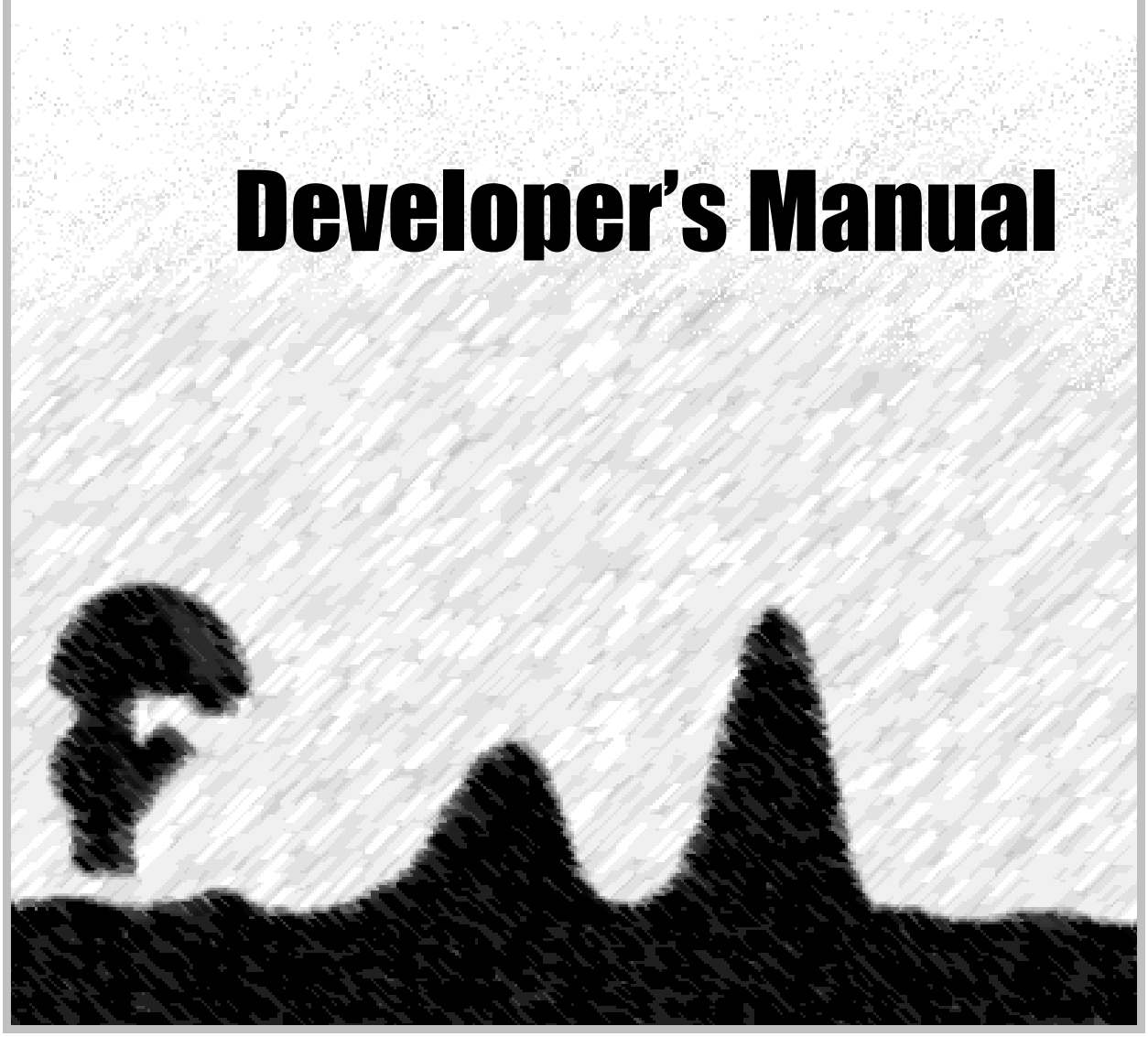
XPS Reduced Data Exchange File

Version 1.1

Developer's Manual



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Developer's Manual

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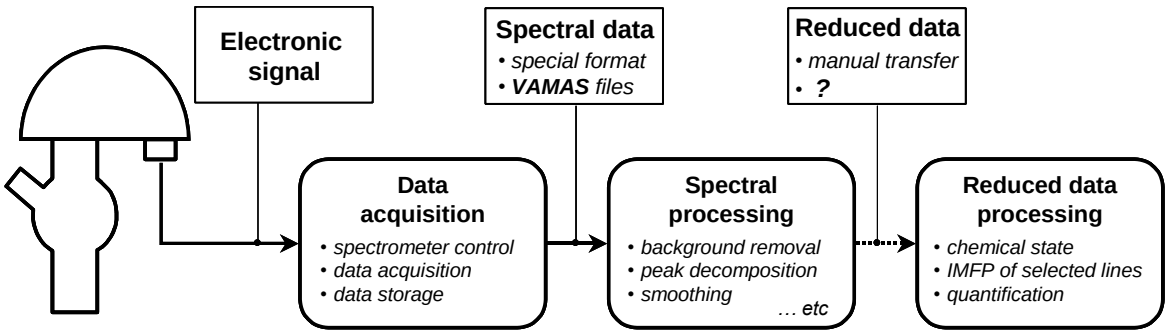
Content

Introduction

The typical data flow in an XPS system and outside is illustrated in the next figure. The data acquisition program controls the instrument's electronics and collects data. The acquired data are usually stored in files with individual format. Application of the programs supplied with the commercial instrument is usually inevitable because of the special requirements needed to control the spectrometers.



However, the programs for spectral processing step can be selected, in general, without restrictions. Lot of these programs can read numerous file formats but the well-known VAMAS file [1] provides a universal solution for transferring spectral data.

The data flow usually stops at this point although transferring of the *reduced data* provided by the spectral processing components, including peak position, FWHM, integral intensity, etc., seems to be trivial task. Looking up line positions in a database [2], calculating IMFP for the determined energies [3], performing special quantification [4-5] usually require manual transfer (i.e., reading and retyping) of data. Transferring larger amount of data by this way is tedious and may be the source of potential errors.

A new file format, the *XPS Reduced Data Exchange File*, is proposed, which defines an "interface" between programs to transfer the derived XPS data.

Although there are several advanced methods available for communication of programs running within one or different computers, a simple way, communication via unformatted character files with defined structure was selected for the proposed task. It has several advantages: it can be applied within one or between more computers, and the latter can be done not only by network but also by offline media. In case of detection computer read errors, the character file can be easily inspected by human reading.

Structure of the XPS Reduced Data Exchange File

