XRFCOMBI
User Manual

M.Bos
Herikebrink 87
7544 ES ENSCHEDE
NETHERLANDS

July 2009

1 INTRODUCTION

The first version of this manual described the installation and use of the set of programs described in the papers *M.Bos, J.A.M. Vrielink, Anal.Chim.Acta 373(1998)291* and *M.Bos, J.A.M.Vrielink, W.E. van der Linden, Anal.Chim.Acta, 412(2000)203*. It now contains additional information concerning corrections for double photon interactions concerning scatter. The user interface is written in Tk/Tcl. Menu buttons give access to the various programs and some utilities to simplify data entry. Data transfer between the various programs is performed by temporary ascii-files that can be inspected (and edited) by any plain ascii text editor.

The calculation methods **XRFSMPLX**, **XRFROUS**, **SMPLX/SCATTER** and **SMPLX/GICAL** handle concentrations of sample components in terms of chemical compounds directly and produces results in terms of the concentrations of chemical compounds. All other programs start with a conversion of the initial estimate of the sample composition to an estimated elemental composition, refine this elemental composition and produce the result also as an elemental composition.

The choice of the program to use for calculating analytical results should be governed by the guidelines given in the abovementioned papers.

In March 2004 the program **xrfcombi** was extended with the incorporation of second order processes comprising one scattering event and one photoelectric absorption based on the work of G.Tirao and G.Stutz, X-Ray Spectrom. 32 (2003)13. For the rayleigh scattering thr RTAB database from L.Kissel is used. (http://www-phys.llnl.gov/Research/scattering). Compton scattering is handled by a closed equation based on the Thomas-Fermi model.

The test version **xrfcombi022** of July 2009 offers the possibility to import intensity data from socalled fitfiles produced by the program Pymca that was developed at ESRF (V.A. Sole, E. Papillon, M. Cotte, Ph. Walter and J. Susini , Spectrochim. Acta Part B 62 (2007) p. 63).

Apart from the user interface **xrfcombi** and its associated programs that can be run from it, the **bin** directory contains 2 standalone programs **simmul** and **xrfmul** that deal with multilayers.

Bug reports and suggestions for improvement of the programs can be sent by e-mail to m.bos@misc.utwente.nl.

2 INSTALLATION

2.1 Linux

The software is available as a gzipped tar archive **xrfcombi021b.tgz** and can be unpacked in a user directory by the command:

```
tar -xvzf xrfcombi020.tgz
```

To function the software needs an installed version of Tk/Tcl. The program **wish** of this package should be reachable via **/usr/XR11R6/bin/wish**. If this is not the place of **wish**, the first line of the script **~/combiscat/bin/xrfcombi** should be adapted to point to the place of **wish**.

The package *gnuplot* should be available if one wants to use the plot option in the File menu of the calibration step to display calibration lines.

The printing of results is routed via the standard unix printer of the **lpr** command. So attention has to be paid to the **printcap** file.

2.2 W95/W98/W2000, XP, Vista

The software is available as a zipped archive and can be unpacked in a user directory. To function the software needs an installed version of Tk/Tcl for Windows. The package *gnuplot* should be available if one wants to use the plot option in the File menu of the calibration step to display calibration lines. The printing of results is routed via a utility program **lprint.exe** which copies the output to be printed in plain ascii to the port **LPT1**. If no printer is connected to this port the program will hang.

3 USING THE PROGRAM

Once installed the program can be started in its working directory **/combiscat/bin** (Linux) or \ **xrf** \ **bin** (Windows) by typing **xrfcombi** (Linux) or **xrfgo** (Windows) after which the main menu bar (see figure 1) shows up.

Figure 1: Main menu of XRFCOMBI

The first thing to do now is to set the spectrometer characteristics by clicking on the **Spectrometer** button with the left mouse button. Now a data-entry form **SPECTROM.PARAM** appears (figure 2) and all items of it should be filled out by mouse clicking on the entry and typing the pertinent

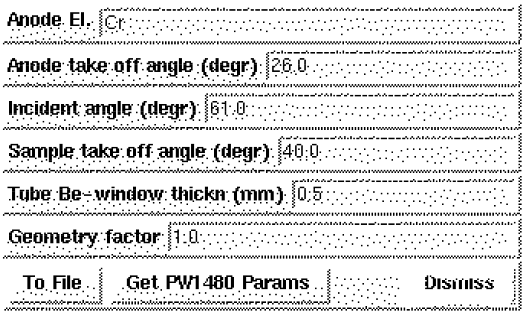

Anode El. Cr
Anode take off angle (degr) 26.0
Incident angle (degr) 61.0
Sample take off angle (degr) 40.0
Tube Be-window thickn (mm) 0.5
Geometry factor 1.0

Figure 2: Entry form for spectrometer data

data in the entries box. When done the **To File** button should be clicked and the window can be dismissed.

