

Moss Winn 4.0 Pre

Manual

revision 2012.03.28

**Written by
Dr. Zoltán Klencsár**

1995–2012

CONTENTS

1. INTRODUCTION	4
2. CONTACTS	5
3. SOFTWARE PROTECTION	5
4. ABBREVIATIONS	5
5. HARDWARE / SOFTWARE REQUIREMENTS	6
5.1. MINIMUM HARDWARE REQUIREMENTS.....	6
5.2. RECOMMENDED HARDWARE.....	6
5.3. SOFTWARE REQUIREMENTS	6
6. INSTALLATION	6
7. DIRECTORIES USED BY MOSSWINN	7
8. CONFIGURATION FILES	9
9. I/O OPERATIONS	13
9.1. DATA FORMATS THAT CAN BE LOADED WITH MOSSWINN.....	13
9.2. TO MAKE MOSSWINN UNDERSTAND OTHER ASCII DATA FORMATS	14
10. THE LOAD MENU	17
11. THE SAVE MENU	18
12. MANAGING THE WINDOWS IN THE MAIN MENU	19
12.1. FUNCTIONALITY OF THE HEADLINE OF THE WINDOWS	19
12.2. ALTERNATIVE OPTIONS INVOKED BY THE RIGHT MOUSE BUTTON.....	20
13. THE ARRANGE MENU	20
14. THE SRE MENU	21
15. THE FOLD MENU	22
16. THE REVERSE MENU	22
17. THE CALIBRATION MENU	22
18. THE ASP MENU	23
19. THE PLOT MENU	23
20. THE EDT MENU	24
21. THE ART MENU	24
22. THE ADD MENU	25
23. THE SBC MENU	26
24. THE SET MENU	26
25. THE DEL MENU	27
26. THE SFT MENU	28
27. THE FIT MENU	30
27.1. FITTING OF CALIBRATION SPECTRA	30
27.2. FITTING OF CALIBRATED MÖSSBAUER SPECTRA	31
27.3. THE MODEL PAGE.....	32
27.3.1. Function of the ADD, REMOVE, SAVE, DB and CONSTRAIN menu boxes	32
27.3.2. Selection of source nuclide.....	37
27.3.3. Spectrum background.....	37
27.3.4. Built in Interactions.....	37
27.3.5. Nuclear parameters of M1, E1, E2, and M1+E2 transitions	41

27.4.	BUILT IN HAMILTONIAN MODELS.....	42
27.4.1.	<i>Static Hamiltonian of mixed magnetic and quadrupole interactions.....</i>	42
27.4.2.	<i>Relative amplitude of the absorption lines of pure M1/E1 transitions.....</i>	43
27.4.3.	<i>Relative amplitude of the absorption lines of mixed M1+E2 transitions.....</i>	44
27.4.4.	<i>The Goldanskii-Karyagin Effect.....</i>	45
27.4.5.	<i>Randomly oriented EFG ($\eta = 0$) in uniaxial magnetic field (^{57}Fe, powdered sample).....</i>	46
27.4.6.	<i>Blume-Tjon two state magnetic relaxation model (^{57}Fe, powdered sample).....</i>	47
27.4.7.	<i>Tjon-Blume Jahn-Teller quadrupole relaxation model (^{57}Fe, powdered sample).....</i>	48
27.4.8.	<i>Pure quadrupole splitting (^{151}Eu, powdered sample).....</i>	49
27.5.	ABSORPTION LINE SHAPES.....	50
27.6.	THIN ABSORBER APPROXIMATION AND TRANSMISSION INTEGRAL.....	52
27.7.	THE PARAMETERS PAGE.....	53
27.8.	FIXING AND RELEASING PARAMETERS, THE MEANING OF DIFFERENT PARAMETER COLORS.....	56
27.9.	SIMULTANEOUS FITTING OF MÖSSBAUER SPECTRA.....	56
27.10.	FITNESS FUNCTIONS OF THE FIT.....	58
27.11.	THE SPECTRUM PAGE.....	59
27.12.	THE INSIGHT PAGES.....	59
27.13.	THE FUNCTIONS PAGE.....	60
27.14.	THE DETAILS PAGE.....	64
27.15.	FITTING OF HYPERFINE FIELD DISTRIBUTIONS.....	68
27.16.	HOW TO COMPLEMENT MOSSWINN WITH USER PROGRAMMED FUNCTIONS.....	69
27.16.1.	<i>How to compile a user written model function.....</i>	69
27.16.2.	<i>How to complement MossWinn with an arbitrary cross-reference function.....</i>	73
28.	THE MÖSSBAUER LINE SHARPENING MENU.....	75
29.	THE NOISE FILTERING MENU.....	77
30.	THE TABLE MAKER MENU.....	78
31.	THE MTX MENU.....	80
31.1.	THE JOB OF THE TRANSFORMATION MATRIX.....	80
31.2.	EXAMPLES FOR TRANSFORMATION MATRICES STORED AS TEXT FILES.....	82
31.3.	OPTIONS AVAILABLE IN THE MTX MENU.....	85
32.	THE MÖSSBAUER PROJECT DESKS MENU.....	86
32.1.	HOW TO ORGANIZE MÖSSBAUER PROJECTS.....	87
33.	THE DATA OPERATIONS MENU.....	88
34.	THE MENU OF HARD DISK OPERATIONS.....	89
35.	PRINTING GRAPHICS.....	89
35.1.	THE PRINTER SETUP DIALOG.....	90
36.	THE EXECUTE MENU.....	92
37.	THE SCANFIT.EXE PROGRAM.....	93
38.	THE HELP MENU.....	95
39.	THE EXIT MENU.....	95
40.	KEYSTROKES APPLICABLE IN MOSSWINN.....	96
41.	NUCLEAR CONSTANTS AS USED IN MOSSWINN 4.0PRE.....	97
42.	QUADRUPOLE SPLITTING CONVERSION CONSTANTS.....	100
43.	REFERENCES.....	101

1. Introduction

Thank you for having chosen the latest version of the MossWinn program, and Congratulations! Today's most accomplished software for Mössbauer spectrum analysis is ready to serve you in your scientific work. Following the release of the first version in 1996, the unique and user-friendly features of MossWinn still remain unrivaled. Building on the strengths of MossWinn 3.0i xp, the first member of the 4.0 series, MossWinn 4.0Pre already takes several further steps ahead to serve scientists worldwide in the field of Mössbauer spectrum analysis, among others by offering the power of 32 bit computing on MS Windows XP, Vista and 7. Precision, productivity, versatility, and ease of the scientific work in the field of Mössbauer spectrum analysis have been further extended in the MossWinn 4.0 series, while the uniquely effective, proven design of the software has been preserved.

Unlike in the case of many other programs, owners of MossWinn 4.0Pre site license do not need to pay for future upgrades of the program: the upgrades are free for license owners.

Your questions and comments concerning MossWinn are welcomed at the E-mail addresses:

AUTHOR@MOSSWINN.COM
Z.KLENC SAR@MOSSWINN.HU

It is recommended to check the site of MossWinn on the web from time to time to get informed about the latest developments in connection with the program. The web site of MossWinn is located at:

HTTP://WWW.MOSSWINN.COM

The MossWinn program was created and tested carefully in order to exclude program errors. However, the author has to state the following usual disclaimer:

The author of the MossWinn program cannot take the responsibility for any consequential, incidental, or other special damages related to the usage of the MossWinn program.

Please, do not tolerate any error or malfunction of the MossWinn program. If you find that the program does not perform as it should, please, contact the author. To get the best performance of the MossWinn program, it is essential that you carefully read this manual.

Finally, let me wish you a fruitful work by using the MossWinn program,

With best regards,

Dr. Zoltán Klencsár
author

2. Contacts

E-mails (preferred contact)	AUTHOR@MOSSWINN.COM Z.KLENC SAR@MOSSWINN.HU
Web	http://www.mosswinn.com http://www.mosswinn.hu
Mail address	Pitvar u. 11., Budapest 1141, Hungary

3. Software protection

Each site license of MossWinn is accompanied by one hardware key. Without having connected this hardware key to the computer, the program runs only in demo mode. (By default MossWinn site licenses are accompanied by an USB type hardware key. Parallel port keys are available at request.)

If the hardware key gets damaged then it can be replaced. In this case, please, send the damaged hardware key back to the author. If guarantee doesn't apply then the cost of the replacement is 80 EUR.

4. Abbreviations

LMC = Left Mouse Click / Click With The Left Mouse Button on . . .

RMC = Right Mouse Click / Click With The Right Mouse Button on . . .

ZVC, ZCh = Zero Velocity Channel (The real-valued channel number that — in theory — belongs to the zero velocity value on the X axis. It is used to describe linear velocity axes of folded spectra.)

CAF, CF = CALibration Factor (The velocity difference between two neighboring channels in a folded spectrum having a linearly calibrated velocity axis.)

DOF = Degree of Freedom

DN = Data Number

ZDN = Zero Data Number (Number of data with a value of zero)

TSA = Total Spectrum Area [**TSA / Base Line**] (calculated on the basis of the fitting curve)

SO = Source nuclide

PAS = Principal Axis System

MSD = Mean Square Displacement Tensor

GKE = Goldanskii-Karyagin Effect

MSCe = $\frac{\mu_N g_e c}{E_\gamma}$ (on fit reports): multiply this value by a hyperfine magnetic field value

(measured in Tesla) in order to obtain the corresponding hyperfine magnetic splitting of the excited state sublevels in mm/s units.

MSCg = $\frac{\mu_N g_g c}{E_\gamma}$ (on fit reports): multiply this value by a hyperfine magnetic field value

(measured in Tesla) in order to obtain the corresponding hyperfine magnetic splitting of the ground state sublevels in mm/s units.

QSCe = $\frac{Q_e c}{(E_\gamma / \text{keV})} \times 10^{21}$ (on fit reports): multiply this value by $V_{zz} / (10^{21} \text{ V/m}^2)$ in order to obtain

$eQ_e V_{zz}$ in mm/s units.

QSCg = $\frac{Q_g c}{(E_\gamma / \text{keV})} \times 10^{21}$ (on fit reports): multiply this value by $V_{zz} / (10^{21} \text{ V/m}^2)$ in order to obtain

$eQ_g V_{zz}$ in mm/s units.

5. Hardware / software requirements

5.1. *Minimum hardware requirements*

The MossWinn program was compiled to run on Intel compatible processors, on PC systems. Among the usual PC components and peripherals, to run MossWinn 4.0Pre the PC system should contain a 32 bit capable Intel compatible processor of ~ 1 GHz or higher core frequency, a hard disk with at least ~ 40 MB free space, at least ~ 256 MB free RAM, mouse with two buttons, a video card and color monitor with at least VGA resolution, a parallel or an USB port, and a CD ROM drive. Thus, the hardware of most PC systems will easily satisfy the hardware needs of MossWinn.

5.2. *Recommended hardware*

Although the MossWinn program will start on a PC having no more power than the minimum requirement stated above, to facilitate efficient work a more powerful system is recommended. Due to the demanding mathematical procedures included in MossWinn, the performance of the program improves considerably with increasing processor speeds. Several procedures of MossWinn can furthermore take advantage of multi-core processor architectures, therefore it is recommended to run the program on a system with a multi-core processor.

In order to check the amount of physical memory available to MossWinn, press **SHIFT+M** either in the **FIT** or in the **Main** menu. The most extensive memory allocation occurs in the FIT menu. To estimate the amount of memory required for a certain fit procedure, take into account that for each fitted spectrum, each added subspectrum would occupy approximately further 80 Kbytes in memory.

5.3. *Software requirements*

Operating systems recommended for **MossWinn 4.0Pre** include 32 bit / 64 bit MS Windows **XP**, **Vista** and **7**. Earlier Windows operating systems (excluding Windows 95 and preceding versions) could do as well. The latest version of the Rainbow Sentinel System Driver (included on the install CD) has to be installed before the licensed version of MossWinn can be started.

6. Installation

Please, read the README.TXT file in the root of the installation CD for detailed instructions concerning installation.

7. Directories used by MossWinn

After the first run of MossWinn the following directories will be present inside the directory

X: \MOSSWINN\

DIRECTORIES AND THEIR FUNCTION

.. \MOSSWINN 4.0\

This directory collects the files and folders MossWinn works with.

.. \MOSSWINN 4.0\DLLS\

This directory contains the dynamic link libraries available to MossWinn. The subspectrum model function libraries should have a name corresponding to the file mask SUB*.DLL, whereas the functional dependence library should have the name DEP_DLL1.DLL. They can be programmed/alterd by the user in order to extend the fitting capabilities of MossWinn by adding new theories and functional dependencies not in the program by default. (See also page 69.)

.. \MOSSWINN 4.0\EXES\

This directory contains executables of tools belonging to the MossWinn program system.

.. \MOSSWINN 4.0\HELP\

This directory contains the html help system of MossWinn.

.. \MOSSWINN 4.0\MIDB\

This directory contains files associated with the MossWinn Internet Database.

.. \MOSSWINN 4.0\USERS\PUBLIC\

This directory contains the configuration and data files associated with MossWinn.

.. \MOSSWINN 4.0\USERS\PUBLIC\ABSORBER\

This directory contains custom calibration-absorber definitions.

.. \MOSSWINN 4.0\USERS\PUBLIC\MODELS\

This directory contains the subspectrum and spectrum fit models which can be defined and saved in the FIT menu of MossWinn via SAVE / SUBSPECTRUM and SAVE / MODEL AS, respectively.

.. \MOSSWINN 4.0\USERS\PUBLIC\PRINT\

This directory contains the printer and clipboard configuration files.

.. \MOSSWINN 4.0\USERS\PUBLIC\PROJECTS\

This directory contains information on the project structure of MossWinn.

.. \MOSSWINN 4.0\USERS\PUBLIC\READONLY

When an attempt is made to load a read-only file, then MossWinn creates a non-read-only copy of the file in question. This copy is placed in a DATE SUBDIRECTORY inside this directory. After that MossWinn will work with this copy instead of working with the original read-only file.

.. \MOSSWINN 4.0\USERS\PUBLIC\STATUS

This directory contains the configuration files of MossWinn. Turn to the **SET** menu in order to edit these files manually.

.. \MOSSWINN 4.0\USERS\PUBLIC\TMATRIX

This directory hosts the version 2.0i style transformation matrices. (See section 31.)

.. \MOSSWINN 4.0\USERS\PUBLIC\TEMP

MossWinn stores temporary files in this directory. By 90 days after their creation, temporary files are moved to the trash directory of MossWinn without notice. Data windows associated with temporary files are denoted by a lightgray - rather than blue - frame in MossWinn.

.. \MOSSWINN 4.0\USERS\PUBLIC\TRASH

This is the trash directory of MossWinn where it places files scheduled for deletion. MossWinn displays a notification when trashed files take up more space than 10 MB.

8. Configuration files

There are several configuration files that can be used to customize MossWinn according to ones needs. Most of the parameters in these files can be set in the MossWinn program itself. The **SET** menu can be used to edit the content of these files manually.

CONFIGURATION FILES AND THEIR FUNCTION

..\MOSSWINN 4.0\USERS\PUBLIC\MOSSWINN.CFG

Main configuration file of the MossWinn program. It contains the following items.

[User]

User title: *Dr.*
 User name: *Zoltán Klencsár*
 User contact: *z.klencsar@mosswinn.hu*

User-specific information that is used in relation with the MossWinn Internet Database (MIDB) service.

[Internet]

Enable MossWinn Internet Database (MIDB) access: YES
 Automatically detect and download updates of help files: YES
 Automatically detect and download updates of exe files: YES
 Next attempt to detect executable update: on startup
 Last downloaded help file version: 2010/03/23

Information concerning internet- and update-related options.

[Startup]

Last maintenance: Sunday
 Start up project group:
 Desk loaded on start up:

Information concerning the startup of the MossWinn program. **Last maintenance** indicates the day when MossWinn last performed maintenance operations on project, fit-model, temporary and trashed files. Maintenance is performed maximum once a day when MossWinn is started. **Start up project group** and **Desk loaded on start up** refer to the project group and the project invoked on startup.

[Appearance]

Fullscreen mode: NO
 Maximized mode: NO
 Application window client width (pixels): 1280
 Application window client height (pixels): 700
 Horizontal position of the application's upper left corner (pixels): 315
 Vertical position of the application's upper left corner (pixels): 298

Settings influencing the initial appearance of the MossWinn program.

[Window attributes]

Window Ratio (200..1000): 540
Headline contains full path: NO
Headline contains history: NO
Headline contains spectrum headline: NO
Headline contains extremum values: NO
Headline contains temperature: YES

Settings influencing the appearance of the data windows displayed by the MossWinn program. **Window Ratio** determines the aspect ratio of the spectrum windows, and influences the way the windows are arranged on the screen when the **ARR** menu option is selected.

[Graphics output]

Default graphics font: Cambria

Settings influencing the appearance of the graphics printed or copied (to the clipboard) by the MossWinn program. Most settings of this kind are printer specific and can therefore be found in the configuration files inside the folder

..\MOSSWINN 4.0\USERS\PUBLIC\PRINT\

[Printing options]

Default printer to be used: PDF
Default printing orientation: LANDSCAPE
An LMC on the Print box in the FIT menu should: print fit results as text

Default printing options. They can be altered in the **SET** menu.

[Calibration options]

Default source matrix: Rhodium
Default calibration absorber: Alpha Iron
Default isomer shift reference material: Alpha Iron

Default calibration options. They can be altered in the **SET** menu.

[Fit attributes]

Standard fitting mode (Area/Amplitude): AREA
Amplitudes must not be negative: YES
Line Widths must be positive: YES
Absolute maximum of parameters: 1.0E+20
Fractional Fit Precision: 1.0E-7
Default number of Monte Carlo iterations: 200

Default options related to mathematical details of spectrum fitting. They can mostly be altered inside the **FIT** menu by pressing on the **SET** box. Parameter values higher than the **Absolute maximum of parameters** will be set to the value given here, which may help avoiding numeric overflows during the fitting procedure. Fits will be considered to be convergent if the relative change of fit parameters, between two iteration steps, is less than the value given here as **Fractional Fit Precision**.