Structure of the *XPS Reduced Data Exchange File* is summarised on the following figure using the BNF notation:

```
XPSRDE  version

TITLE  title of data set

[ PARAMETER ]
[ EXCITATION  mg | al | other energy ]
[ CROSS  none | scofield | evans | wagner | nefedov ]
[ IMFP  none | exp exponent | jablonski element | inorganic | polymer ]
[ ANGLE  none | reilman | ebel ]
[ TRANSMISSION  none | frr | fat | exp exponent | file filename ]
[ CONTAMINATION  none | evans | mohai ]
[ LABEL  {name | time | tilt | temperature} ]

ELEMENT
{ symbol line [state] [b.e.] [cross s.] [asym.] [at.w.] [val.] [ox.] }

INTENSITY
{ { [label] } {intensity} }

[ ENERGY
{ { [label] } {energy} } ]

[ FWHM
{ { [label] } {fwhm} } ]

END
```

Legend

Symbol or convention	Meaning
boldface	Words appearing in boldface are keywords or section names. They must be typed as shown.
italic	Words appearing in italic are parameters. The actual value can be used.
[ ]	Brackets enclose one or more optional items.
|	A vertical bar separates alternatives.
{ }	Items enclosed in braces can be repeated one or more times.

The next chapters give detailed description of each element of the file. The following character formatting conventions are used through the text:

Symbol or convention	Meaning
UPPERCASE	Words appearing in uppercase are keywords. They must be typed as shown.
lowercase	Words appearing in lowercase are parameter keywords. They must be typed as shown.
italic	Words appearing in lowercase italic are parameters. The actual value can be used.
<tab>	Item separator character. It can be tabulator (TAB, ASCII 9) or semicolon (ASCII 59)
<cr/lf>	End of line character(s). It can be carriage return (CR, ASCII 13), linefeed (LF, ASCII 10) or both (CRLF).
...	The previous items can be repeated.

Spaces and empty lines may be inserted between items to improve human readability.

Header keyword

The header keyword identifies the *XPS Reduced Data Exchange File* format, thus it must be the first line of the file. As an exception, all letters of the keyword are significant. The presence of the version number enables further development of the exchange files. The present specification describes the version 1.1.