Depending on the task that has to be performed one can now make a choice with the buttons **Simulate**, **Calibrate** and **Analyze**. **Help** is not implemented yet.

In the **Simulate**, **Calibrate** and **Analyze** tasks one can define samples or standard samples in terms of already defined compounds. The definitions of these compounds are kept by the system in the file **complist.dat**. New entries in this list can only be made via the **Simulate -> Compounds** menu.

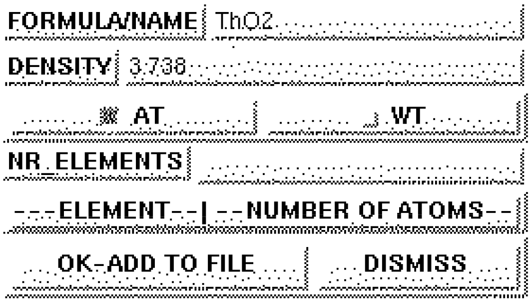
3.1 Simulate

The simulation menu is meant to calculate relative intensities for given lines belonging to elements of a sample with known composition. Clicking on the **Simulate** button of the main menu bar produces the simulation menu (figure 3) via which composition data and the wanted lines can be given.

Figure 3: Bar for Simulation Menu

3.1.1 Compounds

Now the first thing to do is to check whether the systems knows all the compounds of which the sample has to be composed. This can be performed by clicking the **Compounds** button that produces two windows, one named **COMPOUNDS** that shows the list of all known compounds and an entry form to define new compounds (see figure 4). If the list contains all the wanted compounds, the entry form can be dismissed. If not, this entry form should be filled out starting with the name of the compound to be defined in the **FORMULA/NAME** box. Next the density of the compound should be entered in the density box. This quantity is not yet used in the calculations, so at the moment this value is not important, but in the future it will be used to convert mass thickness to normal thickness, so it is better to enter



FORMULA/NAME ThO2

DENSITY 3.738

● AT ○ WT

Figure 4: Entry form for definition of Compounds

the correct value here. Anyhow a value should be entered, otherwise the format of the complist.dat file will be disturbed.

In this release all compounds should be defined in terms of number of atoms of the elements present in the compound, so the radiobutton **AT** should be on(red). If **WT** is chosen the program refuses to accept the entry for now.

Entering the number of different elements present in the compound in the box **NR_ELEMENTS** opens a number of entries in which the symbols of these elements should be entered, followed by the number of atoms of the element in the compound. When the information is entered correctly, then click the **OK-ADD to FILE** button and proceed to the next compound to be defined, overwriting the info in the **FORMULA/NAME** and density box. Clicking in the box **NR_ELEMENTS** removes the old element/number of atoms information and entering a new number of elements for the new compound creates fresh entries for the symbol/ number of atoms items.

When the last new compound has thus been defined and been entered in the list with **OK-ADD TO FILE**, the entry form can be dismissed.

3.1.2 Sample

Clicking the **Sample** button in the **SIMULATION MENU** starts the definition of the composition of the sample for which the intensities have to be calculated. This action opens two windows, the **COMPOUND SELECTION** window (figure 5) and the **DEFINE SAMPLE** window (figure 6). Continue by entering the requested data for **NAME** and **THICKNESS**

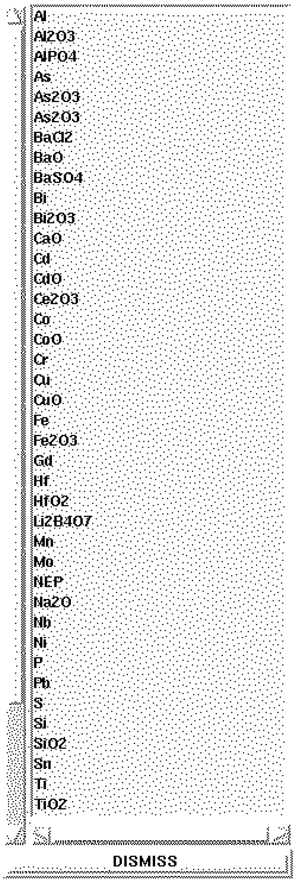
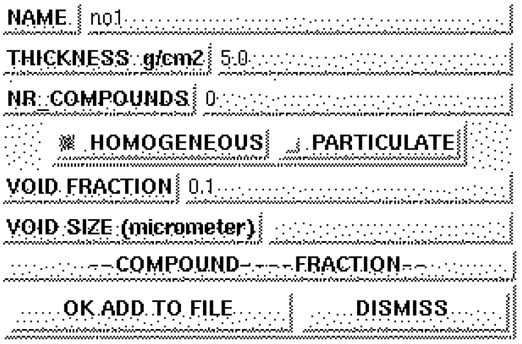