[Sequential fit attributes]

Perform Global fit when doing sequential fit: NO
 Enable Monte Carlo Error Estimation when doing sequential fit: NO
 Enable linking of fits when doing sequential fit: YES
 Ascending ordering when doing sequential fit: YES
 Accept fit results only if chisquare is improved: NO
 When doing sequential fit order spectra with respect to: PH
 Lower limit of the order parameter:
 Upper limit of the order parameter:

Default options related to automatic sequential fitting of spectra. They can be set on the panel invoked by the **SFT** menu.

[Data I/O]

On FLD save file with extension: FLD
 On REV save file with extension: DAT
 Copies of original data files if created should have an extension of: MOS
 Maximum number of windows stored in the TRASH: 9

Default options related to data input and output. They can be altered in the **SET** menu. When a window is removed from a project desk via the **DEL** menu, then it is placed on a TRASH desk where it can be reloaded from. (Press on the **DEL** menu box with the right mouse button in order to achieve this.) **Maximum number of windows stored in the TRASH** determines the maximum number of windows stored on such TRASH project desks. Each project group has its own TRASH desk. When the number of deleted windows placed on this desk exceeds the maximum value given here, then the oldest one will be removed. Deleting a window from a project desk does not alter/influence the associated physical file.

[Performance]

Enable parallel computing on multiple cores: YES

Options related to the performance of MossWinn.

.. \MOSSWINN 4.0\USERS\PUBLIC\STATUS\SPECFRMT.CFG

Contains definitions of special ASCII data formats that make MossWinn able to load ASCII data with a wide range of formats. See section 9.2 for details.

.. \MOSSWINN 4.0\USERS\PUBLIC\STATUS\SPECPRM.CFG

Contains the names of built in and user defined special parameters that can be used to characterize the handled data. They can be manipulated in the **SET** menu. Their value for a given data window can be given in the **EDT** menu.

.. \MOSSWINN 4.0\USERS\PUBLIC\STATUS\EXECUTE.CFG

Contains the path and name information of executable files that can be started from the **EXE** menu of MossWinn.

.. \MOSSWINN 4.0\USERS\PUBLIC\STATUS\EDITPROG.CFG

Contains the path and name of the text editor program that is executed, e.g., when the key 'E' is pressed while in the main menu of MossWinn.

.. \MOSSWINN 4.0\USERS\PUBLIC\STATUS\MASKS.CFG

Contains the file masks that can be selected when the mask edit box is pressed with the right mouse button, e.g., in the **Load** menu.

.. \MOSSWINN 4.0\USERS\PUBLIC\STATUS*.MSK

Files with arbitrary name having the extension **msk** can be used to store the masks for "very special data formats" as described in section 9.2.

.. \MOSSWINN 4.0\USERS\PUBLIC\STATUS\NUCLEAR.CFG

Optional configuration file that can be used to override the default nuclear constants built into MossWinn. See section 41 for details.

9. I/O operations

Original data files encountered by MossWinn at the first time will be copied first: instead of the original, only the copy will be handled by MossWinn. Normally the copy is placed in the host directory of the original file, unless this turns out to be impossible (e.g. because the file is loaded from a read-only storage medium), in which case the copy is placed in a storage directory inside the host directory of MossWinn. The copy will be given the file extension as set in the configuration file **MOSSWINN.CFG**.

9.1. Data formats that can be loaded with MossWinn

MossWinn can be made to understand automatically most of the ASCII data formats used in practice. There are, however, several basic formats that don't need to be defined. The program automatically identifies the following three formats:

(Separators can be commas and spaces as well.)

Data in column	Data in rows	Numbered data in rows
HEADLINE	65987 , 66848 , 68762 . . .	1 , 65987 , 66848 . . .
65987	69000 , 67543 , 67435 . . .	2 , 69000 , 67543 . . .
66848	.	.
67548	.	.
66760	.	.
.	.	.
.	.	.
.	.	.

In the above cases no headline is allowed when data are arranged in rows, and only one headline is allowed in the case when data are arranged in one column.

The first format (*Data in column*) is the default format of MossWinn when one *saves* data with the program. There is a so-called extended format as well, which allows one to save **the velocity scale (in mm/s)** as well as the subspectra together with the original spectrum. This format has the following structure:

Extended format of MossWinn:

```
HEADLINE
-3.2 , 123456 , 123456.432 , . . .
-3.1 , 123478 , 123478.982 , . . .
-3.0 , 134578 , 134578.112 , . . .
. , . , .
. , . , .
. , . , .
```

As in the previous case, in the extended format of MossWinn there is only one headline saved together with the data. The first column contains the velocity of the given channel (in mm/s), the second column contains the data which were measured, the third column contains usually the envelope of the fit, and the fourth and further columns contain the envelope of each subspectra one after the other. The program recognizes this format automatically as well.

9.2. To make MossWinn understand other ASCII data formats

In most cases ASCII data are arranged either in columns or in rows. The data are furthermore preceded by one or more headlines. One of these headlines in the ASCII data file usually contains enough information to identify the format (here called 'special format') in question. This is the idea how the MossWinn program can be made to recognize a high variety of data formats by several simple definitions put in the file: `.. \MOSSWINN 4.0\USERS\PUBLIC\STATUS\SPECFRMT.CFG`

Let's assume that a measuring program produces the following ASCII output:

```
Nov 26 1995      7:06:57 pm      Elt: 01969 Seconds
ID: No spectrum identifier defined
Memory Size: 2048 Chls Conversion Gain: 0512 Adc Offset: 0000 Chls

Chn   Counts   ROI
0,    479857   000
1,    479284   000
2,    479677   000
3,    478015   000
4,    477663   000
.
.
```

Let's assume furthermore that the strings **Memory Size:** and **Conversion Gain:** (case is not relevant) always take part in the third row when the measuring program produces an output like the above one. Then one can use these strings to identify the above data format which contains 5 rows preceding the data, and which contains the data of the measured spectrum in the second column.

To make MossWinn understand the format above, the following lines should be added to the configuration file: **SPECFRMT.CFG**

```
.BEGIN.
Name of the format: Output of spectrometer A
Get spectrum headline from line: 2
Search for identification words in headline: 3
Identification words in the headline: Memory Size: & Conversion Gain:
Irrelevant rows preceding the data: 5
Read data from column number: 2
.END.
```

After these few lines were added to the file **SPECFRMT.CFG**, the MossWinn program assumes that the data have the above form whenever the strings **Memory Size:** and **Conversion Gain:** can be found in the third line of a data file. The name of the format can be any string not longer than 80 characters.

In order to load the X-axis (velocity) data from one of the columns, add the following line to the corresponding format definition:

```
Read X data from column number: n
```

where *n* is the column number of the column containing the velocity data.

As a second example let's assume that the measuring program produces an output like this:

```

SPECTRUM          DATE          TIME          LIVE          REAL
FE12MMS.TXT      97/01/16      13:11:23      52012          0

PHA NO. 1  SEGMENT NO. 1  SIZE 1024
 2 TMS of Fe 12.0 mm/s

 0 45011 45377 45377 45345 45211 45029 45171 44782 45118
 1 44679 45324 45095 45335 45534 44476 44865 45019 45111
 2 45009 45235 45085 45608 45397 45004 45452 45383 45264
 3 44963 44632 44822 45605 44910 45435 45084 44737 44726
. . . . .
. . . . .
. . . . .

```

The corresponding definition, which should be added to the file **SPECFRMT.CFG**, is the following:

.BEGIN.

Name of the format: Data in numbered rows

Get spectrum headline from line: 2

Search for identification words in headline: 4

Identification words in the headline: SEGMENT & SIZE

{& means that both words must be in the fourth line of the data file}

Irrelevant rows preceding the data: 6

Data are arranged in rows.

The rows are numbered.

.END.

If the rows are not numbered then simply omit the sentence: *The rows are numbered.* The maximum number of identification words that can be defined is 4. The identification words cannot be longer than 20 characters. The maximum number of definitions that can be put in the file **SPECFRMT.CFG** is 16.

In the case of the data files defined up to this point, the end of the data should be denoted by a single empty line following the data. This can be changed, if necessary, by putting the following line in any definition in **SPECFRMT.CFG** :

String of termination: MY OWN END LINE

{After MossWinn finds a line equal to 'MY OWN END LINE' the loading terminates}

If the spectrum data file contains also the calibration information, i.e. the calibration factor (CAF) and the zero velocity channel (ZVC), then MossWinn can also be instructed to extract and apply these values. To achieve this, one can add instructions to the corresponding definition in **SPECFRMT.CFG** as follows:

Search for calibration factor in line: 10

{Calibration factor will be looked for in line 10 of the data file.}

Search for calibration factor at character position: 20

{The given character position (20 in line 10) should coincide with one of the characters of the CAF.}

Search for zero velocity channel in line: 10

{Zero velocity channel will be looked for in line 10 of the data file.}

Search for zero velocity channel at character position: 5

{The given character position (5 in line 10) should coincide with one of the characters of the ZVC.}

Further “very special data formats” can be defined as follows. Let’s assume that MossWinn should be able to load the data from the following ASCII file:

```
SOME TEXT NO DATA
SOME TEXT 15678.89 SOME TEXT
DATA14899.9990 SOME TEXT
CHARAC17899TERS NOT19002.43E0BELONGING
TO16999ANY DATA SHOULD BE 19000SKIPPED.
1.6785E+04HOW TO 156435E-01LOAD THESE DATA
WITH MOSSWINN?18888.77
```

Assuming that the above ASCII data file is a data format in which the data are always at the same place we can make MossWinn to extract the data from the file automatically. To do this one has to create a second text file that contains the so-called *mask* matching the above file. The definition of the mask is rather simple: in the file containing the mask there should be a * character wherever a relevant number is present in the data file that should be loaded using the given mask.

In the case of the above example one could create the following mask-file:

```
FIRST ROW. EVERY CHARACTER BUT THE SIGN OF MULTIPLICATION IS SKIPPED
SOME TEXT 156*8.89 SOME TEXT
DATA14899*9990 SOME TEXT
CHARAC17*99TERS NOT19002.4*E0BELONGING
TO16*99ANY DATA SHOULD BE *9000SKIPPED.
1.6785E*04HOW TO 156435E-0*LOAD THESE DATA
WITH MOSSWINN?188*8.77
```

ASCII data file that can be loaded according to the above-defined mask:

```
SOME TEXT NO DATA
SOME TEXT 15678.89 SOME TEXT
DATA14899.9990 SOME TEXT
CHARAC17899TERS NOT19002.43E0BELONGING
TO16999ANY DATA SHOULD BE 19000SKIPPED.
1.6785E+04HOW TO 156435E-01LOAD THESE DATA
WITH MOSSWINN?18888.77
```

In the above case 9 data will be loaded correctly. In the file containing the mask only the * characters are relevant. Other characters were included only to make the comparison of the mask with the data file easier. Save the mask with extension .MSK (name part is arbitrary) inside the folder ..\MossWinn 4.0\USERS\PUBLIC\STATUS\.

One can load data according to the masks saved into the **STATUS** folder by pressing with the right mouse button on the **LOAD FILE** box in the **LOAD** menu.

The maximum number of data that can be loaded with the MossWinn program as one spectrum is 8191.

10. The LOAD menu

Next follows the description of the menu boxes in the **LOAD** menu.

NAME	DESCRIPTION
DRIVE LETTER BOXES	The DRIVE LETTER boxes display the letters for the available drives until the letter R. The current drive can be changed by pressing the DRIVE LETTER box associated with the requested drive or, if the drive letter of the required drive is not visible, either by pressing the corresponding drive letter on the keyboard, or by pressing on the CURRENT DIRECTORY box. Move the mouse pointer over a DRIVE LETTER box to have information displayed about the corresponding drive in the INFO box.
FILE NAME EDIT BOX (THE UPPER BOX)	Shows the name of the selected file.
FILE MASK EDIT BOX (THE LOWER BOX)	Shows the file mask that determines the type of files displayed in the EXISTING FILES box. Press with the right mouse button on the MASK box in order to select one of the predefined file masks listed in the file: <code>.. \MOSSWINN 4.0\USERS\PUBLIC\STATUS\MASKS.CFG</code>
CURRENT DIRECTORY	Indicates the current directory that contains the listed files and folders. Press on it with the mouse in order to create a new directory or to access drives not visible as a DRIVE LETTER box.
EXISTING FILES	Shows the files matching the given file mask and being in the current directory. LMC any of the file names in order to display its preview. RMC the file names in order to select them without preview.
DIRECTORIES	Shows the folders accessible in the current directory.
INFO BOX	The INFO box displays information concerning the visual element over which the mouse pointer is positioned. The visual elements regarding which the INFO box displays information are the DRIVE LETTER boxes, the FILE NAME EDIT box, the FILE MASK EDIT box, the CURRENT DIRECTORY box, the EXISTING FILES box and the DIRECTORIES box.
LOAD FILE	Performs the loading of single data files, file groups, and transformation matrices. To load more than one spectrum in succession without leaving the LOAD menu, LMC the file name of the spectra in the EXISTING FILES box, and then LMC the preview of them appearing on the right side of the screen. To load a file according to a special data format, irrespective of whether the file satisfies the file format criteria (see section 9.2) declared for the format in question, RMC the LOAD box.
X,Y[X]	Performs the loading of data files in X,Y[X] format. First the data are loaded as in the case of the simple LOAD command and after the successful loading process the data in the first column of the data file is loaded separately to serve as the X-axis data of the whole data file. X,Y[X] loading method is selected automatically if the first character in the first row of the data file is the exclamation mark (!). (Spectra saved as X,Y[X] data in the SAVE menu do not require the use of the X,Y[X] method when loading them again. In case of data files loaded as X,Y[X] data the calibration constants have no effect, because the velocity values belonging to the channels are stored in a separate data array in the memory.)
TEXT	Loads text files.
LOAD ALL	Loads all files whose name is currently visible — according to the actual file mask — in the EXISTING FILES list.
EXIT	To leave the LOAD menu.
PREVIEW	Preview of the data & text files is available when the name of a file in the EXISTING FILES box is clicked with the left mouse button (LMC). RMC selects the file, but it does not result in the preview of it.

11. The SAVE menu

NAME	DESCRIPTION
DRIVE LETTER BOXES	The DRIVE LETTER boxes display the letters for the available drives until the letter R. The current drive can be changed by pressing the DRIVE LETTER box associated with the requested drive or, if the drive letter of the required drive is not visible, either by pressing the corresponding drive letter on the keyboard, or by pressing on the CURRENT DIRECTORY box. Move the mouse pointer over a DRIVE LETTER box to have information displayed about the corresponding drive in the INFO box.
FILE NAME EDIT BOX (THE UPPER BOX)	Contains the name by which the file is to save. Press on it to edit.
FILE MASK EDIT BOX (THE LOWER BOX)	Shows the file mask that determines the type of files displayed in the EXISTING FILES box. Press with the right mouse button on the MASK box in order to select one of the predefined file masks listed in the file: <pre> . . \MOSSWINN 4.0\USERS\PUBLIC\STATUS\MASKS.CFG </pre>
CURRENT DIRECTORY	Indicates the current directory that contains the listed files and folders. Press on it with the mouse in order to create a new directory or to access drives not visible as a DRIVE LETTER box. This is the directory where the content of the selected window is saved when the SAVE FILE box is pressed.
EXISTING FILES	Shows the files matching the given file mask and being found in the current directory.
DIRECTORIES	Shows the folders accessible in the current directory.
INFO BOX	The INFO box displays information concerning the visual element over which the mouse pointer is positioned. The visual elements regarding which the INFO box displays information are the DRIVE LETTER boxes, the FILE NAME EDIT box, the FILE MASK EDIT box, the CURRENT DIRECTORY box, the EXISTING FILES box and the DIRECTORIES box.
SAVE FILE	Performs the saving of data files and text files. If the X-axis of the saved spectrum is linearly calibrated, then the basic format of MossWinn is used, that is, data will be saved in one column preceded by one headline.
SAVE X,Y[X]	Performs the saving of data files in the <i>extended</i> format (see section 9.1) of MossWinn. The files saved in this way do not require the use of the X,Y[X] loading method, but they can be loaded using the simple LOAD FILE box in the LOAD menu.
SAVE GROUP	Press on this box to save the list of files associated with the windows on the current project desk to a file group. A <i>file group</i> is a text file with a list of data file names following the code words FILE GROUP being present in the first line of the file. If a file group is selected for load in the Load menu, then MossWinn will load all the files listed in the file group. The direct use of file groups can be considered as to be obsolete: in order to collect files in a group, create instead a new project desk and load the files - to be grouped - onto that.
EXIT	To leave the SAVE menu.

12. Managing the windows in the main menu

When the program starts, the default project gets loaded, and the main menu is displayed. In the main menu spectra and text files are framed in windows with several different colors. The default color of a window (-frame) is blue. The red (i.e. red-framed) window is the *master/target window*, that is, any selected operation gets carried out on the spectrum in this window. The green window is the *source window*, while the red window takes the role of the target window for various operations. Windows referring to files inside the temporary directory of MossWinn (`..\MOSSWINN 4.0\USERS\PUBLIC\TEMP\`) are displayed with a gray frame unless selected to be red- or green-framed.

Unless there are not any windows loaded on the current desk, there is always exactly one master window on the screen. To make a blue-, gray- or green-framed window to be the master window, press on it with the left mouse button. To make a blue- or gray-framed window to be the source window, press on it with the right mouse button. To remove the source status of the window, press on it with the right mouse button again. In order to have the red window display information on the corresponding data, press on it with the left mouse button. A further press on it will make it display the spectrum graph again.

To move a window on the screen, press on it with the left mouse button, and drag it to a new position without releasing the mouse button. To resize a window, press on its frame, and move the mouse while the frame reaches the required size.