Syntax

XPSRDE<tab>***version number***<cr/lf>

Status: obligatory

Parameters

XPS Reduced Data Exchange File version number

Example

```
XPSRDE      1.1
```

Title keyword

The *Title* keyword supplies a name for the XPS quantification dataset. The dataset title can be used for identification purposes by the target application, can be displayed or printed in the header of the reports. If the title is omitted or the source application does not supply a global dataset title, an empty parameter must be entered after the *Title* keyword.

Syntax

```
TITLE<tab>Tile of the dataset<cr/lf>
```

Status: obligatory

Parameters

Title of the dataset

Example

```
TITLE       Al2O3 on Al ion etch series
```

Parameter section

In the *Parameter* section, various optional parameters of the XPS measurements can be passed to the target application. The keywords can be present in any order within the section. This section and all of the parameters are optional. Instead of the missing parameters, the default values can be used in the target application.

Syntax

```
PARAMETER<cr/lf>
keyword<cr/lf>
keyword<cr/lf>
...
```

Status: optional

Parameters

Parameter keywords (optional)

Example

```
PARAMETER
excit    mg
cross    scofield
label    name    tilt
```

Excitation keyword

The *Excitation* keyword specifies the excitation source (and source energy) of the XPS measurements. If the keyword is omitted, the default value is used.

Syntax

EXCITATION<tab>**excitation source**<cr/lf>

Status: optional

Parameters

Name of the excitation source

mg	Mg Kα excitation source (1253.6 eV)
al	Al Kα excitation source (1486.6 eV)
other<tab>***energy***	Other excitation source; the energy must be specified

Example

```
EXCIT   mg
```

```
EXCIT   other   5417.0
```

Cross section keyword

The *Cross section* keyword specifies the cross section or sensitivity factor set. The values of this set will be used when explicit cross sections or sensitivity factors are not supplied. If the keyword is omitted, the default value is used.

Syntax

CROSS<tab>**cross section set**<cr/lf>

Status: optional

Parameters

Name of the cross section or sensitivity factor set

none	No library set is used
scofield	Theoretical relative differential cross sections of *Scofield*, separate sets for Mg Kα and Al Kα excitations [6]
evans	Experimentally based relative differential cross sections of *Evans et al.* for Mg Kα excitation [7]
wagner	Experimentally based relative sensitivity factors of *Wagner et al.* for Mg Kα and Al Kα excitation [8]
nefedov	Experimentally based relative sensitivity factors of *Nefedov et al.* for Al Kα excitation [9,10]

Example

```
CROSS  evans
```

```
CROSS  scofield
```

IMFP keyword

The *IMFP* keyword specifies the basic correction method for the inelastic mean free path of the XPS measurements. If the keyword is omitted, the default method is used. The target application may use more advanced methods (e.g., TPP-2M).

Syntax

IMFP<tab>**IMFP correction method**<cr/lf>

Status: optional

Parameters

Name of the IMFP correction method

none	No IMFP correction
exp<tab>***exponent***	Exponential approach with the specified exponent
jablonski<tab>**class**	*Jablonski*'s exponential approach with pre-set exponents for different material classes [11]

Name of the material class

elem	For elements
inorg	For inorganic materials
poly	For polymers

Example

```
IMFP   exp    0.7
```

```
IMFP   jabl   inorg
```

Angle keyword

The *Angle* keyword specifies the angular correction method for the XPS measurements. If the keyword is omitted, the default method is used.

Syntax

```
ANGLE<tab>angular correction method<cr/lf>
```

Status: optional

Parameters

Name of the angular correction method

none	No angular correction
reilman	Method of *Reilman et al.* [12]
ebel	Method of *Reilman et al.* with correction for elastic scattering by *Ebel et al.* [13,14]

Example

```
ANGLE  reilman
```

Transmission keyword

The *Transmission* keyword specifies the correction method for analyser transmission of the XPS measurements. If the keyword is omitted, the default method is used.

Syntax

TRANSMISSION<tab>**transmission correction method**<cr/lf>

Status: optional

Parameters

Name of the transmission correction method

none	No transmission correction
frr	Fixed analyser transmission or constant analyser energy mode (E^{-1})
fat	Fixed retarding ratio or constant retarding ratio mode (E^{1})
exp<tab>***exponent***	Exponential function is applied with the given exponent (E^{a})
file<tab>***filename***	Exponential or polynomial function is applied with separate coefficient sets for different kinetic energy ranges. Coefficients of the function is described in separate file [5]

Example

```
TRANS   frr
```

```
TRANS   exp    -0.8
```

```
TRANS   file   mytrans.mtr
```

Contamination keyword

The *Contamination* keyword specifies the correction method for surface contaminations of the XPS measurements. If the keyword is omitted, the default method is used.