Figure 5: List box with compounds to select

in their boxes. Next click on the names of those compounds listed in the **COMPOUND SELECTION** listbox that should be included in the sample. These compounds will appear automatically as entries in the **DEFINE SAMPLE** entry form. When all necessary compounds have been selected, dismiss the **COMPOUND SELECTION** box. Then adjust the fractions of the compounds in the **DEFINE SAMPLE** form to the right values either by overwriting the fractions shown or just entering them in their boxes. Now click on the **OK ADD TO FILE** button. If you plan to do calculations on a sample with the same compounds but with different contents or with a different thickness, do not dismiss this entry form to be able to use it later



NAME: no1

THICKNESS g/cm2: 5.0

NR COMPOUNDS: 0

● HOMOGENEOUS ○ PARTICULATE

VOID FRACTION: 0.1

VOID SIZE (micrometer):

Figure 6: Entry form for definition of Sample

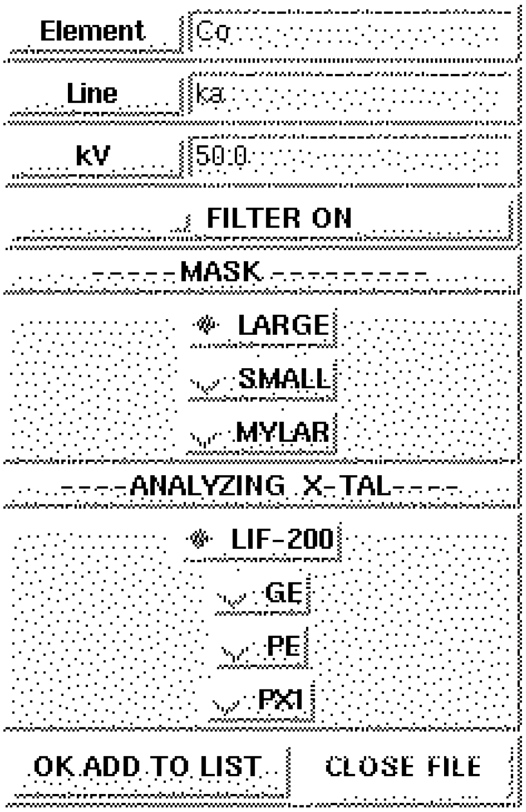
without having to select all compounds again.

The boxes **HOMOGENEOUS**, **PARTICULATE**, **VOID FRACTION** and **VOID SIZE** are not yet used in the program, so don't bother with them.

Now the lines for which the intensities have to be calculated should be entered. Start this process by clicking on the **Lines** button of the **SIMULATION MENU**. This opens the **DEFINE LINES** entry form (figure 7). This entry form is also used in other places in the program where more data is needed than for the simulations that we are dealing with now, so not all entries need to be filled. It suffices to enter the data on **Element** (symbol only), **Line** (line type ka, kb1, kb2, la1, la2, lb1 etc.), **kV** (the voltage the x-ray tube is operated on in kV when the line is measured) and to set the radiobutton **FILTER ON**. When the latter button is red the calculations are performed for the presence of an aluminium filter of 300 μm in the primary beam (we have only this one filter).

Pressing **OK ADD TO LIST** enters this line into the list and when all lines have thus been entered, pressing **CLOSE FILE** writes this list to a diskfile that is used in the calculations. After all lines have been entered the form can be dismissed.

