivatives) will be written in ascii format to tipt.00# and tipt_der.00#. The alignment procedure *does not* add any energy-dependent correction to the post-edge region; i.e., data are aligned in the energy axis but not in the absorption axis. Also the original data can be recovered from the output of FLUO as the pre-edge line and edge-step are written in the header of the output file.

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%% Example 4 for fluo.inp
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
out=cu15c_ali
formin=ascii formout=uwexafs
nor2=800

files
        cu15c.010.xmu           * x=0.15, cpol, 10K
        cu15c.011.xmu           * x=0.15, cpol, 10K
        cu15c.030.xmu           * x=0.15, cpol, 30K
        cu15c.031.xmu           * x=0.15, cpol, 30K
        cu15c.050.xmu           * x=0.15, cpol, 50K
        cu15c.051.xmu           * x=0.15, cpol, 50K
        cu15c.080.xmu           * x=0.15, cpol, 80K
        cu15c.081.xmu           * x=0.15, cpol, 80K
        cu15c.140.xmu           * x=0.15, cpol, 140K
        cu15c.141.xmu           * x=0.15, cpol, 140K
        cu15c.240.xmu           * x=0.15, cpol, 240K
        cu15c.241.xmu           * x=0.15, cpol, 240K

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
```

In this example FLUO will align all the data files (which have ascii format) and write the aligned data and their derivatives in uwxafs format to *cu15c_ali*.

Chapter 4

Program notes

The source code is distributed as a stand alone fortran code. All of the subroutines used in FLUO are written in ANSI standard Fortran-77. The code has been compiled on Intel 486 and Pentium machines running *Linux* using both F2C and GCC and also using GNU Fortran g77 for compilation. The code has also been compiled on Vax-VMS and OPEN-VMS machines.

On VMS machines it is more convenient to open output files with NEW status instead of the UNKNOWN status used in the main program. To change this for use on a Vax-VMS search for the line vaxflg = .false. and change it to vaxflg = .true.

The calculation of the self absorption correction is done by the subroutine *mcfluo* which invokes *mucal* written by Pathikrit Bandyopadhyay. *mucal* uses data from McMaster tables [2] to calculate x-ray cross sections.

Bibliography

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