Syntax

```
CONTAMINATION<tab>contamination correction method<cr/lf>
```

Status: optional

Parameters

Name of the transmission correction method

none	No contamination correction
evans	Static method of *Evans et al.* is applied [7]
mohai	Dynamic method of *Mohai* is applied. Intensity data for C1s line must be present [5,15]

Example

```
CONT   evans
```

Label keyword

The *Label* keyword defines the label sets used to identify the experiments of the XPS measurements. The values of the defined labels must be given in the *Experiment* records. If the keyword is omitted, no labels are used.

Syntax

```
LABEL<tab>label set<tab>label set<tab>...<cr/lf>
```

Status: optional

Parameters

Name of the label sets. Minimum one and maximum four set names must be specified. The order of the set names cannot be altered.

name	The *Name* alphanumeric label set is selected
time	The *Time* numeric label set is selected
tilt	The *Tilt angle* numeric label set is selected
temperature	The *Temperature* numeric label set is selected

Example

```
LABEL  time
```

```
LABEL  time   tilt
```

```
LABEL  name   time   temp
```

```
LABEL  name   time   tilt   temp
```

Element section

The *Element* section enumerates the elements and supplies the basic quantification data for the XPS measurement. At least one and maximum of 20 element records must be present.

Syntax

```
ELEMENT<cr/lf>
element record<cr/lf>
element record<cr/lf>
...
```

Status: obligatory

Parameters

Element quantification data records

Example

```
ELEMENT
C   1s                  0.225
O   1s    OH    531.0   0.624   2.000   16.00   2   0
Al  2p
S   2p    S6+                                   6   3
```

Element record

The *Element* records supply basic quantification data for the elements of the XPS measurement. At least one and maximum of 20 element records must be present. The missing data are replaced by the target application's default values. The energy values in this section are supplied for transmission and IMFP approximation. For chemical state determination, values provided in the *Energy* section can be used.
Items of the *Element* records are positional parameters, i.e., the separator of the omitted parameter must be present if there are any further parameters.

Syntax

symbol<tab>***line***<tab>***state***<tab>***energy***<tab>***cross***<tab>***asym***<tab>***atw***<tab>
valence<tab>***oxygen***<cr/lf>

Status: one obligatory and more optional

Parameters

Element quantification data

symbol	Chemical symbol of the element
line	Photoelectron line assignation of the element
state	*Optional*. Chemical state of the similar elements
energy	*Optional*. Nominal binding energy (eV) of the line
cross	*Optional*. Cross section or sensitivity factor of the line
asym	*Optional*. Asymmetry parameter of the line
atw	*Optional*. Atomic weight of the element
valence	*Optional*. Valence of the element at the given chemical state
oxygen	*Optional*. Number of O atoms in a mol of specified oxide

Example

```
Al  2p
```

```
C   1s                0.225
```

```
O   1s    OH    531.0   0.624   2.000   16.00   2   0
```

Intensity section

The *Intensity* section supplies the integrated intensity data (and also the labels) of the XPS experiments. An experiment (also called *scan* or *level*) is a set of corresponding photoelectron integrated intensity data, e.g., a step in an ion etch series. At least one and maximum 40 intensity records must be present.

Syntax

```
INTENSITY<cr/lf>
experiment record<cr/lf>
experiment record<cr/lf>
...
```

Status: obligatory

Parameters

Intensity (labels and integrated intensity values) data records

Example

```
INTENSITY
Sample-A    0     1000   2000   3000
Sample-A    10    1000   2000   3000
Sample-A    20    1000   2000   3000
Sample-A    30    1000   2000   3000
Sample-B    0     1000   2000   3000   4000
Sample-C    0     1000   2000   3000   5000
Sample-D    0     1000   2000   3000   6000
```

Intensity record

The *Intensity* record supplies the label and integrated intensity data of one experiment (e.g., one step in an ion etch series) of the XPS measurement. At least one and maximum of 40 intensity records must be present.
Items of the *Intensity* records are positional parameters, i.e., the separator of the omitted parameter must be present if there are any further parameters.