At this stage sufficient data has been entered to start the simulation calculations by clicking on the **Simulate** button of the **SIMULATION MENU**. A DropDown Menu opens and a choice between calculations with or without scattering has to be made by click on one of the entries **Simulate no**



Element Ca

Line ka

kV 50.0

FILTER ON

MASK

● LARGE

○ SMALL

○ MYLAR

ANALYZING X-TAL

● LIF-200

○ GE

○ PE

○ PX1

Figure 7: Entry form for definition of lines

scatter and **Simulate with scatter**. When the calculations are ready the results can be inspected by openening the **Viewer** dropdown menu on the **SIMULATION MENU** bar and clicking on the **View Results Simulation** item. This dropdown menu also gives the opportunity to inspect all data files used for the calculation to check for entry errors. The results can also be printed by opening the **Print** dropdown menu and choosing **Print results**.

If the **DEFINE SAMPLE** entry form was not dismissed earlier it is now possible to repeat the calculations for a different composition or thickness just by changing the pertinent data in this entry form, writing it to file by clicking on **OK ADD TO FILE** button of this **DEFINE SAMPLE MENU** form and clicking the **Simulate** button again, followed by Viewing or Printing.

When done with all the needed simulations, dismiss the **DEFINE SAMPLE** entry form and dismiss the **SIMULATION MENU** by clicking on the **Dismiss Sim. Menu** button on its bar.

3.2 Calibrate

The button **Calibrate** opens the menu bar for the calibration process (see figure 8).

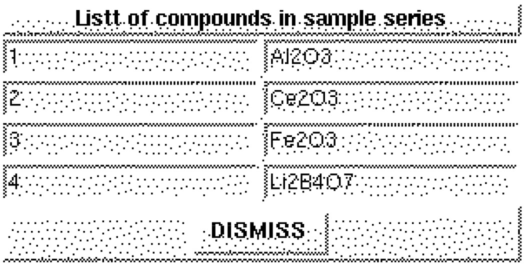
Figure 8: Menu bar for calibration

Data is needed on the composition of the standard samples used for the calibration and on the measured fluorescence lines and their intensities. Entry forms for this data can be opened by clicking on the buttons **Define Sample** (the compounds composing the sample), **Enter Concs** (the fractions of these compounds in the standard), **Define Lines** (the nature of the lines used in the calibration) and **Enter intensities** (the measured intensities for all measured lines for all samples).

The data should be entered in a specific order: **Define Sample** -> **Enter Concs** -> **Define Lines** -> **Enter intensities**.

3.2.1 Define Sample

Clicking on the **Define Sample** button of the **CALIBRATION MENU** bar opens the listbox **COMPOUND SELECTION** (see figure 5 containing all the compounds that the system knows of and a box **SAMPLE COMPOUNDS** that shows the compounds entered thus far (see figure 9). Compounds are entered into the sample by clicking on their name in the listbox **COMPOUND SELECTION**. There is no error correction possibility. On an error just dismiss the **SAMPLE COMPOUNDS** box and start again by clicking on the **Define Sample** button of the **CALIBRATION MENU**. When all compounds that are needed have been entered, dismiss both boxes.

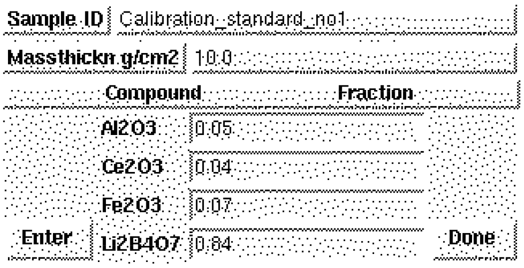

Listt of compounds in sample series

1	Al2O3
2	Ce2O3
3	Fe2O3
4	Li2B4O7

Figure 9: Window showing compounds in sample

3.2.2 Enter Concs

The entry of the composition of the various calibration samples is started by clicking on the **Enter Concs** button of the **CALIBRATION MENU** bar. This action opens an entry form **ENTER CONCS** (see figure 10) and a table **TABLE OF CONCS** (see figure 11) that gives an overview of the composition of the standard samples entered thus far. The entry form should be filled with a sample identification (**Sample ID**), the massthickness in g/cm2 of the sample and the fractions of its constituents. If all entries have been entered correctly the **Enter** button should be pressed to copy the data for this particular sample to the table where it appears automatically. When all standard samples have been treated, the **Done** button of the entry form can be clicked.