Operations, that would change the original spectrum data in the red window, will result in a new window containing the result of the operation in question, so that the original spectrum data remain unaltered.

12.1. Functionality of the headline of the windows

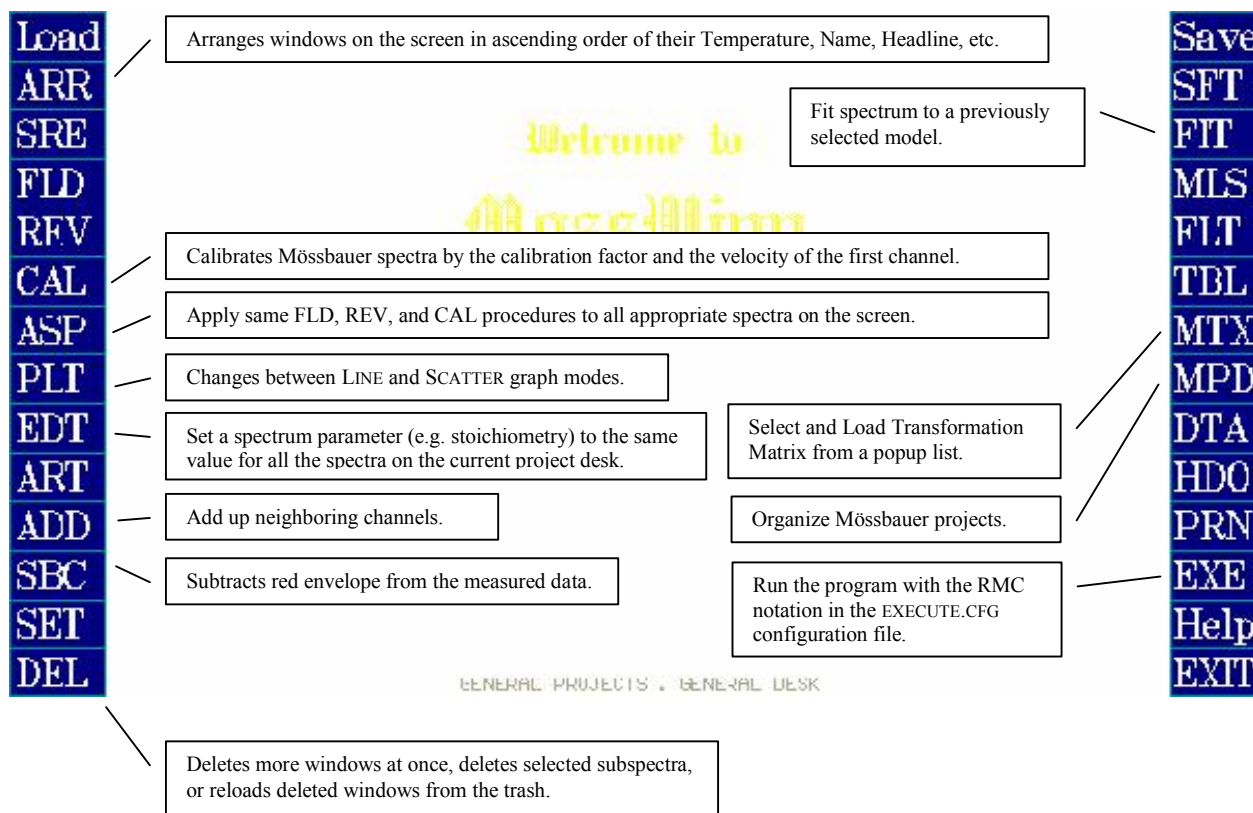
In the bottom of the windows there is a headline that displays information on the corresponding spectrum or text file. Press on the headline to access the following options related to the window in question.

- **Create copy** - to create an independent copy of the window and the associated data file. The newly created data file copy is placed inside the host directory of the original, and is given a name that differs from that of the original by numbering.
- **Create temporary copy** - to create an independent *temporary* copy of the window and the associated data file. The newly created data file copy is placed inside the temporary directory of MossWinn (`..\MOSSWINN 4.0\USERS\PUBLIC\TEMP\`), and is given a name that has the extension of **TMP**. By 90 days after their creation, temporary files are moved to the trash directory of MossWinn without notice. Windows associated with temporary files are denoted by a gray — rather than blue — frame in MossWinn.
- **Rename associated file** - to rename the file associated with the selected window.
- **Update on disk** - to update the content of the file associated with the selected window according to the actual state of the window. If the window does not have an associated file (i.e. it has not been saved yet), then it will be saved as a temporary file.
- **Reload from disk** - to reload the content of the selected window from the file associated with it.
- **Print to printer** - Print image of the selected data window to the default Windows printer.
- **Copy to clipboard** - Copy image of the selected data window into the clipboard of Windows.
- **Show residual** - to show/hide the residual for the selected data window.
- **Recalibrate Y axis** - to adjust the Y axis scale such that all relevant data points are visible.
- **Consider/Ignore zero data points** - to consider/ignore zero valued data points when displaying, fitting, etc. of the selected spectrum. Normally, zero valued data points are ignored, i.e. they are regarded as 'bad points' not to be considered when the spectrum is displayed, fitted or manipulated in any other way.
- **Add to headline content** - to make the selected item to be displayed in the headline of the selected window.
- **Remove from headline content** - to make the selected item *not* to be displayed in the headline of the selected window.
- **Set current as default headline content** - to make the actual headline content to be the default one concerning the items to be displayed. This will influence the window headline of spectra newly loaded/encountered by MossWinn.

12.2. Alternative options invoked by the right mouse button

Throughout the MossWinn program menu boxes appear that have different functionality depending on the mouse button that is clicked (left or right). Such menu boxes can be found in the FIT menu, TBL menu, Load menu, MLS menu, FLT menu, as well as in the main menu.

The picture below emphasizes those menu items that have additional functionality when they are pressed on with the right mouse button in the main menu. A short description of the right mouse button functionality is also given. For a detailed description of these extra options, please, see the description of the corresponding menu system.



13. The ARRRange menu

LMC the ARR box in the main menu of MossWinn in order to make the windows arranged on the screen in rows and columns, according to a predefined shape factor. This shape factor is defined in the MOSSWINN.CFG configuration file (see 'Window attributes' in section 8). RMC the ARR box to arrange the windows on the screen in ascending order of one of their special parameters (alphabetical or numerical order depending on the type of the special parameter). Select the special parameter in question in the appearing popup box. For example, in this way the windows can be made arranged on the screen according to their associated FILE NAME, HEADLINE STRING, TEMPERATURE etc. Whereas special parameters can be defined in the SET menu, their value for the red-framed window can be edited via the EDT menu.

14. The SRE menu

Spectrum Recovery and Editing can be done in the **SRE** menu. In this menu there is the possibility:

- To set the value of selected data points to zero.
- To change the value of any data point.
- To change the channel number of the spectrum.
- To correct overflows by hand.

The next table contains the meaning of the boxes visible on the screen in this menu.

Upper Window	The spectrum that should be recovered. At the edges of this window there is a rectangle that can be managed by the mouse.
Lower Window	The resulted recovered spectrum that reflects promptly the changes made during recovering and editing.
REPLACE ON DISK	Overwrites the original data file with the recovered one on the hard disk. To avoid data loss previously a backup file is saved into the temporary directory of MossWinn.
OVRFLOW	LMC : Adds the overflow number (visible below the word 'OVRFLOW') to all the data counts that are <i>inside</i> the rectangle in the upper window. RMC : Adds the overflow number (visible below the word 'OVRFLOW') to all the data counts that are <i>outside</i> the rectangle in the upper window. The overflow number can be changed after a LMC on its box.
FIX INSIDE	Set the value of those points that are <i>inside</i> the rectangle in the upper window to zero.
FIX OUTSIDE	Set the value of those points that are <i>outside</i> the rectangle in the upper window to zero.
CHANNEL	Press to change the number of channels to a value less than 8191. If one sets fewer channels then the last ones will be cut.
RESET	Reset the value of those points that are inside the rectangle in the upper window.
EXIT & KEEP	Leaves the SRE menu. The original and the recovered data both remain in the memory for further processing.
CANCEL	Leaves the SRE menu without keeping the window containing the recovered spectrum.

When the mouse is positioned above the lower window, then a LMC results in the possibility to edit the value of the selected data point. RMC sets the value of the selected data point to zero.

If the spectrum contains more than 512 channels then difficulties may be encountered by setting the value of individual channels. This is because the resolution of the screen does not allow every data point to have its own pixel on the screen. In these cases one can improve the resolution by a LMC on the '+' sign in the right upper corner of the screen. If the '-' sign is clicked then the original resolution can be recovered. By increasing the resolution, as described above, some part of the spectrum may overstep the edges of the screen. To make the required part of the spectrum displayed, LMC the **arrows** in the left upper corner.

In the case of the '+' and '-' signs as well as in the case of the arrows one can speed up the process by applying RMC rather than LMC. Both mouse buttons can also be pushed at once to achieve an even faster speed.

15. The FoLD menu

LMC the FLD menu box to create a new window containing the folded version of the spectrum in the red window. The program selects the best folding point automatically, but it can as well be set manually on the appearing form. The folding procedure of MossWinn works as follows.

The folding point is supposed to have the mathematical form: $F = N/2$ where N is an integer value. After having entered the folding routine one has the possibility to set the minimum and maximum values of F . The folding point, F , in which case the expression

$$Z(F) = \sum_{i>F}^N (C_i - C_{F-(i-F)})^2$$

is minimum will be accepted. (C_i denotes the counts in the i th channel of the measured spectrum.)

If D_{last} denotes the last channel of the folded spectrum then $D_{\text{last}} = C_F + C_F$ in the case when F is an integer value, and $D_{\text{last}} = C_{F-1/2} + C_{F+1/2}$ in the case when F is a half-integer value. Interpolations between counts in neighboring channels are not made.

After the spectrum has been folded the program attaches a certain number of channels with fixed (zero) value to the left (negative) end of the folded spectrum to make it contain a number of channels equal to 2^n where n is an integer value. (Mainly for the sake of the MLS and FLT menus that rely on the FFT algorithm.) For this reason calibration constants, evaluated by other programs, can not be used automatically in the MossWinn program. (A calibration can usually be correct only if the calibration spectrum was treated exactly the same way as the spectrum to be calibrated.)

The MossWinn program is able to calibrate and fit unfolded spectra in the FIT menu. In this way one can achieve precise fits even if the folding point of the spectrum does not have an integer or half-integer value as assumed in the folding routine. For transmission integral fits, when ultimate precision is required, it is also recommended to fit the unfolded data rather than the folded one. Namely, folding of the spectra always results in a slight broadening of the absorption lines, which could slightly modify the results of transmission integral fits.

16. The REVerse menu

After a spectrum was folded, it is usual to want the channels on the left side of the spectrum to belong to negative velocity values, and the channels on the right side to positive velocities. In the case of some Mössbauer setups the folded spectrum needs to be reversed to achieve this. This reversion can be done via the REV menu.

LMC the REV box to create a new window containing exactly the same data as the original red window did, but in reversed order. If the original spectrum was already calibrated, then the value of the ZVC will be corrected automatically after reversion, so that the – mostly imaginary – channel belonging to the zero velocity will contain exactly the same counts as it did in the case of the original spectrum.

The reversion procedure of MossWinn works as follows. Let C_i denote the original spectrum and D_i denote the reversed spectrum. Then $D_i = C_{N-i+1}$ (N being the number of channels) is true for every i .

17. The CALibration menu

Use the CAL menu to calibrate folded spectra with a linear velocity scale according to known calibration parameters (ZVC and CAF), or to transfer the calibration information from calibrated spectra to uncalibrated ones.

Deselect any green windows on the screen, and LMC the CAL box to set the ZVC and CAF calibration constants for the red window. RMC the CAL box in order to set the CAF constant, along with the velocity value belonging to the first channel, rather than the channel belonging to the zero velocity (ZVC).

To transfer calibration information from one spectrum to the other, select the source spectrum green, and select the uncalibrated target spectrum red. Then LMC the CAL box.

18. The ASP menu

ASP stands for „Apply Same Procedures”. LMC the **ASP** box to carry out **FLD**, **REV** and **CAL** operations for the red window exactly as they were carried out for the green window. RMC the **ASP** box to carry out **FLD**, **REV** and **CAL** operations for all the uncalibrated windows on the screen exactly as they were carried out for the green window.

Typical application of this menu is the following. Load a calibration spectrum, and carry out the **FLD** and **REV** operations on it as required. Enter the **FIT** menu and calibrate the velocity axis of the calibration spectrum. Exit the **FIT** menu, and load all the raw (unfolded, non-reversed, and non-calibrated) spectra that were measured according to the same velocity settings as the calibration spectrum. LMC the window of one of the newly loaded spectra in order to make it red. RMC the window of the calibration spectrum to make it green. Then RMC the **ASP** box. As a result, all the newly loaded spectra will be folded, reversed and calibrated exactly according to the calibration spectrum in the green window. The resulted calibrated spectra will be placed in new windows, whereas the original ones will remain unaltered. (As the processed version of the spectra will be positioned above their respective originals, it is convenient to select the option ‘DEL → Delete invisible windows on the current desk’ in order to remove the original — uncalibrated — spectra from the desk.)

19. The PLoT menu

RMC the **PLT** box to make data points in the red window connected/disconnected. When a text file is being shown in the red window a LMC on the **PLT** box makes the red window transparent/not-transparent. A RMC on the **PLT** box makes a text window maximized/minimized in size. LMC the **PLT** box to change the following options of plotting data in the red window.

- **Apply to all** - to apply the selected option to all the windows.
- **Consider/Ignore zero points** - to consider/ignore zero valued data points when displaying, fitting, etc. of the red-framed spectrum. Normally, zero valued data points are regarded as 'bad points' not to be considered when the spectrum is displayed, fitted or manipulated in any other way. 'Fixing' data in the SRE menu also means that the value of the selected data points are set to zero.
- **Show/Hide horizontal line at Y = 0.0** - to show/hide a horizontal line at the ordinate value of $Y = 0.0$ in the red-framed data window. If the Y axis range does not contain the value of $Y = 0.0$, then the line won't appear. This option is useful e.g. for inspecting residuals created via the SBC menu box.
- **Connect/Disconnect points** - toggle between scatter and line graph modes for the red-framed window.
- **Show/Hide residual** - to show/hide the residual for the red-framed spectrum window. The residual is calculated by subtracting the red fitting envelope from the measured data, then it is shifted to be positioned above the spectrum data. A magenta-colored horizontal line denotes the zero level of the residual, while a grey stripe indicates (approximately) the levels of +1 Std and -1 Std around the zero level. The residual is visible only if the spectrum window contains a fitting envelope.
- **Show/Hide Y axis** - to show/hide the Y (vertical) axis of the red-framed spectrum window.
- **Use/Hide suffix** - to use/hide suffix notation in the numerical labels of the Y axis of the red-framed spectrum window. Suffix notations include k (kilo, 10^3), M (Mega, 10^6), G (Giga, 10^9), T (Tera, 10^{12}), P (Peta, 10^{15}) and E (Exa, 10^{18}). On graphical outputs the suffix notations appear as a $/10^n$ extension after the Y-axis title.
- **Show percentage/absolute values** - toggle between percentage (i.e. relative) and absolute numerical representation of the Y (ordinate) values in the red-framed spectrum window. In percentage representation the ordinate values are meant relative to the (signed) maximum of the data, $y_i(\%) = 100 \times (y_i/y_{\max})$. (According to the above, for negative valued data the percentage representation may result in values lower than -100%).
- **Transparent/Not transparent** - to make the red-framed window transparent/not transparent. In transparent mode the white background of the window is not drawn, such that windows being below the transparent window can be seen as well.
- **Ungroup window** - to create a separate data window for all or only one of the fitting envelopes being present in the red-framed spectrum window. To create a separate window for all of the fitting envelopes, click directly on this item, whereas to create a separate window only for a single fitting envelope, select one of them in the appearing list.

- **Group with green** - to add all the data series being part of the green-framed spectrum window to the red-framed spectrum window. In the red-framed window the newly added data series will appear as additional fitting envelopes. Fitting envelopes can be removed from a data window via the menu list of the DEL menu box (accessible by a click with the right mouse button).
- **Make a copy of red** - to create an independent copy of the red-framed data window.

20. The EDT menu

Press on the **EDT** box with the *left mouse button* in order to edit special spectrum parameters, headline content, X-axis and Y-axis titles, and history string of the spectrum shown in the red-framed window. Press on the **EDT** box with the *right mouse button* in order to set a selected special parameter to the same value for all the spectra/datasets shown on the current project desk.

21. The ART menu

ART stands for **ARiThmetical Operations**. Click the **ART** menu to carry out one of the following operations.