Syntax

```
label<tab>label<tab>...<tab>intensity<tab>intensity<tab>...<cr/lf>
```

Status: one obligatory and more optional

Parameters

Label and intensity data

label	*Optional.* Labels for each label set specified by the *Label* keyword in the *Parameter* section
intensity	Integrated photoelectron intensity data (counts) for each element specified in the *Element* section

Example

```
Sample-A   0    1000    2000    3000
```

```
10     1000     2000     3000    4000    5000
```

```
1000    2000    3000    4000           6000
```

Energy section

The *Energy* section supplies the actual line position data (and also the labels) for each XPS experiment. An experiment (also called *scan* or *level*) is a set of corresponding photoelectron binding energy data, e.g., a step in an ion etch series. At least one and maximum 40 energy records can be present.

Syntax

```
ENERGY<cr/lf>
energy record<cr/lf>
energy record<cr/lf>
...
```

Status: optional

Parameters

Energy (labels and binding energy values) data records

Example

```
ENERGY
Sample-A    0    284.6    531.0    103.1
Sample-A    10   284.6    531.0    103.1
Sample-A    20   286.5    531.5    101.4
Sample-A    30   286.5    531.5    99.2
Sample-B    0    284.6    531.0    103.2    74.3
Sample-C    0    284.6    531.3    103.1    74.1
Sample-D    0    284.6    531.2    103.3    74.5
```

Energy record

The *Energy* record supplies the label and actual line position data of one experiment (e.g., one step in an ion etch series) of the XPS measurement. At least one and maximum of 40 energy records must be present.
Items of the *Energy* records are positional parameters, i.e., the separator of the omitted parameter must be present if there are any further parameters.

Syntax

```
label<tab>label<tab>...<tab>energy<tab>energy<tab>...<cr/lf>
```

Status: one obligatory and more optional

Parameters

Label and line position data

label	*Optional.* Labels for each label set specified by the *Label* keyword in the *Parameter* section
energy	Photoelectron line position data (binding energy, eV) for each element specified in the *Element* section

Example

```
Sample-A   0   284.6   531.0   103.1
```

```
10    284.6    531.0    103.1    74.3
```

```
284.6    531.0   103.1          71.8
```

FWHM section

The *FWHM* section supplies the correct line width (full width at half maximum) data (and also the labels) for each XPS experiment. An experiment (also called *scan* or *level*) is a set of corresponding photoelectron line width data, e.g., a step in an ion etch series. At least one and maximum 40 FWHM records can be present.

Syntax

```
FWHM<cr/lf>
fwhm record<cr/lf>
fwhm record<cr/lf>
...
```

Status: optional

Parameters

FWHM (labels and full width at half maximum values) data records

Example

```
FWHM
Sample-A    0     2.1   1.9   1.8
Sample-A    10    2.1   2.0   1.8
Sample-A    20    2.2   2.1   1.9
Sample-A    30    2.2   2.1   2.0
Sample-B    0     2.1   1.9   1.8   3.0
Sample-C    0     2.1   1.9   1.8   2.95
Sample-D    0     2.34  2.15  1.86  1.87
```

FWHM record

The *FWHM* record supplies the label and line width (full width at half maximum) data of one experiment (e.g., one step in an ion etch series) of the XPS measurement. At least one and maximum of 40 FWHM records must be present.
Items of the *FWHM* records are positional parameters, i.e., the separator of the omitted parameter must be present if there are any further parameters.

Syntax

```
label<tab>label<tab>...<tab>fwhm<tab>fwhm<tab>...<cr/lf>
```

Status: one obligatory and more optional

Parameters

Label and line width data

label	*Optional.* Labels for each label set specified by the *Label* keyword in the *Parameter* section
fwhm	Photoelectron line full width at half maximum data (eV) for each element specified in the *Element* section

Example

```
Sample-A   0    0    2.1   1.9   1.8
```

```
10     2.34    2.15   1.86   1.87
```

```
1.43    1.37   1.29   1.35          1.38
```

End of file keyword

The end of file keyword identifies the end of the *XPS Reduced Data Exchange File*.

Syntax

```
END<cr/lf>
```

Status: obligatory

Parameters

None

Example

```
END
```

Notes on File Structure

- In version 1.0 of the *XPS Reduced Data Exchange File*, the *Intensity* section was named *Experiment* section and the *Energy* and *FWHM* sections were not implemented.

- Any of the *Intensity*, *Energy* or *FWHM* sections can be omitted from the *XPS Reduced Data Exchange File* but at least one of them must be present, depending on the purpose of the target application. (E.g., a quantification application does not need FWHM data; a chemical state database does not need intensity values; etc.)

- The number of the experiment records must be the same in the *Intensity*, *Energy* and *FWHM* sections.

- The content of labels in the *Intensity*, *Energy* and *FWHM* sections must be identical because the target application may process only one of these sections.