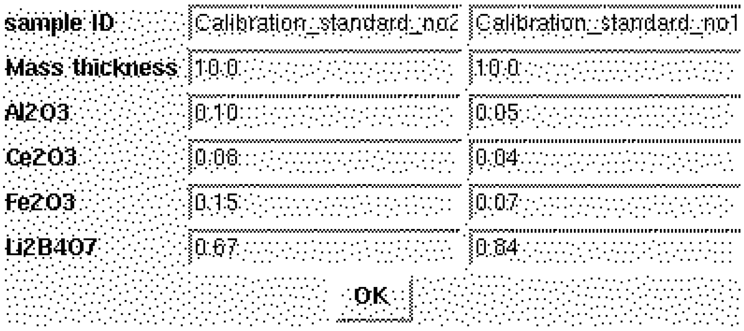

Sample ID: Calibration_standard_no1

Massthickn g/cm2: 10.0

Compound	Fraction
Al2O3	0.05
Ce2O3	0.04
Fe2O3	0.07
Li2B4O7	0.84

Figure 10: Entry form for concentrations of compounds in sample

The next step is to check the contents of the table **TABLE OF CONCS**. If there are mistakes, then correct them by clicking on the pertinent box and



sample ID	Calibration_standard_no2	Calibration_standard_no1
Mass thickness	10.0	10.0
Al2O3	0.10	0.05
Ce2O3	0.08	0.04
Fe2O3	0.15	0.07
Li2B4O7	0.67	0.84

Figure 11: table of entered sample compositions

type the correct value. When all is ok, then click on the **OK** button of the table.

3.2.3 Define Lines

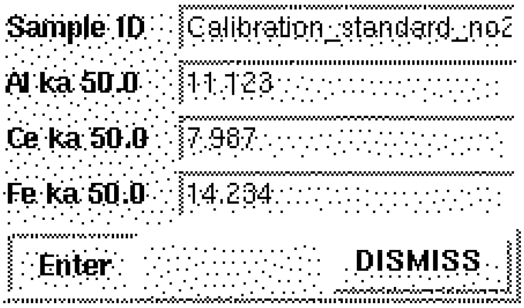
With the **Define Lines** button the same entry form as used in the Simulate menu is opened to indicate which X-Ray Fluorescence Lines haven been measured (see figure 7). Now, however, we are dealing with specific measurements, so all information should be entered correctly. In our laboratory we we either measure with a large mask or a small one, or we measure in cups closed with a mylar film. The choice can be indicated by clicking on the correct radiobutton.

Furthermore we have the choice between four analyzing crystals. The choice is indicated to the system by clicking on one of the radiobuttons **LIF-200**, **GE**, **PE** or **PX1**.

The only thing the system does with this data is to mark calculated calibration constants as belonging to these specific conditions (in the file **listio.dat**), so that in the analyzing phase the correct calibration constants can be found for a given set of measurement conditions. So if you don't find your wanted conditions concerning masks and analyzing crystals here, just pick one and be consistent in using it.

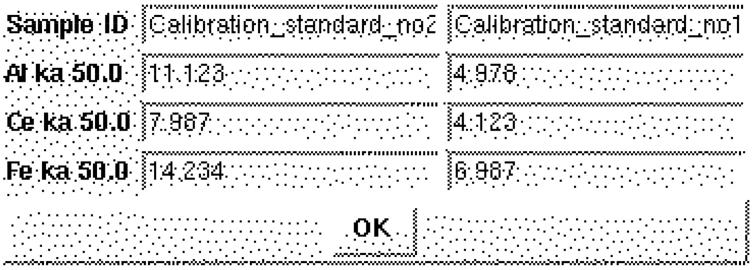
3.2.4 Enter intensities

The final thing to do before the calculations can be started is to enter the measured intensities for all standard samples. The process is started by clicking on the **Enter intensities** button of the **CALIBRATION MENU** bar. This opens and entry form **ENTER INTENSITIES** in which the intensities measured for the indicated sample should be given (see figure 12). Clicking on the **Enter** button of this form copies the data to the **TABLE OF INTENSITIES** (figure 13). If all standard samples have been treated the entry box shrinks and can be dismissed.



Sample ID	Calibration_standard_no2
Al ka 50.0	11.123
Ce ka 50.0	7.987
Fe ka 50.0	14.234

Figure 12: Entry form for measured intensities



Sample ID	Calibration_standard_no2	Calibration_standard_no1
Al ka 50.0	11.123	4.978
Ce ka 50.0	7.987	4.123
Fe ka 50.0	14.234	6.987

Figure 13: Table of measured intensities

After checking the contents of the **TABLE OF INTENSITIES** and correcting the mistakes, this table can be dismissed by clicking its **OK** button. The data is now written to a file which is used in the calibration calculations.