- **Multiply by a constant** - to multiply each data value in the red-framed data window by the same constant, and place the result in a new data window.
- **Multiply RED by GREEN** - to multiply each data value in the red-framed data window by the respective data value in the green-framed data window, and place the result in a new data window. Note that this operation disregards the calibration of the X (velocity) axis.
- **Normalize spectrum** - to normalize the red-framed spectrum and place the result in a new window. Normalization is based on an estimated base line value (BL) that can be overruled by the user. The normalized spectrum is calculated as $Y_i(\text{normalized}) = \text{MAX}(BL - Y_i, 0) / \text{MAXIMUM}_k(BL - Y_k)$, where $\text{MAX}(a, b)$ denotes a if $a > b$ and it denotes b otherwise, whereas $\text{MAXIMUM}_k(a_k)$ denotes the maximum of a_k considering all possible values of k . Consequently, the Y (ordinate) values of the normalized spectrum will all lie in the range of $[0, 1]$. Normalization does not work for negative valued data sets.
- **Divide by a constant** - to divide each data value in the red-framed data window by the same constant, and place the result in a new data window.
- **Divide RED by GREEN** - to divide each data value in the red-framed data window by the respective data value in the green-framed data window, and place the result in a new data window. Note that this operation disregards the calibration of the X (velocity) axis.
- **Strip data...** - to strip off the selected subspectrum envelope curve from the measured data in the red-framed spectrum window, and place the result in a new data window. The stripped spectrum is calculated as $Y_i(\text{stripped}) = Y_i - Y_i[\text{SUB}] + \text{MAXIMUM}_k(Y_k[\text{SUB}])$ (for transmission spectra) and $Y_i(\text{stripped}) = Y_i - Y_i[\text{SUB}] + \text{MINIMUM}_k(Y_k[\text{SUB}])$ (for scattering – e.g. CEMS – spectra), where [SUB] refers to the subspectrum stripped off.
- **Set minimum to zero** - to subtract the minimum of the data in the red-framed data window from every data value of the window, and place the result in a new data window.
- **Set negative to zero** - to set all the negative valued data in the red-framed data window to zero, and place the result in a new data window.
- **Set negative to positive** - to take the absolute value of the data in the red-framed data window, and place the result in a new data window.
- **Horizontal reflection of data** - to turn absorption peaks into emission peaks and vice versa for the red-framed spectrum window, and place the result in a new data window. The transformation is carried out as $Y_i(\text{transformed}) = \text{MAXIMUM}_k(Y_k) - Y_i + \text{MINIMUM}_k(Y_k)$. (Note that applying the transformation twice will give back the original spectrum.)
- **Set zeros equal to red envelope** - to set zeroed data equal to the corresponding value of the red fitting envelope of the red-framed spectrum. This option can be used to eliminate bad/zeroed data points after the spectrum was satisfactorily fitted in the FIT menu, which may prove to be useful when one exports the corresponding spectrum data to an external grapher software.
- **Convolution with a Gaussian** - to convolve the data in the red window with a Gaussian curve, and place the result in a new data window. The convolution is carried out simply by adding up Gaussian curves with

appropriate weight factors: $Y_k(\text{result}) = \sum_j (Y_j \times \text{Gaussian}(v_j, v_k))$ where $\text{Gaussian}(v_j, v_k)$ denotes the value of a Gaussian function centered at v_j and having an **area** of 1, as calculated for the abscissa of v_k . The width (FWHM) of the Gaussian is given by the user.

- **Convolution with a Lorentzian** - to convolve the data in the red window with a Lorentzian curve, and place the result in a new data window. The convolution is carried out simply by adding up Lorentzian curves with appropriate weight factors: $Y_k(\text{result}) = \sum_j (Y_j \times \text{Lorentzian}(v_j, v_k))$ where $\text{Lorentzian}(v_j, v_k)$ denotes the value of a Lorentzian function centered at v_j and having an **amplitude** of 1, as calculated for the abscissa of v_k . The width (FWHM) of the Lorentzian is defined by the user.
- **Add normally distributed noise** - to add normal statistical noise to the data in the red-framed window by assuming that for a given data the variance of the noise distribution and the value of the data are equal (referring to the underlying Poisson distribution), and place the result in a new data window.
- **Add noise with fixed variance** - to add normal statistical noise to the data in the red-framed window by assuming that the variance of the noise probability distribution is the same for all data points, and place the result in a new data window. The value of the uniform variance is defined by the user.
- **Recover original baseline** - to estimate and recover the original baseline of a spectrum that was obtained by dividing the measured spectrum data by a constant factor (e.g. the baseline itself). In order to recover the baseline value of a spectrum that was normalized in this way, it has to be fitted to some model previously, so that the red envelope of the fit estimates well the measured data. Then select this option to calculate and place the spectrum with the recovered baseline in a new window.
- **Recover original baseline (in case of overflows)** - to estimate and recover the original baseline of a spectrum that was obtained by subtracting a constant from the spectrum data (this happens, e.g., during overflows). In order to recover the baseline value of a spectrum, it has to be fitted to some model previously, so that the red envelope of the fit estimates well the measured data. Then select this option to calculate and place the spectrum with the recovered baseline in a new window.
- **Shift velocity axis...** - to add a certain (positive or negative) constant to the velocity value of each channel of the spectrum in the red-framed window, and place the result in a new data window. By the use of this option one can modify the calibration of the velocity axis. For example, in order to transform a calibration relative to alpha iron to a calibration relative to Stainless Steel (SS), one would add *IS* (isomer shift of alpha-Fe relative to SS) = + 0.09 mm/s to the velocity value of each channel.
- **Restrict velocity axis...** - to restrict the velocity axis (either only of the spectrum in the red-framed window or of all spectrum windows on the current desk) to a velocity range to be defined by the user as $[v_{\min} \dots v_{\max}]$ on the appearing dialog. The resulted spectra are placed in new windows, while the original spectra (and the corresponding files) remain unaltered. The number of channels in the processed spectrum copies will be changed in accordance with the user-defined velocity interval.

22. The ADD menu

The **ADD** menu can be used to add two spectra channel by channel, to add a constant to the data points of the spectrum in the red window, as well as to add up neighboring channels of the red window, thus reducing statistical noise.

Deselect any green-framed window on the screen, and click on the **ADD** box with the left mouse button to add a constant to the spectrum in the red window. RMC the **ADD** box to add up the neighboring channels of the spectrum in the red window. In this latter case the resulted spectrum will contain half as many channels as the original spectrum did. If A_i and B_i denote the original spectrum and the resulted spectrum respectively, then $B_i = A_{2i-1} + A_{2i}$.

In the presence of a green-framed window containing another spectrum, a LMC on the **ADD** box results in a new window containing the sum of the spectra of the red and green windows. Every channel in this new spectrum bears a value that equals to the sum of the counts in the corresponding channel in the red and in the green windows. If A_i , B_i and C_i denote the spectrum in the red window, the spectrum in the green window and the resulted spectrum respectively, then $C_i = A_i + B_i$. Only those spectra can be added which contain exactly the same number of channels.

23. The SBC menu

The **SBC** menu can be used to subtract a constant value from each data point of the spectrum in the red window, to subtract the green window from the red one, and to subtract the red envelope from the spectrum in the red window.

Deselect any green-framed windows and LMC the **SBC** box to subtract a constant from every data point in the spectrum being in the red window. RMC the **SBC** box to subtract the red envelope (if any) from the original spectrum both being present in the red window.

In the presence of a green framed window, LMC the **SBC** box to subtract the spectrum in the green window from the spectrum in the red window. If A_i , B_i and C_i denote the spectrum in the red window, the spectrum in the green window and the resulted spectrum respectively, then $C_i = A_i - B_i$. Only spectra with the same number of channels can be subtracted.

24. The SET menu

The SET menu can be used to alter configuration data of MossWinn, as well as to define or delete special parameter types. The following options are available:

- **Set user title, name and contact** - to set your preferred title (e.g. Dr.), your name and E-mail address that identify you when you publish data in the MossWinn Internet Database. It is recommended that you give your real name and E-mail here.
- **Set internet access options** - to enable/disable internet access related functions. When enabled, these functions allow MossWinn (1) to automatically detect, download and install updates of its files from the internet, as well as (2) to access the MossWinn Internet Database via the internet.
 - Automatically download updates of MossWinn help files. [Enabled]
 - Automatically check for updates of MossWinn executables. [Enabled]
 - MossWinn Internet Database (MIDB) access. [Enabled]
- **Set performance options...** - to set options influencing the performance of MossWinn, e.g. whether MossWinn is allowed to utilize its parallel computing routines to speed up the corresponding calculations on multi-core processor systems.
 - Parallel computation on multiple cores [Enabled]
- **Enable/disable libraries** - to enable the loading and calling of those dynamic link libraries that one intends to use for the calculation of the corresponding subspectrum curve(s) in the FIT menu. The libraries in question should have a file name corresponding to the mask SUB*.DLL, and they should be present in the code library directory of MossWinn.
- **Set mouse type...** - to set whether the mouse is to be treated as a left-handed or as a right-handed mouse. When in Windows the function of the left and right mouse buttons are swapped, then MossWinn will start by assuming a left-handed mouse. Setting the mouse to be left-handed or right-handed in MossWinn will not alter the corresponding (system-wide) setting in Windows.
 - Left-handed - if the mouse is set to be left-handed, then the functions attributed to the left and right mouse buttons are swapped (compared to what is described in this manual).
 - Right-handed - if the mouse is set to be right-handed, then the left and right mouse buttons function as described in this manual.
- **Set ASCII keyboard layout** - to display the Customize ASCII keyboard layout dialog that can be used to redefine character inputs in which keystrokes result in MossWinn. When the dialog is displayed, press a key (or shift + key) and then, by using the mouse, in the ASCII list select the character in which the pressed key should result in when entered in MossWinn. Select **Restore** to invalidate all changes and restore the default layout.
- **Set autosave options...** - to set the file extensions used when spectra are saved automatically by MossWinn. (The auto-save and auto-copy features cannot be disabled.)
- **Set default calibration options...** - to set the default attributes of calibration spectra:
 - ^{57}Co source matrix (rhodium, chromium or palladium)
 - Calibration material (e.g. Alpha Iron)
 - Isomer shift reference (e.g. Alpha Iron)

- **Default graphics font...** - to set the font that is used when graphical images of spectra are printed to printer, saved to file or copied into the clipboard.
- **Default printer to be used...** - to set the Windows printer that is used when text or graphics is printed by MossWinn.
- **Page orientation when printing...** - to set the default page orientation (portrait or landscape) when graphics is printed by MossWinn.
- **Special parameters...** - to define, delete or set the value of special parameters.
- **Configuration setting series** - to invoke the configuration setting series that enables the setting of a multitude of options.
- **Edit configuration file...** - to directly edit the content of one of the configuration files, by invoking either the text editor program selected in the EXE menu, or the system's default text editor program (in the case of EDITPROG.CFG).
- **Reload configuration files** - to reload all configuration files in order to make MossWinn aware of their actual state. This option is useful especially after one has directly edited the content of some configuration file and wants the changes to take effect without restarting MossWinn. Normally, configuration files are loaded only when MossWinn starts up.

25. The DEL menu

LMC the **DEL** box to delete the red-framed window from the current desk. The window will be placed onto the TRASH desk of the corresponding project group. The file on the hard disk belonging to the red window won't be altered. RMC the **DEL** box to activate one of the following procedures (trashing of the windows won't take place by applying these procedures).

- **Delete all windows on all of the desks** - to delete all the windows loaded in MossWinn. This will make all active project desks empty. With the exception of the *General Projects* . *General Desk* and the *Trash* desks, empty project desks do not get updated on closing the program.
- **Delete all windows on the current desk** - to delete all the windows loaded in MossWinn on the current desk.
- **Unload from memory all desks but current** - to make the actually displayed desk to be the only one that is active. When a new project desk is selected, then the old one may remain in memory, i.e. it may remain active. There can be a maximum of 16 *active project desks* loaded in MossWinn. Press the **TAB** and **Backspace** keys to navigate (i.e. go forward and backward, respectively) among the active project desks.
- **Delete text windows** - to delete all text windows (i.e. windows whose content is not interpreted/displayed as a function of numerical data) on the current project desk.
- **Delete blue-framed windows** - to delete blue-framed windows on the current project desk.
- **Delete gray-framed (temporary) windows** - to delete gray-framed, i.e. temporary windows on the current project desk.
- **Delete invisible windows on the current desk** - to delete those windows on the current project desk that are fully covered by other windows.
- **Delete Subspectrum** - to delete one, all or all but the red one of the fitting envelopes (subspectra) being part of the red-framed window.
- **Reload deleted window** - to reload a formerly deleted window from the Trash desk of the current project group.

26. The SFT menu

SFT stands for „Sequential Fit of spectra” The **SFT** menu can be used to sequentially fit Mössbauer spectra being on the current desk according to a selected model. The models that are available are those, which were saved in the **FIT** menu previously. The fit of the spectra will happen one after the other, and the fit results will be saved automatically via **ACCEPT** in the **FIT** menu, so that after all the spectra get fitted, one can immediately turn to the **TBL** menu to create a table of the obtained fit results. To break the fitting of the spectra keep pressing the ESC key on the keyboard.

LMC the **SFT** box to enter the dialog box that can be used to customize the sequential fit. The following options are available.

Option	Functionality
Fit spectra to the model... 1A ... selected here: 1B ... that was used to fit the spectrum in the red window. 1C ... that was accepted for them previously.	Choose this option to fit all spectra to the fit model selected in the popup box on the right. Choose this option to fit all spectra to the fit model that was accepted previously for the spectrum in the red window. Choose this option to refit all spectra to the specific fit model accepted for them previously.
2A All fits start with the model saved for the red window. 2B Fit [n+1] takes the end result of Fit [n] as the start. These options are not effective if 1C is selected.	Choose this option to start all fits with the parameters accepted for the spectrum in the red window. Choose this option to perform a chain-fitting of spectra, in which the (n+1) th fit takes the parameters of the end result of the n th fit as initial fit parameters.
3A Analyze spectra in ascending order of... 3B Analyze spectra in descending order of... 3C Analyze only those in the range...	With the help of the options 3A and 3B one can determine the order in which spectra get analyzed. Select the order parameter (e.g. “Temperature [K]” or “File Name”) in the popup box on the right. This has importance especially in the case of chain-fits (2B selected) when the spectrum of Fit [n+1] should be as close as possible to the spectrum of Fit [n]. Select this option if only a subset of the spectra on the current desk should be fitted in the sequential fit procedure. Set the extreme values for the order parameter in the string boxes on the right. One can select a numerical value or a non-numerical string value depending on the type of the order parameter.

Option	Functionality
<p>4A Recreate distributions without fitting</p> <p>4B Do not perform global fitting.</p> <p>4C Do not perform Monte Carlo Error Calculation.</p> <p>4D Accept fit results only if chisquare is improved.</p>	<p>Select this option to recreate and invoke distribution curves (if any) associated with fits accepted earlier for the spectra on the current project desk.</p> <p>Select this option to prevent the FIT menu to perform a global search for the optimum set of fit parameters at the beginning of each fitting session. If the initial parameters for the fits can be estimated to be close to the optimum values, then it is recommended to have this option selected.</p> <p>If the standard error calculation routine fails to give reliable results for the standard deviation of the fitting parameters, then Monte Carlo Error Estimation procedure is invoked automatically in the FIT menu. The Monte Carlo Error Calculation, however, can take considerable amount of time depending on the complexity of the applied fit model. Select this option to prevent the program to perform the time consuming Monte Carlo Error calculation even in cases when the standard method failed.</p> <p>Select this option to prevent the program to automatically accept the obtained fit result in cases when a fit accepted earlier for the actual spectrum provided a lower normalized chi-square value.</p>
<p>5A Fix Parameter</p> <p>5B Unfix Parameter</p>	<p>Use these options to Fix (5A) or Unfix (5B) a fit parameter in all of the spectra on the current desk without entering the fit menu for each of the spectra individually. The fit model, for which the parameters are shown in the popup boxes, is taken from the spectrum of the red window.</p> <p>A typical example for the application of this option is when one fits a series of spectra to a fit model in which one of the fit parameters is fixed in order to achieve a better stability of the fit. Then, using this option, the parameter in question gets unfixed, and the sequential fit procedure is repeated to fine-tune the value of the formerly fixed parameter.</p>

A typical application of the **SFT** menu is the following. Let's assume that Mössbauer spectra of the same material were taken at 20 different temperatures, and that all the spectra are already calibrated. All the spectra display the same structure, e.g. two doublets, so that they all can be analyzed using the same fit model, and they will differ only in the derived model parameters (e.g. Isomer Shift and Quadrupole Splitting). To let MossWinn do the analysis automatically, LMC the **SFT** box and select the appropriate model. By clicking on **START** the fit will begin immediately, and will proceed automatically until all the spectra get analyzed.

27. The FIT menu

Enter the FIT menu with a LMC in order to fit already calibrated Mössbauer spectra, or in order to fit calibration spectra to calibrate the velocity axis. To fit a spectrum according to a model saved previously in the FIT menu, one can also RMC the FIT box and select the required fit model.

27.1. Fitting of calibration spectra

MossWinn allows the calibration fitting of Mössbauer spectra measured with a $^{57}\text{Co}(^{57}\text{Fe})$ — in the followings ^{57}Fe — Mössbauer source. During calibration-fitting the physical model describing the measured reference material (e.g. α -Iron) is assumed to be known, and by fixing the position type parameters (e.g. isomer shift and hyperfine magnetic field) of the model, the velocity axis of the Mössbauer spectrum gets determined by the fit.

In order to calibrate the velocity axis of a calibration spectrum, proceed as follows. Select the — yet uncalibrated — calibration spectrum to be the master window (red framed) in the main menu. Deselect any source (green framed) windows. LMC the FIT box. In the FIT menu click on the CALIBRATION tab in the right upper corner of the screen. Select the **Matrix** (e.g. Rhodium) of the ^{57}Fe Mössbauer source that was used for the measurement. If the used matrix is not among those displayed, then click on **Define Matrix...** to define the source matrix. After the source matrix has been selected, select the **Absorber** (e.g. α -Iron) used for calibration purposes. MossWinn also supports the calibration of the velocity axis according to simultaneously measured reference absorbers. This means, that the velocity axis can be calibrated on the basis of a spectrum that was measured for example with α -Iron and Stainless Steel (SS) used simultaneously as absorbers. If the absorber material — used for calibration purposes — is not among those listed, then do the followings. Go to the **MODEL** page and set the known model of the used absorber material (e.g. one doublet). Then set the known, correct values of position type parameters (e.g. isomer shift and quadrupole splitting). The isomer shift value(s) should be set relative to α -iron. Fix all the position type parameters that were set in this way (click on the name of them with the left button of the mouse). Go back to the CALIBRATION page, invoke the **Absorber** popup (click on the text **Unknown Absorber**), and select **Define Absorber**.