- The energy values given in the *Element* section are *nominal* energy data for transmission and IMFP approximation, while the values in the *Energy* section are the actual, accurate line positions for chemical state determination.

Example Exchange files

A general example with four elements (O is in two separate chemical states) and four experiments labelled with name and time. All optional parameters, intensity, energy and FWHM data are specified. Basic quantification data of the first O1s line are also specified.

```
XPSRDE    1.1

TITLE     Test experiments

PARAMETER
EXC       mg
CROSS     evans
IMFP      jabl   inorganic
ANGLE     reilman
TRANS     exp    -0.8
CONT      mohai
LABEL     name time

ELEMENT
O    1s     OH    531   0.624   2   16   2   0
O    1s     =O
C    1s
Al   2p

INTENSITY
aaa    0     1000    1500    2000    2500
bbb    10    1500    2000    2500    3000
ccc    20    2000    2500    3000    3500
ddd    30    3500    4000    4500    5000

ENERGY
aaa    0     284.6   531.0   103.1   74.3
bbb    10    284.6   531.2   103.2   71.4
ccc    20    284.6   531.2   101.9   71.2
ddd    30    284.6   531.5   99.4    71.2

FWHM
aaa    0     2.1     1.9     1.8     3.0
bbb    10    2.1     2.0     1.8     3.1
ccc    20    2.2     2.0     1.9     3.1
ddd    30    2.2     2.1     1.9     3.1

END
```

An example with two elements and two experiments with the minimal additional information from the source application.

```
XPSRDE   1.1
TITLE
ELEMENT
O    1s
C    1s
INTENSITY
1000   1500
2000   3000
END
```

In the next example semicolon is used as item separator. Spaces are also added for readability. Separators after the omitted positional parameters are included (O1s record).

```
XPSRDE; 1.1
TITLE; Semicolon and spaces as item separator
PARAMETER
EXCIT;  other; 5417.0
IMFP;   exp; 0.7
ANGLE;  none
TRANS;  exp;  -0.8
CONT;   none
LABEL;  name; time
ELEMENT
C; 1s; CH
O; 1s; ; ; 0.123
INTENSITY
aaa; 10; 1000.1; 1500.1
bbb; 20; 1500.1; 2000.1
ccc; 30; 2000.1; 2500.1
ENERGY
aaa; 10; 284.6; 531.5
bbb; 20; 284.6; 531.4
ccc; 30; 284.6; 531.2
END
```

Comma is applied as decimal separator. Empty lines are added before sections.