3.2.5 Results

The calibration results can now be obtained by clicking on the **Results** menubutton of the **CALIBRATION MENU** bar. This opens a pull down menu with which the right type of calculations can be started or the results can be inspected and printed. The button **Normal calibration** starts a calibration procedure that uses the normal relative intensities based on the intensities of the pure elements. With the button **Gi-factor calibration** the calibration method from the paper "Non-destructive analysis of small irregularly shaped homogeneous samples by X-ray fluorescence spectrometry", M.Bos, et.al. in Anal.Chim.Acta 412(2000)203, is carried out. It is very well possible to perform the calibration calculation in both ways. The results are kept in different files, i.e. **listio.dat** resp. **listgi.dat** the list of calibration constants (**listio.dat**) that the system uses in the analyzing phase. If scatter corrections are wanted in the analyzing phase, the calibration should be carried out using the menu choices **Calibrate** -> **Results** -> **Scatter calibration**.

3.2.6 File

The **CALIBRATION MENU** bar has a **File** menubutton that gives access to some maintenance functions via a dropdown menu. The last item on this menu **Quit calibration** closes the calibration menu bar. All files used in the calibration calculations can be archived by clicking on the **Save Calib Data** entry of this menu. The entry **Load Calib Data** restores archived calibration to the standard files, which then can be edited by hand if necessary so that a recalculation of calibration constants can be performed.

Finally the calibration constants can be inspected graphically via the gnuplot program by clicking on the **Plot Calib Data** entry of the **File** menubutton.

3.3 Analyze

The button **Analyze** on the main menu bar (figure 1) opens the **ANALYZE SAMPLES** menu bar (see figure 14). This bar shows a number of buttons that give access to the entry forms that should be filled out to enter data on the qualitative composition of the sample (**Compounds in Sample**), the

Figure 14: Analyze menu bar

quantitative composition of the sample for those components of which the concentration is known together with the indication of the quantities to be calculated from the measurements, i.e. unknown concentrations and maybe the massthickness of the sample (**Enter Concs**), the definition of the lines that were used in the measurements (**Define Lines**) and the intensities of the measured lines (**Enter intensities**).

As an alternative for **Enter intensities** the intensities can be imported from socalled *fitfiles* from the ESRF program Pymca for batch processing of spectra measured under the same conditions and samples containing the same compounds. In this case **Enter intensities** should be skipped. To use this facility the form **ENTER CONCS** has to be filled out only **once**.

These entries should be dealt with in the order given.

The **Results** button gives access to the various calculation methods and with the **File** button data that has been entered can be archived or saved data can be retrieved and/or edited.

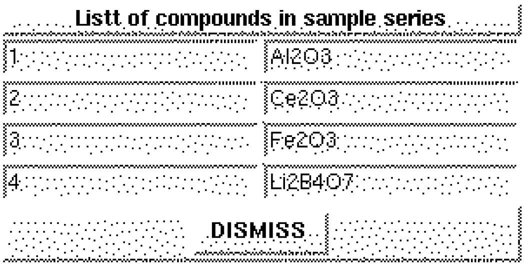
Details for the various entry forms are given below.

3.3.1 Compounds in sample

The first thing to do in an analyzing session is clicking on the **Compounds in sample** button of the **ANALYZE SAMPLES** menu bar and this produces the same **COMPOUNDS SELECTION** listbox with compounds from which the samples can be composed as was used in the calibration menu (figure 5). Clicking on the names of the wanted compounds enters them in the **SAMPLE COMPOUNDS** table (see figure 15). Both windows should be dismissed before continuing.

3.3.2 Enter Concs

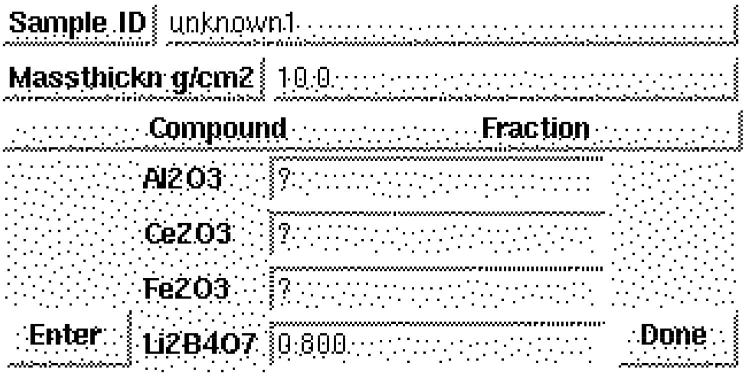
The **Enter Concs** button of the **CALIBRATION MENU** bar opens an entry form and a table. The entry form **ENTER CONCS** shows entries for the sample identification, the massthickness and the concentration of the


Listt of compounds in sample series

1	Al2O3
2	Ce2O3
3	Fe2O3
4	Li2B4O7

Figure 15: Table of sample compounds

constituents of the sample (see figure 16). Unknown concentrations or an unknown massthickness should be given as question marks. Concentrations that are known (i.e. the Li2B4O7 content) should be given as fractions and are kept fixed during the calculations.