After the correct absorber material was set, the **Isomer Shift Reference** material should be selected. (When the calibration fit is accepted, then the velocity axis will be calibrated so that isomer shift values will be relative to the reference material selected here.) If the spectra, which are going to be calibrated according to the actually fitted calibration spectrum, were measured with a ^{57}Fe Mössbauer source, then it is recommended to select α -iron as the calibration material. In all other cases it is recommended to select the **Source material** here as the **Isomer Shift Reference** material. In the latter case the velocity axis will be calibrated according to the real — absolute — velocity of the source, that is the velocity values on the X-axis will denote the real velocity the source was moved towards the absorber with while the counts in the particular channel were collected.

After the reference material has been selected, the **Waveform** of the movement of the source should be set. This can be **Triangle** (constant absolute acceleration in time) or **Sinusoid** (Cosine acceleration in time).

Then, it should be set whether the spectrum has been **Folded** (electronically or by software) or it is **Unfolded** displaying all the four quarter periods of the movement of the source.

Then, it should be set whether the very **first channel** of the spectrum bears a negative or positive velocity. (Mössbauer spectra are recorded usually with the negative velocities encountered first. But this may be not the case depending on the settings of the electronics used.) In the folded case a spectrum can display velocities according to the schemes of $-/+$ and $+/-$. In the unfolded case, however, the velocity axis can correspond to $-/+ +/-$ or $+/- -/+$ schemes.

When all the above settings are completed, the **Cal Mode** should be set active, in order to activate the selected model. As a result the **Velocity Axis** parameter group appears with three parameters at the top of the parameter list. **Max. Velocity [mm/s]** denotes the maximum velocity of the source during its movement. **Delay [Dwell Time]** denotes a possible time difference in units of Dwell Time (time of continuous counting in a particular channel in one cycle of movement) between the start of the source-movement-period and the start of the counting period. Such delays are not uncommon, and even with good value electronics it may very well have an order of magnitude of 1.0 (one channel sweep).

Period Length [Channels] determines the number of channels the whole movement period of the source is divided into. This usually equals to the number of channels in the spectrum. **However, some spectrometers produce an ASCII spectrum output with 512 or 1024 channels, but at the same time divide the whole period into only 500 and 1000 channels, respectively (the rest of the channels are redundant and they are usually zeroed). In such a case the correct setting of the *Period Length [Channels]* parameter (500 instead of 512, and 1000 instead of 1024) is essential to achieve precise calibration.**

To complete the calibration fitting, the calibration spectrum should be fitted according to the model selected as described above. Usually very good fits can be achieved, with $\chi^2 \approx 1.0$. If this is not the case it is recommended to check carefully whether all the calibration parameters are set correctly.

To finalize the result of calibration fitting, click on **ACCEPT**. As a result the program will calibrate the velocity axis according to the selected reference material. If the reference material is not the same as the source material, then the fitting will worsen, as the isomer shift parameters of the fit will not be the correct ones relative to the **Isomer Shift Reference** material anymore. This effect, however, does not influence the correctness of the velocity axis calibration.

To transfer the obtained calibration information to other spectra measured with the same velocity settings, exit the **FIT** menu, and in the **main** menu turn either to the **CAL** or to the **ASP** menu.

27.2. Fitting of calibrated Mössbauer spectra

Depending on the existence and content of the master (red) and source (green) windows in the main menu, the FIT menu will proceed as listed below.

Content of the red window	Content of the green window	What happens after a LMC on the FIT box
Yet unfitted spectrum	None	Fitting of the spectrum according to a model to be selected later on in the FIT menu.
Yet unfitted spectrum	Transformation matrix (text file)	Fitting of the spectrum according to the model represented by the selected transformation matrix.
Yet unfitted spectrum	A previously fitted spectrum	Fitting of the spectrum according to the former fit of the spectrum shown in the green framed window
Previously fitted spectrum	None	Fitting of the spectrum according to its former fit.
Previously fitted spectrum	Transformation matrix (text file)	Fitting of the spectrum according to the model represented by the selected transformation matrix.
Previously fitted spectrum	A previously fitted spectrum	Fitting of the spectrum according to the former fit of the spectrum shown in the green framed window.

A **FIT** can be reloaded only if it was accepted previously by a click on the **ACCEPT** box in the fit menu. To fit a spectrum according to a model selected from the models saved previously in the **FIT** menu, RMC the FIT box and select the required fit model.

The FIT menu is divided into five main pages from which only four are visible by default. The fifth can be invoked by a mouse click on the **DETAILS** box. The **PARAMETERS PAGE** occupies the left of the screen. On the right of it, in the center of the screen, the blue colored menus of the **FUNCTIONS PAGE** can be seen. On the right of it the **MODEL PAGE**, then two identical **INSIGHT PAGES (D,E)**, then the **CALIBRATION PAGE** is located. On the right bottom corner of the screen the **SPECTRUM PAGE** is situated followed by the **RESIDUAL PAGE** and three identical **INSIGHT PAGES (A,B,C)**.

In the followings, the functionality of these pages is described.

27.3. The Model page

The Model page can be used to set the physical model according to which the spectrum should be fitted. At the top of the page the **Model Group Popup** box is located. Click on it to select the required model group, or to select directly the previously saved model according to which the current spectrum should be fitted. Below the Model Group Popup box the **Model Popup** box is located, which lists all the models contained by the Model Group actually selected in the Model Group Popup box. On the right of the Model Group Popup box there is the **Source Popup** box in which the nuclide should be selected on which the Mössbauer effect was measured in the case of the current spectrum. Below the Model Popup box the **Subspectrum Popup** box is located. This can be used to select the **actual subspectrum**. The **Background** and **Velocity Axis** parameter groups are also treated formally as subspectra. Below the Subspectrum Popup box the **Parameters List** box is located, which lists all the parameters belonging to the actual subspectrum. On the right of the Parameters List box, the **Constraints List** box is located that lists the constraints set for the **actual parameter** selected in the Parameters List box. On the right of the Subspectrum Popup box, above the Constraints List box, the **Interaction Popup** box is located. This can be used to select the interaction — physical model — of the actual subspectrum. When the actual subspectrum is the parameter group of Background, then on the right of the Interaction Popup box the Calculation Mode Popup box is displayed. This popup box can be used to select **Transmission Integral** calculation mode or **Thin Absorber Approximation** calculation mode. When the actual subspectrum is neither the parameter group of Background nor the parameter group of Velocity Axis, then on the right of the Interaction Popup box the **Line Shape Popup** box is displayed. This popup box can be used to select the shape of absorption lines the absorption pattern of the actual model is built from. Below the Parameters List box there are the **ADD**, **REMOVE**, **SAVE**, and **CONSTRAIN** popup boxes, along with the **DETAILS** box. The latter should be clicked to invoke the **DETAILS** page that can be used to fine-tune linear models.

27.3.1. Functions of the ADD, REMOVE, SAVE, DB and CONSTRAIN menu boxes

ADD

New Subspectrum	To add a new subspectrum only to the model of the current spectrum. The subspectrum can be selected from the collection of previously saved subspectra, or — by simply clicking on „New Subspectrum” — it will be a singlet.
New Subspectrum (DLL)	To add a new subspectrum available in user programmed and compiled dynamic link libraries, being saved in the code library directory (. . \MOSSWINN 4.0 \DLLs \) with a name corresponding to the mask SUB*.DLL, to the model of the current spectrum.
New Subspectrum Group	To add a subspectrum group only to the model of the current spectrum. The subspectrum group can be selected from the collection of previously saved subspectrum groups (multiple subspectra with arbitrary constrains between them).
New Shared Subspectrum	To add a new shared subspectrum to the model of all the spectra fitted simultaneously. The subspectrum can be selected from the collection of previously saved subspectra, or — by simply clicking on „New Subspectrum” — it will be a singlet.
New Shared Subspectrum (DLL)	To add a new shared subspectrum available in user programmed and compiled dynamic link libraries to the model of all the spectra fitted simultaneously.
New Shared Subspectrum Group	To add a shared subspectrum group to the model of all the spectra (with the same SOURCE setting as the actual one) fitted simultaneously. The subspectrum group can be selected from the collection of subspectrum groups saved earlier via the SAVE \ SAVE SUBSPECTRUM GROUP... option.

Extra Fit Parameter	A special parameter can be added to the parameter group of the Background.
New Spectrum to fit	To add a new spectrum to the list of spectra that are fitted simultaneously. Only those spectra are available which are loaded on the current desk in the main menu.

REMOVE

Subspectrum	To remove a shared/unshared subspectrum from the model of the fitted spectra/current spectrum.
All subspectra	To remove all shared and unshared subspectra from the fit model associated with the current spectrum.
Spectrum from fit	To remove a spectrum from the list of spectra fitted simultaneously.
Subspectrum from collection	To remove a previously saved subspectrum from the collection of subspectra. A separate collection is maintained for each of the nuclides.
Subspectrum Group from collection	To remove a previously saved subspectrum group from the collection of subspectrum groups. A separate subspectrum group collection is maintained for each of the nuclides.
Fit model from model group	To remove a previously saved fit model from the model group actually selected in the Model Group Popup.
Model group	To remove a whole model group with all of its models.
Parameter	To remove a parameter from the list of parameters. This function is used first of all to remove Extra Parameters added previously to the list of parameters.

SAVE

Save Spectrum	To save the current spectrum to disk with a different name according to its present state.
Save Subspectrum	To save one of the subspectra of the model of the current spectrum to the collection of subspectra belonging to the actually selected SOURCE.
Save Subspectrum Group...	To save one or more of the subspectra of the current model as a group (unit) to the collection of Subspectrum Groups belonging to the actually selected SOURCE.
Save Model As	To save the model of the current spectrum either to one of the existing model groups or in a newly created model group.
Insight Page...	To save the content of one of the insight pages to disk in ASCII format, according to its present state.

DB

The DB menu box provides access to functions of the **MossWinn Internet Database (MIDB)** service. Access to the MIDB service requires subscription that can be requested e.g. via the **REQUEST MIDB DATABASE SUBSCRIPTION FOR THE ATTACHED KEY...** submenu of the **HELP** menu in the main menu.

Find and apply best match Considering own records Considering all records Considering all transmission / conversion type records	To search through the MIDB database records in order to find the spectrum that best matches the fitted spectrum currently on the screen, and to set the corresponding fit model as included in the database record returned by the search. The fitness of the database records with respect to the current spectrum is evaluated by considering the isomer shift of the isomer shift reference material that can be set via the ISOMER SHIFT REFERENCE submenu option of the SET menu. A press directly on the FIND AND APPLY BEST MATCH menu item is equivalent to the option CONSIDERING OWN RECORDS . The fit model returned as the best match will be saved automatically as a new model of the MIDB [*] model group where * stands for the corresponding source nuclide. Apart from the best match, the search will also return several further records in descending order of their fitness. Select this menu again in order to see the corresponding list and apply another one of the returned records.
---	---

Open compound class in database browser	Turn to this option in order to select one of the records returned by the FIND AND APPLY BEST MATCH function, and open the corresponding compound class in the database browser.
Browse the internet database	Select this option in order to display the database browser that allows one to search through the MIDB database records according to various criteria. The database browser also provides the possibility to try/apply the fit models, represented by the database records, to the fitted spectrum currently on the screen.
Publish record in the internet database	Select this option in order to publish the current fit model and/or a downsampled version of the current spectrum in the MossWinn Internet Database. If along with the fit parameters you also want to publish their standard deviation in the database, calculate the corresponding standard deviations via the CAL STD menu before turning to this option. Once the option is selected, first the DATABASE RECORD INPUT FORM becomes displayed on which one can set various parameters associated with the record to be published. Then, the next form provides the possibility to set the resampled form of the measured spectrum, and to declare whether one wants to publish only the fit model, only the resampled spectrum, or both. On the next form a preview of the record is displayed, where one can check how the record will appear when published. The record becomes finally published when on the preview form the PUBLISH RECORD button is pressed. Once a record is published in the database, it may appear in the MIDB database browser of MIDB subscribers all around the world. The MIDB Publisher's Guide (http://www.mosswinn.hu/midbguide.htm) contains useful information on recommended practices concerning the publication of MIDB records.
Withdraw record from the internet database	Select this option in order to withdraw a MIDB record published earlier by using the hardware key that is currently attached to the computer (own record). The own record that is to be withdrawn can be selected on the appearing form. Withdrawal of own records from the MIDB database does not require subscription to the database.
Edit record published in the internet database	Select this option to edit one of the own MIDB records by changing the record parameters that can be set on the DATABASE RECORD INPUT FORM . The fit model and the resampled spectrum associated with the record cannot be edited in this way. The own record that is to be edited can be selected on the appearing form.
Synchronize local data with the internet database	Select this option to carry out pending MIDB publication and withdrawal operations, and to synchronize local data with the MIDB host server. The frequency of such synchronization events may be subject to a limitation.
Open MIDB Compound Summary in the default browser	Select this option to open the MIDB Compound Summary in the default browser. (http://www.mosswinn.hu/midbsummary.htm)
Help on the DB menu box	Select this option in order to open the html help concerning the DB menu box.

CONSTRAIN

Distribution	Select one of the listed distribution types to fit a distribution of the actual parameter. The left and right boundaries of the distribution will be equal to the actual minimum and maximum values of the actual parameter, respectively.
Unrestricted (UNR)	No restriction will be applied when the distribution is derived. Identical to the original method of Hesse and Rübartsch. The Smoothing factor can not be fitted in this case.
Positive, Free Boundaries (PFB)	Only positive valued distributions will be considered.
Positive, Zero Left Boundary (PZLB)	Only those positive valued distributions will be considered, which approaches zero at the left boundary (at the minimum value of the X axis).
Positive, Zero Right Boundary (PZRB)	Only those positive valued distributions will be considered, which approaches zero at the right boundary (at the maximum value of the X axis).
Positive, Zero Left & Right Boundaries (PZLRB)	Only those positive valued distributions will be considered, which approaches zero at the left and right boundaries (at the minimum and maximum values of the X axis).
Split distribution	Select this option in order to split the distribution at some intermediate value by adding the SPLIT [x] directive to the parameter constraints list box, where <i>x</i> denotes an intermediate distribution-parameter value. As a result, the distribution will contribute to the fitting curve by two separate subspectra: one belonging to distribution-parameter values higher than <i>x</i> , and the other belonging to distribution-parameter values lower than or equal to <i>x</i> .

CONSTRAIN

Relative	Available only for Amplitude type parameters. The internal absolute value of the selected Amplitude type parameter will be calculated by multiplying its displayed relative value with the absolute value of the <i>first</i> of the Amplitude type parameters in the host subspectrum. If the selected parameter is the first Amplitude type parameter in the current subspectrum, then its absolute value will be calculated by multiplying its displayed relative value with the value of the BASE LINE.
-----------------	---

CONSTRAIN

Is Equal to	:= constraint will be added to the list of constraints of the actual parameter. Click on the Constraints List box to set the value that the actual parameter should be equal to.
Is in the Range	[,] constraint will be added to the list of constraints of the actual parameter. Click on the Constraints List box to set the minimum and maximum values of the actual parameter.
INclude Range	INC[,] constraint will be added to the list of constraints of the actual parameter. Click on the Constraints List box to set the minimum and maximum values of the interval which should be enabled for the actual parameter.
EXclude Range	EXC[,] constraint will be added to the list of constraints of the actual parameter. Click on the Constraints List box to set the minimum and maximum values of the interval which should be excluded from the enabled values of the actual parameter.
Higher Than	> constraint will be added to the list of constraints of the actual parameter. Click on the Constraints List box to set the value that the actual parameter should exceed.
Higher or Equal	>= constraint will be added to the list of constraints of the actual parameter. Click on the Constraints List box to set the value that the actual parameter should exceed or equal.
Less Than	< constraint will be added to the list of constraints of the actual parameter. Click on the Constraints List box to set the value that the actual parameter should be lower than.
Less or Equal	<= constraint will be added to the list of constraints of the actual parameter. Click on the Constraints List box to set the value that the actual parameter should not exceed.
Hard constraint	HARD constraint will be added to the list of constraints of the actual parameter. The above 8 constraints in constraint lists marked with the HARD constraint will be considered whenever the value of the corresponding parameter is set (e.g. during local fitting via the FIT menu). The above 8 constraints in constraint lists without the HARD constraint are in effect only when the Global Fitting procedure is executed via the GLOBAL menu.

CONSTRAIN

Higher Than #PARAMETER	The value of the actual parameter will have to exceed the value of the selected parameter. To remove this constraint click on the name of the actual parameter in the list of parameters.
Higher or Equal #PARAMETER	The value of the actual parameter will have to be higher or equal to the value of the selected parameter. To remove this constraint click on the name of the actual parameter in the list of parameters.
Less Than #PARAMETER	The value of the actual parameter will have to be less than the value of the selected parameter. To remove this constraint click on the name of the actual parameter in the list of parameters.
Less or Equal #PARAMETER	The value of the actual parameter will have to be less than the value of the selected parameter. To remove this constraint click on the name of the actual parameter in the list of parameters.
Not Equal to #PARAMETER	The value of the actual parameter must not be equal to the value of the selected parameter.
Is Close to #PARAMETER	The value of the actual parameter must remain close to the value of the selected parameter. What is „close” and what is „far” is determined by the enabled range of #PARAMETER.
Is Far from #PARAMETER	The value of the actual parameter must remain far from the value of the selected parameter. What is „far” and what is „close” is determined by the enabled range of #PARAMETER.