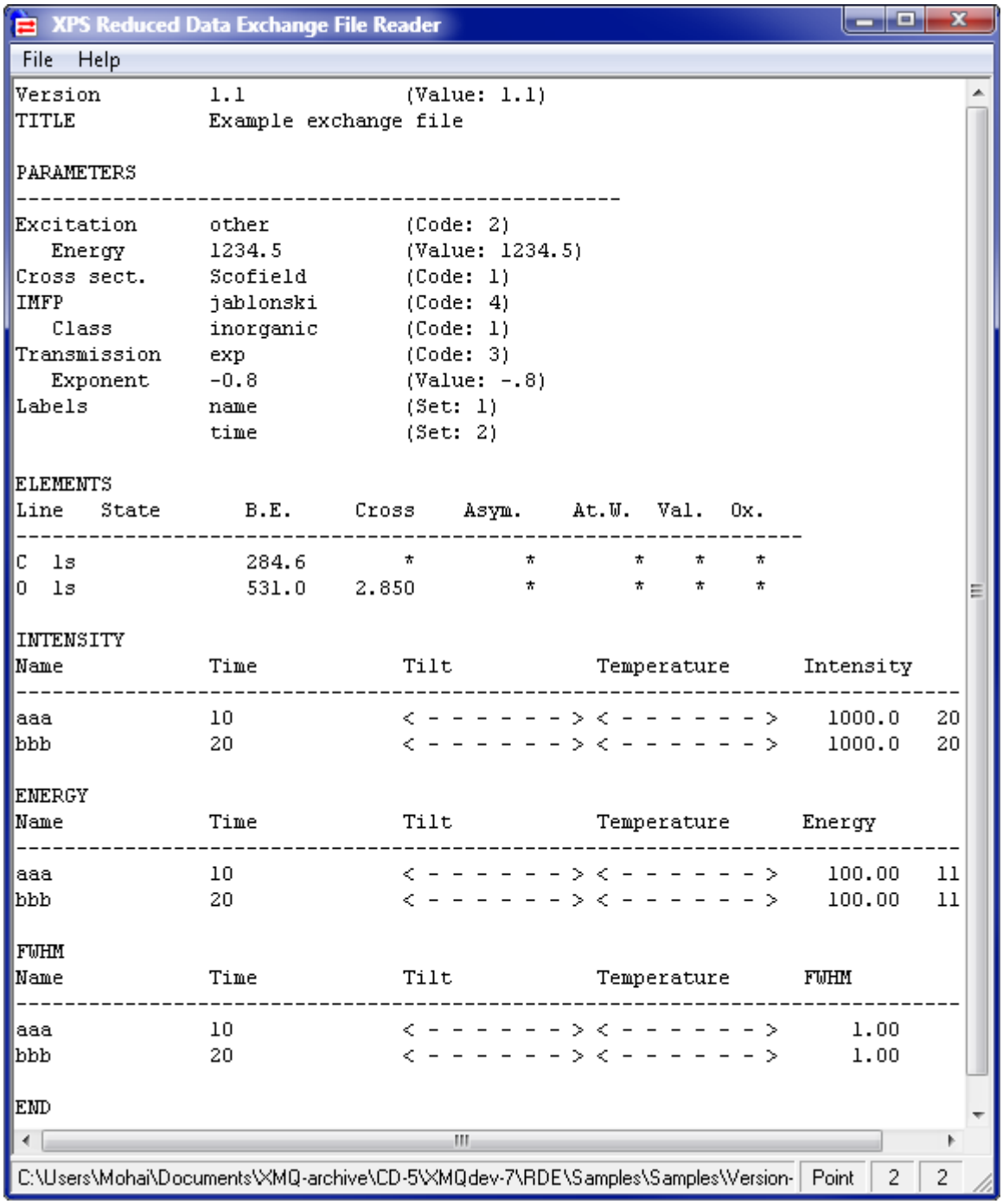
```
XPSRDE    1.1
TITLE     Comma as decimal separator

PARAMETER
IMFP      exp    0,5
TRANS     exp    -0,8
CONT      none
LABEL     name   time

ELEMENT
C    1s     C
O    1s

INTENSITY
aaa    10    1000,1   1500,1
bbb    20    1500,1   2000,1
ccc    30    2000,1   2500,1

END
```

An example of version 1.0 XPS Reduced Data Exchange file. The keyword EXPERIMENT is used instead of INTENSITY and no Energy or FWHM sections are allowed.

```
XPSRDE   1.0
TITLE
ELEMENT
O    1s
C    1s
EXPERIMENT
1000   1500
2000   3000
END
```

The Exchange file reader program

The *XPS Reduced Data Exchange File Reader* program can be used to verify the exchange files and analyse the possible errors. Target applications, including XPS MultiQuant, usually do not give detailed error descriptions when reading incorrect exchange files, thus the author of the exchange files (source application) is responsible for the accurate content and format.
The program uses the same parsing engine as built into XPS MultiQuant.



Menus

File / Open…
This command invokes the *Open XMQ Exchange file* dialog box for selecting files to read. Files can also be opened by drag and drop the file from the Windows Explorer to the main window.

File / Re-read
This command opens and reads again the current file. It is useful when the same file is under test.

File / Exit
Quits the program.

Help / About…
This command invokes the program's about box, showing the version numbers of the program and the exchange files.

Copy
The *Copy* command is available in the pop-up menu (*right click*).

Main window

The content of the file, together with the interpreted values are listed in the main window. Section names are underlined and header rows are provided for the *Element, Intensity, Energy* and *FWHM* records for better readability. In the *Parameter* section, after the name of a keyword its parameter is printed, as found in the file. Next, in parenthesis, the interpreted value is displayed. The names of the sub-parameters are intended.

Code
The *Code* item shows the numeric codes assigned to the different parameters by the parser. They must be equal with the numbers enumerated in the following table if interpretation was correct.

Keyword	Parameter	Code
Excitation	*Mg*	0
	Al	1
	other	2
Cross section	*none*	0
	Scofield	1
	Evans	2
	Wagner	3
	Nefedov	4
IMFP	*none*	0
	exponential	2
	Jablonski	4
Class	*element*	0
	inorganic	1
	polymer	2

Keyword	Parameter	Code
Angle	*none*	0
	Reilman	1
	Ebel	2
Transmission	*none*	0
	FAT	1
	FRR	2
	exponential	3
	file	4
Contamination	*none*	0
	Evans	1
	Mohai	2

Value
The *Value* item shows the interpreted (numeric) version of the preceding parameter. They must be identical, in spite the conversion differences (e.g., decimal separator). The decimal separator in the *Value* item is always point.