Sample ID: unknown1

Massthickn g/cm2: 10.0

Compound	Fraction
Al2O3	?
Ce2O3	?
Fe2O3	?
Li2B4O7	0.800

Figure 16: Entry form for sample composition/unknowns

When this form has been completed for a sample to be analyzed the button **Enter** of this form should be pressed to copy the data to the **TABLE OF CONCS**. As soon as the data of the last sample has been entered this form can be dismissed by clicking on its **Done** button.

The next step is to inspect the **TABLE OF CONCS** for errors, correcting them if there are any and copying them to a system file used in the calculations by clicking on its **OK** button.

As was mentioned above only one sample has to be provided if the insities are imported from Pymca fitfiles.

3.3.3 Define Lines

The definition of the characteristics of the measured lines proceeds exactly as in the calibration section. It is stressed here that entering multiple lines for one element is only possible for the calculation methods that use the simplex algorithm (**XRFSLMPX**, **SMPLX/GICAL** and **SMPLX/SCATTER**). The other calculation methods don't converge if multiple lines for one element are used.

3.3.4 Enter intensities

The procedure to enter the measured intensities is also the same as in the calibration menu. If intensities are to be imported from Pymca fitfiles this step can be skipped.

3.3.5 Import Intens. from Pymca

Data from fitfiles generated by the Pymca software from spectra measured under the same conditions for samples having the same qualitative composition can be processed in a single batch by importing them in xrfcombi using this button. All previous steps except **Enter intensities** should have been carried out before the import. One has to make sure that the file containing the list of the fitfiles to be processed should be in the **\xrf\bin\data** directory. It should have the name **fitfilelist.py** and the format as generated by Pymca . Also make sure that the references to the fitfiles in this list are correct (no forward but backslashes between subdirectories).

3.3.6 Results

The button **Results** of the **ANALYZE SAMPLE** menu bar gives access to the various calculation methods as described in the Anal.Chim.Acta papers and a calculation method that includes the contribution of scatter to the intensities of the measured lines **SMPLX/SCATTER**. The latter calculation method should only be used if the calibration has also been carried out including the contribution for scatter. Only in case the calibration is carried out with the pure element concerned as the only standard this is not necessary.

Choose the wanted calculation method. The calculation results are available when the **Results** button returns from its raised state to the flat state and then can be inspected with the **View** item of the **Results** menu or printed with the **Print** item.

N.B. Only the method **SMPLX/SCATTER** includes scatter contributions and should be used with the corresponding calibration method.

3.3.7 File

The **File** menu button of the **ANALYZE SAMPLE** menu bar gives access to utilities for editing, storing and retrieving the system files that are used in the calculation of the results.

The **Quit** item dismisses the **ANALYZE SAMPLE** menu bar.

4 MULTILAYERS

Apart from the user interface **xrfcombi** and its associated prgrams that can be run from it, the **bin** directory contains 2 standalone programs **simmul** and **xrfmul** that deal with multilayers.

Both programs can only be run from the commandline and rely on the presence of some data files in the **bin/data** directory to provide the needed input data.

4.1 simmul

simmul needs the following datafiles in the ./bin/data directory: (1) **simsampl.dat** and (2) **deflines.dat**. The first contains the structure and quantitative composition of a multilayer sample, the second contains the names of the lines for which the relative fluorescence intensities will be calculated.

The file **simsampl.dat** should contain the following data:

1. Line 1 - number of layers of the sample

2. Line 2 - number of components of toplayer massthickness of toplayer followed by n times a name of a compound from the list **complist.dat** and its fraction in the toplayer. n stands for the number of compounds that the toplayer consists of.
3. Line 3 - same structure as line 2 but now for the layer beneath the toplayer.
4. Line 4 - same structure als line 2 but now for the 3rd layer from the top etc.