CONSTRAIN

:= #PARAMETER	The value of the actual parameter must be equal to the value of the selected parameter.
:= #PARAMETER + CONST	The value of the actual parameter must be equal to the value of the selected parameter + a constant. The constant will be added to the parameter list of the actual subspectrum.
:= #PARAMETER * CONST	The value of the actual parameter must be equal to the value of the selected parameter * a constant. The constant will be added to the parameter list of the actual subspectrum.
:= #PARAMETER * CONST1 + CONST2	The value of the actual parameter must be equal to the value of the selected parameter * Constant m + Constant b . The constants m and b will be added to the parameter list of the actual subspectrum.
:= User Programmed Function [Quadratic]	<p>The value of the actual parameter will be equal to Φ (SELECTED PARAMETER, NEW PARAMETERS 1..N) where the function Φ can be an arbitrary function programmed by the user in DEP_DLL1.DLL. The default Φ function is Quadratic:</p> $\text{ACTUAL PARAMETER} := \text{CONSTANT} + \text{LINEAR} * \text{SELECTED PARAMETER} + \text{QUADRATIC} * (\text{SELECTED PARAMETER})^2$ <p>See page 73 for further details.</p>
:= #Percentage constrained	The area of the actual subspectrum will be constrained by a percentage parameter, and the first of the amplitude type parameters will be fixed. The rest of the amplitude type parameters (if any) will serve as a RELATIVE parameter: to get their real value multiply their displayed relative value with that of the first amplitude type parameter. To remove the percentage constraint, click on the name of the first amplitude type parameter of the corresponding subspectrum in the list of parameters, and select the first row in the appearing popup box.

27.3.2. Selection of source nuclide

On the **MODEL** page click on the **SOURCE** popup box to set the source nuclide used for the Mössbauer measurement. The correct setting of the source nuclide is essential in order to obtain correct values for the fit parameters. The available models in the Interaction Popup depend on the selected source nuclide. The program also passes the source-nuclide information to user written Dynamic Link Libraries (see page 69).

27.3.3. Spectrum background

When the parameter list of the background is selected formally as the actual subspectrum, then the Interaction Popup box serves for the selection of various background types. The following types are available. (The v velocity is measured in [mm/s]).

Constant	Constant baseline with one parameter: BASE LINE $Background = BaseLine$
Slope	Baseline with slope, with two parameters: BASE LINE, SLOPE $Background = BaseLine + Slope \cdot v$
Curvature	Baseline modeling slope and curvature, with three parameters: BASE LINE, CURVATURE, CENTER $Background = BaseLine + Curvature \cdot (v - Center)^2$
Third Order	Baseline modeled by a third order polynomial, with four parameters: BASE LINE, CURVATURE, CENTER, CUBIC COEFFICIENT $Background = BaseLine + Curvature \cdot (v - Center)^2 + CubicCoefficient \cdot (v - Center)^3$
Unfolded	Baseline that can be used to model backgrounds of unfolded spectra that are calibrated. Power of a cosine function with five parameters: BASE LINE, COSINE AMPLITUDE, COSINE EXPONENT, MAXIMUM VELOCITY, CENTER [MM/S] $BaseLine \pm COSINEAMPLITUDE \cdot \left[\cos\left(\frac{\pi}{2} \cdot \frac{(v - Center)}{MaximumVelocity}\right) \right]^{COSINEExponent}$
Unfolded + Slope	Unfolded background with slope, described by six parameters (v_0 depends only on the velocity axis, and it is determined internally. Its value is close to the value of the MAXIMUM VELOCITY): BASE LINE, COSINE AMPLITUDE, COSINE EXPONENT, MAXIMUM VELOCITY, CENTER [MM/S], SLOPE $BaseLine \pm slope \cdot ABS(v - v_0) \pm COSINEAMPLITUDE \cdot \left[\cos\left(\frac{\pi}{2} \cdot \frac{(v - Center)}{MaximumVelocity}\right) \right]^{COSINEExponent}$

27.3.4. Built in Interactions

For each selected source nuclide, MossWinn provides several interactions that can be selected for any fitted subspectra. Some of these are linear models that can be fine-tuned further on the **DETAILS** page. Others, which cannot be modified on the **DETAILS** page, are based on Hamiltonian calculations. To add a new custom subspectrum model to those already available in the Interaction Popup box, save the model in question to the **Subspectrum Collection** of the corresponding source nuclide (via SAVE → SAVE SUBSPECTRUM). Then the saved model will be available in the Interaction Popup box under SUBSPECTRUM FROM COLLECTION. One can add any subspectrum model to the fitting capability of MossWinn by writing and compiling the corresponding code as DLL (see page 69 for details).

The following table lists the interactions available by default for the various nuclides. The interaction when there is no splitting in the absorption line is called MONOPOLE in MossWinn.

Source nuclides: ⁵⁷Fe, ¹¹⁹Sn, ¹²⁵Te, ¹⁵¹Eu, ¹²¹Sb, ¹²⁹I, ¹⁴¹Pr, ²³⁷Np, ¹⁹⁷Au, ¹⁶¹Dy (25.655 keV), M1/E1, M1+E2, E2	
Monopole	Linear model. Single absorption line, with three parameters: AMPLITUDE, ISOMER SHIFT, LINE WIDTH
Quadrupole (Powder) (Available only for ⁵⁷ Fe, ¹¹⁹ Sn, ¹²⁵ Te, ¹⁹⁷ Au, ¹⁵¹ Eu)	For ⁵⁷Fe, ¹¹⁹Sn, ¹²⁵Te, ¹⁹⁷Au : Linear model Symmetrical quadrupole doublet with four parameters: AMPLITUDE, ISOMER SHIFT, Q. SPLITTING, LINE WIDTH For ¹⁵¹Eu : Hamiltonian, non-linear model. The model is calculated by solving the static Hamiltonian for pure quadrupole interaction. Powdered material is assumed. The model is described with five parameters: AMPLITUDE, ISOMER SHIFT, VZZ [10 ^{^21} V/M2], ETA [0..1], LINE WIDTH
Magnetic (Powder) (Not available for M1/E1, M1+E2, E2)	Linear model. Magnetically split absorption pattern described with four parameters: AMPLITUDE, ISOMER SHIFT, MAGNETIC FIELD [T], LINE WIDTH
First Order Mixed M+Q (Powder) (Available only for ⁵⁷ Fe, ¹¹⁹ Sn, ¹²⁵ Te)	Linear model. Magnetically split absorption pattern displaying quadrupole splitting for the case of ETA = 0, with 6 absorption lines having the amplitude ratio of 3:2:1:1:2:3, with five parameters: AMPLITUDE, ISOMER SHIFT, MAGNETIC FIELD [T], Q. SPLITTING, LINE WIDTH
Mixed M+Q Static Hamiltonian (Powder)	Hamiltonian, non-linear model. <u>H</u> based system The model is calculated by solving the static Hamiltonian for mixed magnetic and quadrupole interactions with arbitrary relative orientation. The z axis is assumed to be parallel to the magnetic field. BETA (EFG) denotes the polar, and ALPHA (EFG) denotes the azimuthal angle of V _{zz} relative to the direction of the magnetic field. The model is described with eight parameters: AMPLITUDE, ISOMER SHIFT, MAGNETIC FIELD [T], VZZ (EFG) [10 ^{^21} V/M2], ETA (EFG), BETA (EFG), ALPHA (EFG), LINE WIDTH
Mixed Q+M Static Hamiltonian (Powder)	Hamiltonian, non-linear model. <u>V_{zz}</u> based system. The model is calculated by solving the static Hamiltonian for mixed magnetic and quadrupole interactions with arbitrary relative orientation. The z axis is assumed to be parallel with the V _{zz} (that is with the e _z unit vector of the coordinate system in which the EFG is diagonal and V _{xx} ≤ V _{yy} ≤ V _{zz}). BETA (MF) denotes the polar, and ALPHA (MF) denotes the azimuthal angle of the magnetic field relative to e _z . The model is described with eight parameters: AMPLITUDE, ISOMER SHIFT, MAGNETIC FIELD [T], VZZ (EFG) [10 ^{^21} V/M2], ETA (EFG), BETA (MF), ALPHA (MF), LINE WIDTH
Blume-Tjon Two State Magnetic Relaxation (Powder) (Available only for ⁵⁷ Fe)	Hamiltonian, non-linear model. Blume-Tjon relaxation model assuming a relaxing magnetic field with two possible, opposite directions for the magnetic field at the place of the nucleus. The model is described with eight parameters: AMPLITUDE, ISOMER SHIFT, MAGNETIC FIELD [T], VZZ (EFG) [10 ^{^21} V/M2], ETA (EFG), JUMP UP RATE, JUMP DOWN RATE, LINE WIDTH
Tjon-Blume Jahn-Teller Quadrupole Relaxation (Powder) (Available only for ⁵⁷ Fe)	Hamiltonian, non-linear model. Tjon-Blume relaxation model assuming an electric field gradient whose main component (V _{zz}), although fixed in magnitude, reorients dynamically and randomly between the e _x , e _y and e _z directions of the eigensystem of the EFG tensor. The hyperfine magnetic field and η are assumed to be zero. The model is described with five parameters: AMPLITUDE, ISOMER SHIFT, VZZ (EFG) [10 ^{^21} V/M2], JUMP RATE, LINE WIDTH

<p>Random EFG in uniaxial external magnetic field (Powder) (Available only for ^{57}Fe)</p>	<p>Hamiltonian, non-linear model. The analytical expression for the line shape of the ^{57}Fe Mössbauer spectrum of a powdered sample, with randomly oriented EFG and $\eta = 0$, subjected to a uniaxial (external) magnetic field, as given by Blaes et al. in N. BLAES, H. FISCHER, U. GONSER: NIM B 9 (1985) 201. The model is described with seven parameters ($\eta = 0$ is a dummy parameter):</p> <p>AMPLITUDE, ISOMER SHIFT, MAGNETIC FIELD [T], VZZ (EFG) [10^{21} V/M²], ETA (EFG), THETA (GAMMA RAY), LINE WIDTH</p>
<p>Quadrupole (Single crystal) (Available only for ^{57}Fe, ^{119}Sn, ^{125}Te, ^{197}Au)</p>	<p>Linear model. Asymmetrical quadrupole doublet with five parameters: AMPLITUDE (1), AMPLITUDE (2), ISOMER SHIFT, Q. SPLITTING, LINE WIDTH</p>
<p>Magnetic (Single crystal) (Available only for ^{57}Fe, ^{119}Sn, ^{125}Te)</p>	<p>Linear model. Magnetically split absorption pattern with 6 absorption lines having the amplitude ratio of 3:x:1:1:x:3, with five parameters: AMPLITUDE (1,3,4,6), AMPLITUDE (2,5), ISOMER SHIFT, MAGNETIC FIELD [T], LINE WIDTH</p>
<p>First Order Mixed M+Q (Single crystal) (Available only for ^{57}Fe, ^{119}Sn, ^{125}Te)</p>	<p>Linear model. Magnetically split absorption pattern displaying quadrupole splitting for the case of $\text{ETA} = 0$, with 6 absorption lines having the amplitude ratio of 3:x:1:1:x:3, with six parameters: AMPLITUDE (1,3,4,6), AMPLITUDE (2,5), ISOMER SHIFT, MAGNETIC FIELD [T], Q. SPLITTING, LINE WIDTH</p>
<p>Mixed M+Q Static Hamiltonian (Single crystal)</p>	<p>Hamiltonian, non-linear model. \underline{H} based system The model is calculated by solving the static Hamiltonian for mixed magnetic and quadrupole interactions with arbitrary relative orientation. The z axis is assumed to be parallel to the magnetic field. BETA (EFG) denotes the polar, and ALPHA (EFG) denotes the azimuthal angle of V_{zz} relative to the direction of the magnetic field. THETA (GAMMA RAY) denotes the polar, and PHI (GAMMA RAY) denotes the azimuthal angle of the gamma-ray direction relative to the direction of the magnetic field. The model is described with ten parameters: AMPLITUDE, ISOMER SHIFT, MAGNETIC FIELD [T], VZZ (EFG) [10^{21} V/M²], ETA (EFG), BETA (EFG), ALPHA (EFG), THETA (GAMMA RAY), PHI (GAMMA RAY), LINE WIDTH</p>
<p>Mixed Q+M Static Hamiltonian (Single crystal)</p>	<p>Hamiltonian, non-linear model. \underline{V}_{zz} based system. The model is calculated by solving the static Hamiltonian for mixed magnetic and quadrupole interactions with arbitrary relative orientation. The z axis is assumed to be parallel with the V_{zz} (that is with the e_z unit vector of the coordinate system in which the EFG is diagonal and $V_{xx} \leq V_{yy} \leq V_{zz}$). BETA (MF) denotes the polar, and ALPHA (MF) denotes the azimuthal angle of the magnetic field relative to e_z. THETA (GAMMA RAY) denotes the polar, and PHI (GAMMA RAY) denotes the azimuthal angle of the gamma-ray direction relative to e_z. The model is described with ten parameters: AMPLITUDE, ISOMER SHIFT, MAGNETIC FIELD [T], VZZ (EFG) [10^{21} V/M²], ETA (EFG), BETA (MF), ALPHA (MF), THETA (GAMMA RAY), PHI (GAMMA RAY), LINE WIDTH</p>
<p>Mixed M+Q Static Hamiltonian (Mosaic)</p>	<p>Hamiltonian, non-linear model. \underline{H} based system The model is calculated by solving the static Hamiltonian for mixed magnetic and quadrupole interactions with arbitrary relative orientation. The z axis is assumed to be parallel to the magnetic field. BETA (EFG) denotes the polar, and ALPHA (EFG) denotes the azimuthal angle of V_{zz} relative to the direction of the magnetic field. THETA (GAMMA RAY) denotes the polar angle of the gamma-ray direction relative to the direction of the magnetic field. The azimuthal angle of the gamma-ray direction is assumed to be random and evenly distributed between 0 deg and 360 deg in the sample (mosaic sample), so that the amplitudes are averaged with respect to this angle {PHI (GAMMA RAY)}. The model is described with nine parameters: AMPLITUDE, ISOMER SHIFT, MAGNETIC FIELD [T], VZZ (EFG) [10^{21} V/M²], ETA (EFG), BETA (EFG), ALPHA (EFG), THETA (GAMMA RAY) LINE WIDTH</p>

Mixed Q+M Static Hamiltonian (Mosaic)	<p>Hamiltonian, non-linear model. \underline{V}_{zz} based system.</p> <p>The model is calculated by solving the static Hamiltonian for mixed magnetic and quadrupole interactions with arbitrary relative orientation. The z axis is assumed to be parallel with the \underline{V}_{zz} (that is with the e_z unit vector of the coordinate system in which the EFG is diagonal and $V_{xx} \leq V_{yy} \leq V_{zz}$). BETA (MF) denotes the polar, and ALPHA (MF) denotes the azimuthal angle of the magnetic field relative to e_z. THETA (GAMMA RAY) denotes the polar angle of the gamma-ray direction relative to e_z. The azimuthal angle of the gamma-ray direction is assumed to be random and evenly distributed between 0 deg and 360 deg in the sample (mosaic sample), so that the amplitudes are averaged with respect to this angle {PHI (GAMMA RAY)}. The model is described with nine parameters: AMPLITUDE, ISOMER SHIFT, MAGNETIC FIELD [T], VZZ (EFG) [10^{21} V/M²], ETA (EFG), BETA (MF), ALPHA (MF), THETA (GAMMA RAY), LINE WIDTH</p>
Mixed M+Q Static Hamiltonian (Powder+GKE)	<p>Hamiltonian, non-linear model with Goldanskii-Karyagin Effect. \underline{H} based system</p> <p>The model is calculated by solving the static Hamiltonian for mixed magnetic and quadrupole interactions with arbitrary relative orientation. The z axis is assumed to be parallel to the magnetic field. BETA (EFG) denotes the polar, and ALPHA (EFG) denotes the azimuthal angle of \underline{V}_{zz} relative to the direction of the magnetic field.</p> <p>The MSD Tensor is assumed to be diagonal in the PAS, and furthermore it is assumed to display axial symmetry. D(z,x) (MSD) denotes $k^2 \cdot [\langle z^2 \rangle_{av} - \langle x^2 \rangle_{av}]$. The model is described with nine parameters: AMPLITUDE, ISOMER SHIFT, MAGNETIC FIELD [T], VZZ (EFG) [10^{21} V/M²], ETA (EFG), BETA (EFG), ALPHA (EFG), D(z,x) (MSD), LINE WIDTH</p>
Mixed Q+M Static Hamiltonian (Powder+GKE)	<p>Hamiltonian, non-linear model with Goldanskii-Karyagin Effect. \underline{V}_{zz} based system</p> <p>The model is calculated by solving the static Hamiltonian for mixed magnetic and quadrupole interactions with arbitrary relative orientation. The z axis is assumed to be parallel with the \underline{V}_{zz} (that is with the e_z unit vector of the coordinate system in which the EFG is diagonal and $V_{xx} \leq V_{yy} \leq V_{zz}$). BETA (MF) denotes the polar, and ALPHA (MF) denotes the azimuthal angle of the magnetic field relative to e_z.</p> <p>The MSD Tensor is assumed to be diagonal in the PAS, and furthermore it is assumed to display axial symmetry. D(z,x) (MSD) denotes $k^2 \cdot [\langle z^2 \rangle_{av} - \langle x^2 \rangle_{av}]$. The model is described with nine parameters: AMPLITUDE, ISOMER SHIFT, MAGNETIC FIELD [T], VZZ (EFG) [10^{21} V/M²], ETA (EFG), BETA (MF), ALPHA (MF), D(z,x) (MSD), LINE WIDTH</p>
External libraries	<p>Turn to this menu option in order to access theories (subspectrum models) programmed and compiled as external dynamic link libraries (see page 69).</p>
Subspectrum from collection	<p>To select any subspectrum saved earlier into the subspectrum collection of the selected source nuclide.</p>

27.3.5. Nuclear parameters of M1, E1, E2, and M1+E2 transitions

When M1/E1, M1+E2, or E2 is selected formally as the source in the FIT menu, then one has the possibility to customize (or even fit if required) the values of the nuclear parameters of the selected nuclear transition. MossWinn adds/removes the necessary nuclear parameters automatically to/from the parameter list of the background. The name and meaning of these parameters — as used in MossWinn — are as follows.