Set
The *Set* item shows the code (1-4) of the label set. Numbers in the *Set* items must be in ascending order and unique (i.e., the order of the label sets cannot be changed and label set names cannot be repeated).

Special notes in the main window

< - - - - - - >	empty label marker
*	missing (default) element, intensity, energy or FWHM data
********** *keyword*	unknown keyword marker

Status bar

The status bar shows the name and path of the current file, the decimal separator (*point* or *comma*) of the current locale and the number of detected elements and experiments. If the path is long and the filename cannot be read, double click to alter the alignment of the text. The *Tool Tip* (appearing when the mouse pointer paused over the status bar panels) helps to identify the items.

Example files

Several *XPS Reduced Exchange Files* are available to test various features of the files. The feature to test is identified by the parameter of the TITLE keyword. Examples are divided into three categories: correct, acceptable and erroneous files.

Calling target application

The source application, after preparing the *XPS Reduced Data Exchange File*, may call the target application (e.g., XPS MultiQuant) passing the file name as parameter.

The following example illustrate the *Shell* function of the Visual Basic language to perform the above task:

```
TaskID = Shell("XMQ.exe testfile.mqx", 1)
```

Error messages

Element section must precede experiment sections
Element section must be before the *Intensity*, *Energy* or *FWHM* sections.

Element section not found
The ELEMENT keyword is missing in the Exchange file. The element records regarded as unknown keywords.

END keyword not found
The end of file is reached but the END keyword not found.

Error [*Number***] [***Description***]**
An unexpected error occurred.

Illegal angular correction method
The specified angular correction method is unknown. Method is set to *None*.

Illegal contamination correction method
The specified contamination correction method is unknown. Method is set to *None*.

Illegal cross section set
The specified cross section set is unknown. *None* is selected.

Illegal exchange file header
The file header is not the expected character sequence or the file is not an *XPS Reduced Data Exchange* file. Fatal error; the file is abandoned.

Illegal exchange file version
The version number is not the expected value. The file may be corrupted or too old. Fatal error; the file is abandoned.

Illegal excitation code
The specified excitation code is unknown. Excitation is set to *Mg*.

Illegal IMFP material class
The IMFP material class is unknown. Class is set to *Element*.

Illegal IMFP method
The specified IMFP correction method is unknown or the method is not allowed in *XPS Reduced Data Exchange* files. Method is set to *None*.

Illegal label set
The specified label set is unknown or the set is not allowed in *XPS Reduced Data Exchange* files. No label set is selected; labels are mixed with intensity values.

Illegal transmission correction
The specified transmission correction method is unknown. Method is set to *None*.

Invalid excitation energy
The specified excitation energy is less or equal with zero.

No experiment section (Intensity, Energy, FWHM) found
One of the experiment sections (*Intensity, Energy* or *FWHM*) must be present in the XPS Reduced Data Exchange files.

Number of experiments not equal in sections
The number of the experiment records must be the same in the *Intensity*, *Energy* and *FWHM* sections.

TITLE keyword not found
Using of the TITLE keyword is obligatory.

Too many elements
There are too many (>20) element records in the ELEMENT section.

Too many experiments in [*section name***] section**
There are too many (>40) experiment records in one of the experiment sections (*Intensity*, *Energy* or *FWHM*).

Unknown keyword: [*word***]**
The word is not recognised as valid keyword.

Compatibility issues

The target applications, including *XPS Reduced Data Exchange* file reader program and XPS MultiQuant, should be designed to read files prepared on various computer systems, if possible, without any previous conversion.

Character encoding

The *XPS Reduced Data Exchange* files are usually simple ASCII files but files with Unicode Little Endian, Unicode Big Endian and UTF-8 encoding can be also read without conversion.

Line terminators

Line terminator characters can be LF (linefeed), CR (carriage return) and CRLF characters, thus files written under DOS, Windows, Unix, Linux and Macintosh operating systems can be read without conversion.

Decimal separators

The decimal separator character can be either point or comma, regardless of the current locale settings. However, using of digit grouping symbols should be avoided because they may cause unpredictable results.

Item separators

The item separator character can be TAB (tabulator) or semicolon.

Keywords and parameters

All keywords and parameters are case insensitive. Usually the firs four characters are significant, except the header and when the keyword is less than four characters.

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