An example of **simsampl.dat** is given below:

```
3
2 0.0005  Cu 0.8  Zn 0.2
3 0.001  Cu 0.1 Al 0.1 Zn 0.8
1 10.0 BaTiO3 1.0
```

This files describes a sample with a toplayer of 0.0005 g/cm2 Cu/Zn consisting of 80% Cu and 20% Zn , a middle layer of 0.001 g/cm2 Cu/Al/Zn 10/10/80 % on a substrate of 10.0 g/cm2 pure bariumtitanate.

The file **deflines.dat** should contain the data on the fluorescence lines for which the relative intensity will be calculated. It can be built by hand using an ascii editor, but it can also be constructed using **xrfcombi** -> Simulate -> Lines. Its structure is as follows:

- Line 1 - Element symbol line symbol kV setting
- Line 2 - Element symbol Line symbol kV setting
- etc.

An example for the file **deflines.dat**:

```
Cu ka 50.0
Zn ka 50.0
Al ka 50.0
Ba la1 50.0
Ti ka 50.0
```

Using these files with simmul produces:

```
Rel. int Cu ka is 9.691811e-02
Rel. int Zn ka is 1.469369e-01
Rel. int Al ka is 2.873800e-04
Rel. int Ba la1 is 3.212512e-01
Rel. int Ti ka is 7.387456e-02
```

4.2 xrfmul

The program **xrfmul** can be used to calculate the composition and thickness of the layers of a multilayersample if sufficient measurement data is provided. This program needs 2 data files in de ./bin/data directory: (1) **sample.dat** and (2) **lines.dat**. The structure of the **sample.dat** file is as follows:

- Line 1 - number of layers of the sample
- Line 2 - number of compounds of toplayer , massthickness of toplayer followed by eiher 0 or 1, name of compound #1 fraction of compound #1 in toplayer followed by either 0 or 1, name of compound #2 in toplayer , etc.
- line 3 same structure as line 2 but for layer beneath toplayer
- etc.

massthicknesses and fractions followed by a 0 are refined, those followed by a 1 are kept fixed. For the quantities to be refined an estimate should be given.

An example for the same multilayer as given in the example for **simmul**:

```
3
2 0.0001 0 Cu 0.5 0 Zn 0.5 0
3 0.0001 0 Al 0.33 0 Cu 0.33 0 Zn 0.8 1
1 10.0 1 BaTiO3 1.0 1
```

This setup determines the thickness and composition of the toplayer and the thickness of the second layer and its Al and Cu content. The Zn content is fixed at 80% and so are the thickness and composition of the substrate BaTiO3.

The measurement data should be put in the file **lines.dat** in the format:

- Line 1 - Element Symbol Line symbol kV setting relative intensity
- Line 2 - same structure for next fluorescence line

For the same example:

```
Ti ka 50.0 7.387456E-2
Ba la1 50.0 3.212512E-1
Al ka 50.0 2.8738E-4
Zn ka 50.0 1.469369E-1
Cu ka 50.0 9.691911E-2
```

The relative intensity given in this file for each line should be calculated by hand from the measured intensity by dividing by the slope of the corresponding calibration line.

Running **xrfmul** with both these files in the ./bin/data directory produces:

```
0 Z: 22 line ka rel int. 0.0738746
1 Z: 56 line la1 rel int. 0.321251
2 Z: 13 line ka rel int. 0.00028738
3 Z: 30 line ka rel int. 0.146937
4 Z: 29 line ka rel int. 0.0969181
Line nr 0 RXI found 0.0738745 RXI meas 0.0738746
Line nr 1 RXI found 0.321251 RXI meas 0.321251
Line nr 2 RXI found 0.00028738 RXI meas 0.00028738
Line nr 3 RXI found 0.146937 RXI meas 0.146937
Line nr 4 RXI found 0.0969183 RXI meas 0.0969181
Layer 0 has 2 compounds and a massthickness of 0.0005  g/cm2
Compound Cu wfract 0.8
Compound Zn wfract 0.2
Layer 1 has 3 compounds and a massthickness of 0.001  g/cm2
```

```
Compound Al wfract 0.0999999
Compound Cu wfract 0.100001
Compound Zn wfract 0.8
Layer 2 has 1 compounds and a massthickness of 10  g/cm2
Compound BaTiO3 wfract 1
Ssq is 1.43745e-15
```

It is stressed that the calculations with **xrfmul** and **simmul** do not include scatter contributions.