Parameters used for each type (M1/E1, E2, M1+E2) of nuclear transition:

Parameter name	Meaning
Energy (Gamma ray) [KeV]	Energy of the γ ray emitted during the Mössbauer transition.
Spin (Excited state)	Nuclear spin of the excited state of the Mössbauer nuclide in units of \hbar . Constrained to $I_e \leq 9/2$.
Spin (Ground state)	Nuclear spin of the ground state of the Mössbauer nuclide in units of \hbar . Constrained to $I_g \leq 9/2$.
g factor (Excited state)	Gyromagnetic factor of the excited state of the Mössbauer nuclide.
g factor (Ground state)	Gyromagnetic factor of the ground state of the Mössbauer nuclide.
Q.Mom. (Excited state) [barn]	Nuclear quadrupole moment of the excited state of the Mössbauer nuclide.
Q.Mom. (Ground state) [barn]	Nuclear quadrupole moment of the ground state of the Mössbauer nuclide.
Natural Line Width [mm/s]	(Experimental) Natural line width, as measurable in an experiment (e.g. 0.194 mm/s for ^{57}Fe).

Additional nuclear parameters used only for the M1+E2 type nuclear transition:

Parameter name	Meaning
Amplitude (E2/M1)	AMPLITUDE (δ) of the E2 / M1 mixing ratio of a mixed M1+E2 Mössbauer transition. It should be non-negative. Equals to the absolute value of the ratio of the corresponding reduced matrix elements: $ \delta \cdot e^{i\zeta} = \frac{\langle I_g \mathbf{M} (E2) I_e \rangle}{\langle I_g \mathbf{M} (M1) I_e \rangle}$ (Most literature quotes δ^2 . For ^{197}Au , for example, $\delta^2 \approx 0.11$)
Phase angle (E2/M1) [deg]	PHASE difference between the E2 and M1 radiations. MEASURED IN DEGREES. $180 \cdot \frac{\zeta}{\pi}$ where ζ appears in $\delta \cdot e^{i\zeta}$. For ^{99}Ru , for example, Phase angle (E2/M1) [deg] ≈ 180 . (For ^{99}Ru see O.C. KISTNER: PHYS. REV. 144 (1966) 1022.)

27.4. Built in Hamiltonian models

27.4.1. Static Hamiltonian of mixed magnetic and quadrupole interactions

The model of mixed magnetic and quadrupole interaction is solved in MossWinn by the diagonalization of the nuclear Hamiltonian matrix. In the system where the e_z unit vector is chosen to be parallel to the direction of the magnetic field the Hamiltonian is expressed as follows [R.W. GRANT: MÖSSBAUER SPECTROSCOPY IN MAGNETISM: CHARACTERIZATION OF MAGNETICALLY-ORDERED COMPOUNDS, IN MÖSSBAUER SPECTROSCOPY, ED. U. GONSER, SPRINGER-VERLAG, 5 (1975) PP. 97.]:

$$\begin{aligned}
 H(I)_{m,m} &= -\omega_H \hbar \cdot m + \frac{\omega_Q \hbar}{2} (3 \cos^2 \beta - 1 + \eta \cdot \sin^2 \beta \cdot \cos 2\alpha) [3m^2 - I(I+1)] \\
 H(I)_{m,m+1} &= \frac{3\omega_Q \hbar}{2} \sin \beta \cdot \left\{ \cos \beta - \frac{\eta}{6} [(1 + \cos \beta) e^{2\alpha i} - (1 - \cos \beta) e^{-2\alpha i}] \right\} (2m+1) \sqrt{(I-m)(I+m+1)} \\
 H(I)_{m,m+2} &= \frac{3\omega_Q \hbar}{4} \left\{ \sin^2 \beta + \frac{\eta}{6} [(1 + \cos \beta)^2 e^{2\alpha i} + (1 - \cos \beta)^2 e^{-2\alpha i}] \right\} \sqrt{(I+m+2)(I+m+1)(I-m)(I-m-1)} \\
 \omega_H &= \frac{g_N(I) \cdot B \cdot \mu_N}{\hbar} & \omega_Q &= \frac{1}{\hbar} \cdot \frac{eV_{zz}Q}{4I(2I-1)}
 \end{aligned}$$

where B denotes the flux density of the hyperfine magnetic field, β denotes the polar, and α denotes the azimuthal angle of V_{zz} **relative to e_z** , I denotes the angular momentum quantum number of the excited or ground state of the Mössbauer nucleus, and m goes through the values of $-I, -I+1 \dots I-1, I$. The rest of the elements in the upper triangle are zero. The elements in the lower triangle of the $\mathbf{H}(I)$ matrix are calculated in the following way:

$$\mathbf{H}(I)_{i,j} [\text{lower triangle}] = \mathbf{H}(I)_{j,i} [\text{upper triangle}]^*$$

where * denotes the operation of complex conjugation (with other words, $\mathbf{H}(I)$ is a Hermitian matrix). In the system where the e_z unit vector is chosen to be parallel to the V_{zz} (to the e_z unit vector of the coordinate system in which the EFG is diagonal and $|V_{xx}| \leq |V_{yy}| \leq |V_{zz}|$) the Hamiltonian is expressed as follows [based on the paper: W. KÜNDIG: NUCLEAR INSTRUMENTS AND METHODS 48 (1967) 219.]:

$$\begin{aligned}
 H(I)_{m,m} &= \omega_Q \hbar [3m^2 - I(I+1)] - \omega_H \hbar m \cos \beta \\
 H(I)_{m,m+1} &= \frac{-\omega_H \hbar \sin \beta}{2} \sqrt{I(I+1) - m(m+1)} \cdot e^{i\alpha} \\
 H(I)_{m,m+2} &= \frac{\omega_Q \hbar}{2} \cdot \eta \cdot \sqrt{[I(I+1) - (m+2)(m+1)] \cdot [I(I+1) - m(m+1)]}
 \end{aligned}$$

where the same notations were used as in the previous case, except that here β denotes the polar, and α denotes the azimuthal angle of the **magnetic field relative to e_z** . The rest of the elements in the upper triangle are zero. The matrix elements of the lower triangle are calculated in the same way as described in the previous case.

MossWinn calculates the Hamiltonian for the excited as well as for the ground state of the nucleus, and solves the corresponding eigenproblems numerically. Then the position of the absorption lines is calculated from the obtained eigenvalues. Then at each position a Lorentzian, a Lorentzian with dispersion, a Pseudo-Voigt function, or a Cosine Smeared Lorentzian function — depending on the corresponding setting in the FIT menu — is placed. The relative amplitudes of the lines are calculated with the help of the eigenvectors derived during the solution of the eigenproblem. For each handled nuclide three different cases are handled as explained below: Single crystal, Mosaic, and Powder samples.

27.4.2. Relative amplitude of the absorption lines of pure M1/E1 transitions

Single Crystal case

In the case of a single crystal the electric field vector of the dipole radiation field can be expressed as follows [R.M. HOUSLEY, R.W. GRANT, U. GONSER: PHYS. REV. 178 (1969) 514.]:

$$\begin{aligned} \mathbf{E}(\underline{r})_{i \rightarrow j} = R(\underline{r}) \cdot \{ & [a_M(1,1)e^{i\varphi} + a_M(1,-1)e^{-i\varphi}] \cdot \hat{\Psi} + \\ & + i \cdot [a_M(1,1)e^{i\varphi} \cos(\vartheta) + a_M(1,0)\sqrt{2} \sin(\vartheta) - a_M(1,-1)e^{-i\varphi} \cos(\vartheta)] \cdot \hat{\Xi} \} \end{aligned}$$

where $\hat{\Psi}$ and $\hat{\Xi}$ are spherical unit vectors that are both perpendicular to the propagation direction of the radiation, as well as they are perpendicular to each other. θ and φ are the polar and azimuthal angles of the γ -ray direction relative to the quantization axis (in our case either the direction of \underline{H} , or the direction corresponding to V_{zz}). The complex coefficients $a_M(1,1)$, $a_M(1,0)$ and $a_M(1,-1)$ are calculated from the eigenvectors of the actual Hamiltonian matrix:

$$a_M(1,m)_{i \rightarrow j} = \sum_{m_e - m_g = m} \alpha_i(m_e) \cdot \alpha_j^*(m_g) \cdot \text{Clebsch}(I_e, 1, I_g, m_e, m, m_g)$$

where $i \rightarrow j$ denotes the transition from the i th eigenstate of the excited nucleus, to the j th eigenstate of the nucleus in its ground state. $\alpha_i(m_e)$ equals to the scalar product of the i th eigenstate of the excited nucleus with $|I_e, m_e\rangle$. $\alpha_j(m_g)$ equals to the scalar product of the j th eigenstate of the nucleus in its ground state with $|I_g, m_g\rangle$. * denotes the operation of complex conjugation.

The relative amplitude of the absorption line belonging to the transition $i \rightarrow j$ is then proportional to $\mathbf{E}^*(\underline{r})_{i \rightarrow j} \mathbf{E}(\underline{r})_{i \rightarrow j}$.

Mosaic Sample case

In the model for a mosaic sample the relative amplitude of the absorption line belonging to the transition $i \rightarrow j$ is proportional to $\int_0^{2\pi} \mathbf{E}_{i \rightarrow j}^* \mathbf{E}_{i \rightarrow j} \cdot d\varphi$ that is, the amplitudes get averaged with respect to the azimuthal angle of the γ -ray direction.

Powder Sample case

In the model for a powder sample the relative amplitude of the absorption line belonging to the transition $i \rightarrow j$ is proportional to $\int_0^{2\pi} d\varphi \cdot \int_0^\pi \mathbf{E}_{i \rightarrow j}^* \mathbf{E}_{i \rightarrow j} \cdot \sin(\vartheta) \cdot d\vartheta$ that is, the amplitudes get averaged with respect to the azimuthal angle as well as with respect to the polar angle of the γ -ray direction.

True for all the three cases

For the case of Hamiltonian models, independent of the setting of the AREA/AMPLITUDE mode, the relative amplitudes of the absorption lines get normalized so that the area of their sum — that is the area of the whole subspectrum — will be equal to the AMPLITUDE parameter of the corresponding subspectrum.

27.4.3. Relative amplitude of the absorption lines of mixed M1+E2 transitions

In the case of a mixed M1+E2 nuclear transition — apart from a constant factor — the electric radiation field can be expressed as follows:

$$\vec{E}(\mathcal{G}, \varphi) = \sum_{m=-2}^{+2} i \cdot [\delta \cdot e^{i\cdot\zeta} \cdot a(2, m)] \cdot (\vec{X}_{2,m} \times \vec{e}_r) - \sum_{m=-1}^{+1} a(1, m) \cdot \vec{X}_{1,m}$$

(For pure E2 nuclear transition the radiation field is expressed as $E(\mathcal{G}, \varphi) = \sum_{m=-2}^{+2} i \cdot a(2, m) \cdot (\vec{X}_{2,m} \times \vec{e}_r)$)

where $\vec{e}_r = \vec{e}_r(\mathcal{G}, \varphi)$ is the direction of propagation of the radiation, $\vec{X}_{1,m} = \vec{X}_{1,m}(\mathcal{G}, \varphi)$ denotes the vector spherical harmonics (for their definition, see for example J.M. BLATT, V.F. WEISSKOPF: THEORETISCHE KERNPHYSIK, TEUBNER VERLAG, LEIPZIG 1959, PP. 500). The ratio of the reduced matrix elements appears as:

$$\delta \cdot e^{i\cdot\zeta} = \frac{\langle I_g | \mathbf{M}(E2) | I_e \rangle}{\langle I_g | \mathbf{M}(M1) | I_e \rangle}$$

$a(1, m) = a_M(1, m)$ is defined as described in the previous section, and $a(2, m)$ is expressed as:

$$a(2, m)_{i \rightarrow j} = \sum_{m_e - m_g = m} \alpha_i(m_e) \cdot \alpha_j^*(m_g) \cdot \text{Clebsch}(I_e, 2, I_g, m_e, m, m_g)$$

For single crystals the relative amplitudes of the absorption lines are then proportional to

$$\text{Amplitude} \propto \vec{E}^*(\mathcal{G}, \varphi) \cdot \vec{E}(\mathcal{G}, \varphi)$$

Powder and Mosaic geometries are handled in a way similar to that described in the previous section.

27.4.4. The Goldanskii-Karyagin Effect

The Goldanskii-Karyagin Effect (GKE) is implemented for all the handled (M1, E1, E2, M1+E2) Mössbauer transitions for powder geometry. The Mean Square Displacement (MSD) Tensor is assumed to be DIAGONAL in the Principal Axis System (PAS) (fixed either to the EIGENSYSTEM of the EFG or to the \underline{H} magnetic field), and furthermore it is assumed to display AXIAL SYMMETRY.

Accordingly, for a given $i \rightarrow j$ (excited state level \rightarrow ground state level) transition, in the case of a powder sample the relative intensity of the absorption lines can be expressed as:

$$\text{Amplitude}_{i \rightarrow j} \propto \int_0^{\pi} d\vartheta \cdot \left[e^{-k^2 \cdot [\langle z^2 \rangle_{\text{av}} - \langle x^2 \rangle_{\text{av}}] \cos^2(\vartheta)} \cdot \sin(\vartheta) \cdot \int_0^{2\pi} \mathbf{E}_{i \rightarrow j}^* \mathbf{E}_{i \rightarrow j} \cdot d\varphi \right]$$

where k is the absolute value of the wave vector of the radiation, $\langle z^2 \rangle_{\text{av}}$ and $\langle x^2 \rangle_{\text{av}}$ denote the average of the squared displacement of the Mössbauer nucleus from its equilibrium state in the \underline{e}_z and \underline{e}_x direction of the PAS, respectively. As before, θ and φ are the polar and azimuthal angles of the γ -ray direction relative to the quantization axis.

In MossWinn $D(z, x)(\text{MSD}) = k^2 \cdot [\langle z^2 \rangle_{\text{av}} - \langle x^2 \rangle_{\text{av}}]$ appears as fitting parameter when one of the following models is selected:

- 1, MIXED M+Q STATIC HAMILTONIAN (POWDER + GKE)
- 2, MIXED Q+M STATIC HAMILTONIAN (POWDER + GKE)

References:

H.-D. PFANNES, U. GONSER: APPL. PHYS. **1** (1973) 93.

G.K. SHENOY, J.M. FRIEDT: NUCLEAR INSTRUMENTS AND METHODS **136** (1976) 569.

27.4.5. Randomly oriented EFG ($\eta = 0$) in uniaxial magnetic field (^{57}Fe , powdered sample)

The analytical expression for the line shape of the ^{57}Fe Mössbauer spectrum of a powdered sample, with randomly oriented EFG and $\eta = 0$, subjected to a uniaxial (external) magnetic field has been given in

N. Blaes, H. Fischer, U. Gonser: NIM B **9** (1985) 201.

This analytical expression is implemented in MossWinn as

$$F(\nu) = \frac{A}{8\pi} \cdot \text{Re}(N_0(H) + N_0(-H))$$

where A is the area of the corresponding subspectrum (having the name AMPLITUDE as a fit parameter), and apart from the 8π normalization factor, the remaining quantities are essentially the same as those in Eq. (5) of the above mentioned paper of Blaes *et al.* In the FIT menu of MossWinn the model is described with the following parameters:

AMPLITUDE	Area of the subspectrum.
ISOMER SHIFT	^{57}Fe isomer shift.
MAGNETIC FIELD [T]	The amplitude H of the uniaxial magnetic field.
Vzz (EFG) 10^{21} [V/m ²]	The main component of the EFG in the EFG eigensystem.
ETA (EFG)	Asymmetry parameter of the EFG, fixed to zero.
Theta (Gamma ray)	Polar angle of the γ -ray direction relative to the direction of the H magnetic field.
LINE WIDTH	Internal line width (Γ).

To initialize a subspectrum with the above model select RANDOM EFG IN UNIAXIAL EXTERNAL MAGNETIC FIELD (POWDER) in the interaction popup on the MODEL PAGE.

27.4.6. Blume-Tjon two state magnetic relaxation model (⁵⁷Fe, powdered sample)

The ⁵⁷Fe Blume-Tjon two state magnetic relaxation model implemented in the MossWinn program describes the physical model for a powdered sample that contains ⁵⁷Fe nuclei experiencing fluctuating hyperfine magnetic field. The theoretical background and calculation of this model can be found in:

M. BLUME, J.A. TJON: PHYS. REV. **165** (1968) 446.

It is assumed that the ⁵⁷Fe nucleus experiences a magnetic field that relaxes between two values: $H_1 = -h$ and $H_2 = +h$. That is, the magnetic field can either point „upwards” (+ h) or „downwards” (- h). The direction of the magnetic field is assumed to be along one of the principal axes of the EFG. The relaxation between the two states + h and - h is described by the two transition rates $W_1 = 2\pi f_1$ and $W_2 = 2\pi f_2$, expressed as angular frequencies associated with the corresponding f_1 and f_2 transition frequencies.

MossWinn fits the following model:

$$W(p(v)) \propto \text{Re} \sum_{m_0, m_1} \frac{1}{4} \left| \langle I_0 m_0 | H | I_1 m_1 \rangle \right|^2 \cdot \sum_{i,j} p_i \cdot \langle j | [A^{-1}(p) + 3Q^2 \eta^2 B(p)]^{-1} | i \rangle$$

Without giving a detailed explanation of the above expression, we simply note that this function is essentially identical with expression (B1) of APPENDIX B in the above-mentioned paper of Blume and Tjon. The model makes it possible to describe relaxation effects in the presence of nonzero electric field gradient and an arbitrary asymmetry parameter η . It contains eight parameters.

AMPLITUDE	Area of the subspectrum
ISOMER SHIFT	⁵⁷ Fe isomer shift
MAGNETIC FIELD [T]	The amplitude h of the relaxing magnetic field.
VZZ (EFG) [10 ²¹ V/m ²]	The component of the EFG in the direction of the magnetic field + h .
ETA (EFG)	Asymmetry parameter of the EFG
JUMP UP RATE	$\log_{10} W_2$
JUMP DOWN RATE	$\log_{10} W_1$
LINE WIDTH	Internal line width (Γ)

The quantities $\log_{10} W_1$ and $\log_{10} W_2$ are called *Jump down rate* and *Jump up rate* in MossWinn, respectively. The total relaxation frequency of the process is given by $f_{\text{total}} = f_1 + f_2$, whereas the corresponding characteristic relaxation time is given by $\tau_r = 2\pi / (W_1 + W_2) = 1 / (f_1 + f_2) = 1 / f_{\text{total}}$.

Note that some relaxation time values given in the literature (see, e.g., Blume 1965 and Wickman 1966) are apparently in accordance with a relaxation time calculated as $\tau = 1 / (W_1 + W_2)$, whereas other works (see, e.g., Stoian *et al.* 2005) quote relaxation time as $\tau_r = 1 / (f_1 + f_2)$.

The *Jump up rate* and *Jump down rate* values are forced to be equal by default. In this case $W_1 = W_2 = W$, and the τ_r relaxation time is given by $\tau_r = 1 / f_{\text{total}} = \pi / W$.

Similarly to other Hamiltonian models, area fitting mode is the default mode when fitting Blume-Tjon magnetic relaxation model, independent of the setting of the AREA/AMPLITUDE mode. Consequently, the Amplitude parameter denotes the area of the corresponding subspectrum.

M. Blume: *Phys. Rev. Lett.* **14** (1965) 96.

H.H. Wickman (1966): Mossbauer Paramagnetic Hyperfine Structure, In: MÖSSBAUER EFFECT METHODOLOGY (ed. I.J. Gruverman), Vol. 2, p. 39. (See Figure 6 on page 55.) The same figure is reprinted in: S. Mørup, J.A. Dumesic, H. Topsøe (1980) Magnetic Microcrystals, In: APPLICATIONS OF MÖSSBAUER SPECTROSCOPY (ed. R.L. Cohen), Vol. 2, p. 1. (See Figure 4 on page 18.)

S.A. Stoian, Y. Yu, J.M. Smith, P.L. Holland, E.L. Bominaar, E. Münck: *Inorganic Chemistry* **44** (2005) 4915.

27.4.7. Tjon-Blume Jahn-Teller quadrupole relaxation model (⁵⁷Fe, powdered sample)

The ⁵⁷Fe Tjon-Blume Jahn-Teller quadrupole relaxation model implemented in the MossWinn program describes the physical model for a powdered sample that contains ⁵⁷Fe nuclei experiencing an electric field gradient whose main component (V_{zz}), although fixed in magnitude, reorients dynamically and randomly between the \mathbf{e}_x , \mathbf{e}_y and \mathbf{e}_z directions of the eigensystem of the EFG tensor. All the three directions are assumed to be equally probable. The asymmetry parameter, η , and the hyperfine magnetic field, H , are both assumed to be equal to zero. The ‘‘Jahn-Teller’’ effect enters the name of the model because the assumptions of the model are expected to get realized in the presence of a dynamic Jahn-Teller effect. The theoretical background and calculation of this model can be found in:

J.A. TJON, M. BLUME: PHYS. REV. **165** (1968) 456.

MossWinn fits the following absorption shape:

$$W(p(\nu)) \propto \text{Re} \sum_{m_0, m_1} \frac{1}{4} \left| \langle I_0 m_0 | H^{(+)} | I_1 m_1 \rangle \right|^2 \cdot \sum_{i,j} p_i \cdot \langle j | A(p) \cdot [1 + 3\alpha^2 B(p) A(p)]^{-1} | i \rangle$$

Without giving a detailed explanation of the above expression, we simply note that this function is essentially identical with equation (15) of the above-mentioned paper of Tjon and Blume. (MossWinn evaluates the above expression by utilizing equation (16) of the same paper.)

The model is described with five parameters.

AMPLITUDE	Area of the subspectrum
ISOMER SHIFT	⁵⁷ Fe isomer shift
VZZ (EFG) [10 ²¹ V/m ²]	The main component of the EFG.
JUMP RATE	$\log_{10} W$, logarithm of the angular relaxation frequency , $W = 2\pi f$, where f is the transition frequency between the different states.
LINE WIDTH	Internal line width (Γ)

Similarly to other Hamiltonian models, AREA fitting mode is the default mode when fitting Tjon-Blume Jahn-Teller relaxation model, independent of the setting of the AREA/AMPLITUDE mode. Consequently, the Amplitude parameter denotes the area of the corresponding subspectrum.

27.4.8. Pure quadrupole splitting (^{151}Eu , powdered sample)

This routine was originally implemented in MossWinn 2.0 . In order to preserve compatibility with earlier versions, it appears in MossWinn 4.0Pre in an unchanged form.

A quadrupole split spectrum of ^{151}Eu in general consists of 12 Lorentzian lines (8 when $\eta = 0$) according to the $7/2 \rightarrow 5/2$ nuclear transition. MossWinn displays only the envelope of the 12 absorption lines on the screen. Zero magnetic field and randomly oriented powdered sample is assumed in the calculations. The model is described with five parameters:

AMPLITUDE	Denotes the whole area of the subspectrum.
ISOMER SHIFT	^{151}Eu isomer shift
Vzz [10^{21} V/m ²]	V_{zz} denotes the element with the highest absolute value in the diagonal form of the EFG (Electric Field Gradient) tensor. The V_{zz} parameter has the unit: 10^{21} [V/m ²].
ETA [0..1]	ETA denotes the asymmetry parameter (η) of the EFG: $ETA = \frac{V_{xx} - V_{yy}}{V_{zz}} \quad (0 \leq ETA \leq 1)$ V_{xx} , V_{yy} and V_{zz} being the diagonal elements of the EFG tensor, defined as usual.
LINE WIDTH	Line width of the absorption lines building up the quadrupole split absorption pattern of ^{151}Eu . Each of the 12 lines has the same line width.

In this routine MossWinn solves the Hamiltonian of the ^{151}Eu nucleus as described in the paper:

J. LINDEN *et al.*: PHYS. REV. B **46** (1992) 8534.

27.5. Absorption line shapes

In MossWinn the following functions can be selected as the line shape of the absorption lines:

<p>Lorentzian (LOR)</p>	<p>For AMPLITUDE calculation mode:</p> $\frac{\Gamma^2}{4} \cdot \frac{Amplitude}{(v-IS)^2 + \frac{\Gamma^2}{4}}$ <p>For AREA calculation mode:</p> $\frac{\Gamma}{2\pi} \cdot \frac{Area}{(v-IS)^2 + \frac{\Gamma^2}{4}}$
<p>Pseudo-Voigt (PVOI)</p>	<p>The Pseudo-Voigt line shape approximates the Voigt line profile, which latter is resulted by the convolution of a Lorentzian line ($l(y)$) with a Gaussian line profile ($g(x-y)$):</p> $V(x) = \int_{-\infty}^{\infty} l(y) \cdot g(x-y) \cdot dy$ <p>This line shape can describe small distributions in the measured sample (e.g. quadrupole splitting distribution). The MossWinn program uses the Pseudo-Voigt Line Shape described in the paper: W. I. F. DAVID: J. APPL. CRYST. 19 (1986) 63-64.</p> <p>When the Pseudo-Voigt line shape is selected for a subspectrum, then the former line width parameters will determine the line width (FWHM) of the Gaussian that takes part in the convolution above. The Lorentzian line width is then added to the parameter list of the subspectrum as an additional parameter.</p> <p>If the subspectrum model contains more than one absorption line, then they all can have different Gaussian line widths, but all of them will share the same Lorentzian line width. The value of this common Lorentzian line width in this case should be close to the line width obtained by fitting a spectrum corresponding to a caliber (e.g. α-iron foil) which was measured using the same radioactive source. The remaining width of the individual lines in the spectrum will be present then in the Gaussian line and will be characteristic of the distribution of Mössbauer nuclides in the measured sample.</p> <p>By setting the Lorentzian Line Width of the Pseudo-Voigt function to zero one obtains a perfect Gaussian line shape that can be used to decompose previously calculated distributions.</p> <p>In AMPLITUDE calculation mode the amplitude type parameters will denote the height of the Pseudo-Voigt peak. In AREA calculation mode the amplitude type parameters will denote the area of the Pseudo-Voigt peak.</p>
<p>Lorentzian with dispersion (LOR-DI)</p>	<p>If there is a considerable interference between the nuclear resonance absorption of γ rays and the atomic photoelectric effect (most pronounced in the case of E1 type nuclear transitions), then a so called "Dispersion term" appears in the Mössbauer absorption line. The resulted line shape can be expressed as follows (see for example F.E. WAGNER, B.D. DUNLAP, G.M. KALVIUS, H. SCHALLER, R. FELSCHER, H. SPIELER: PHYS. REV. LETT. 28 (1972) 530. and D.J. ERICKSON, M.W.J. PRINS, L.D. ROBERTS: PHYS. REV. C 8 (1973) 1916.):</p> <p>For AMPLITUDE calculation mode:</p> $\frac{\Gamma^2}{4} \cdot \frac{Amplitude \cdot \left(1 - 2 \cdot \xi \cdot (v-IS) \cdot \frac{2}{\Gamma}\right)}{(v-IS)^2 + \frac{\Gamma^2}{4}}$ <p>For AREA calculation mode:</p> $\frac{\Gamma}{2\pi} \cdot \frac{Area \cdot \left(1 - 2 \cdot \xi \cdot (v-IS) \cdot \frac{2}{\Gamma}\right)}{(v-IS)^2 + \frac{\Gamma^2}{4}}$ <p>where ξ is called "DISPERSION AMPLITUDE" in MossWinn.</p>

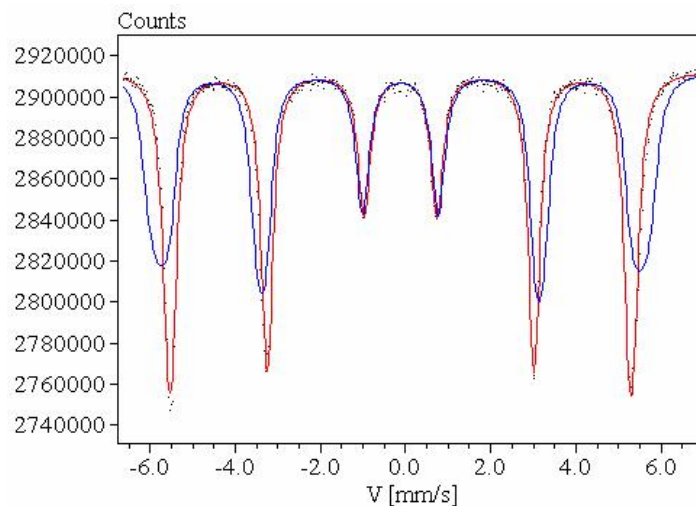
Table continued on the next page.

**Lorentzian with
Cosine smearing
(LOR-CS)**

This line shape is available only in thin absorber approximation mode. The smeared Lorentzian line shape can be used to model *cosine broadening* caused by geometrical effects. MossWinn fits the line shape described by D. CRESPO AND J. PARELLADA IN HYP. INT. **29** (1986) 1539. (Eq. 3). This line shape is exact in the case of a point source moving along the line defined by the center of a circular absorber, placed normally and coaxially to the source velocity, and the point source itself. However, as the authors point out in the above paper, this line shape works well even if the conditions are not exactly those mentioned above.

In the case of this smeared Lorentzian line shape the amplitude, area and percentage values displayed or printed by MossWinn are exactly those which you would get for a Lorentzian line if cosine smearing was not present in the spectrum. That is, apart from possible f factor differences, relative areas in this case reflect the relative occurrence of Mössbauer nuclides in different microenvironments just as in the case of Lorentzian lines when Cosine broadening is not present. At the same time the area values are not equal to the apparent spectral area.

When smeared Lorentzian is selected as line shape in MossWinn, a new parameter — **VISUAL ANGLE [deg]** — will be added to the parameter list of the subspectrum in question. This is the visual angle of the absorber or the detector aperture (which is smaller depending on the actual geometrical conditions) viewed from the point source. Certainly, in real geometrical conditions this value will be only some kind of average mainly because the source always has a finite diameter, which often makes it differ strongly from the ideal picture of a point source. An example of the cosine broadened line shape can be seen below.



⁵⁷Fe Mössbauer spectrum of alpha iron recorded using bad geometrical conditions. The red curve has been calculated using the „Lorentzian with Cosine smearing” line shape (Visual Angle=16°). The blue curve shows the case when Visual Angle=30°.

In **AMPLITUDE** calculation mode the amplitude type parameters will denote the height of the corresponding Lorentzian peak. This may deviate from the actual, apparent height of the peak. In **AREA** calculation mode the amplitude type parameters will denote the area of the corresponding Lorentzian peak. This may deviate from the actual, apparent area of the peak.

27.6. Thin Absorber Approximation and Transmission Integral

To change between thin absorber approximation (**Thin A.**) and transmission integral (**T-INT**) calculation mode, select the parameter list of the background as the formal actual subspectrum. As a result, in the place of the former Line Shape Popup box, the actual calculation mode (Thin A. or T-INT) will be displayed. Press on the box to change the calculation mode.

In thin absorber approximation mode the spectra are calculated by adding (in REFLECTION mode) / subtracting (in TRANSMISSION mode) the absorption lines to / from the background. The transmission integral mode is available only for TRANSMISSION mode. In transmission integral mode, the calculation is done in the following way.

First the absorption lines are calculated as in the case of the thin absorber approximation mode, but without subtraction from the baseline. In the resulted absorption curve, denoted below as $A(v)$, the absorption peaks point upwards. $A(v)$ gets then normalized to have a full area equal to

$$\int_{-\infty}^{+\infty} A(v) \cdot dv = \frac{\pi}{2} \cdot \Gamma_0$$

where Γ_0 equals to the Lorentzian line width (full width at half maximum) of the corresponding nuclear transition (for ^{57}Fe , for example, Γ_0 equals to 0.097 mm/s). The resulted normalized function, $A_n(v)$, is then used to calculate the transmission spectrum, $N(v)$, in the following way.

$$N(v) = N(\infty) \cdot \left((1-b) \cdot \frac{T(v)}{T(\infty)} + b \right)$$

where

$$T(v) = (1 - f_s + f_s \cdot \int L_s(w-v, \Gamma_s) \cdot e^{-\tau \cdot A_n(w)} \cdot dw)$$

where

$$L_s(w-v, \Gamma_s) = \frac{\Gamma_s}{2\pi} \cdot \frac{1}{(w-v)^2 + \frac{\Gamma_s^2}{4}}$$

$N(v)$ = The envelope of the fitting curve

$N(\infty)$ = BASE LINE of the Background parameter list.

b = Background fraction of γ quanta [0..1].

τ = Effective thickness of the absorber (> 0).

Γ_s = Full width at half maximum of the peak emitted by the source.

f_s = Mössbauer-Lamb factor of the source [0..1].

References

G.K. SHENOY, J.M. FRIEDT, H. MALETTA, S.L. RUBY: CURVE FITTING AND THE TRANSMISSION INTEGRAL: WARNINGS AND SUGGESTIONS, IN MÖSSBAUER EFFECT METHODOLOGY, VOLUME 9, (EDITED BY I.J. GRUVERMAN, C.W. SEIDEL, D.K. DIETERLY) PP. 277

S.MARGULIES, J.R.EHRMAN: NUCL. INST. METH. **12** (1961) 131.

S.MARGULIES, P.DEBRUNNER, H.FRAUENFELDER: NUCL. INST. METH. **21** (1963) 217.

A. VERTES, D.L. NAGY (EDS.): MÖSSBAUER SPECTROSCOPY OF FROZEN SOLUTIONS, AKADEMIAI KIADO, BUDAPEST (1990) PP. 34.

27.7. The Parameters page

The **Parameters Page** occupies the left side of the **FIT** menu. It displays the parameters of the fitted model grouped according to different schemes. To select a scheme, LMC the **GROUP BOX** in the left upper corner, and select the required scheme. Available schemes are the followings.

Group by Subspectra	The parameters will be grouped by subspectra. After the parameter groups of the VELOCITY AXIS (present only when calibration is being performed) and the BACKGROUND , the subspectra are listed one after the other. For each subspectra first the amplitude type parameters, then the position type parameters, then the line width type parameters, and at last the extra parameters are displayed. Each subspectrum has its own color that corresponds to the color used to draw the subspectrum on the spectrum graph. In case of simultaneous fitting of spectra the color of the subspectra are determined individually for each spectrum. That is, shared subspectra do not have necessarily the same color in each of the spectra. However, shared subspectra have the same name in all of the spectra where they exist.
Group by Parameter	The parameters will be grouped by their type. First the amplitude type parameters, then the position type parameters, then the line width type parameters, and at last the extra parameters are displayed. In each of the type-groups the parameters belonging to the same subspectrum follow each other.
Group by Name	The parameters will be grouped by their type first, then they will be ordered according to their name. First the amplitude type parameters, then the position type parameters, then the line width type parameters, and at last the extra parameters are displayed. In each of the type-groups the parameters follow each other in alphabetical order.

The box, right beside the Group box, displays the number of the current spectrum and the number of the simultaneously fitted spectra in the following form:

„S” *Serial number of the current spectrum displayed / Number of the spectra fitted simultaneously*

The box right beside displays the number of fitted parameters in the following form:

„P” *Number of fitted parameters*

Further, right beside there are two tabs for the following two tab pages:

Bars	Std
After the parameters bars are displayed that can be used to set the values of parameters. LMC the bar and move the mouse left or right to change the value of the parameter inside the range defined by the relations of the parameter in question, and monitor the changes in the corresponding subspectrum continuously on the Spectrum Page. To increase the maximum of the parameter, draw the corresponding bar beyond its maximum and, without releasing the left mouse button, press the right mouse button until the required maximum is reached. To modify the minimum, draw the bar beyond its minimum towards the left, and modify the minimum by pressing the right mouse button without releasing the left one.	<p><i>During fitting:</i></p> <p>When a parameter changes during fitting, the difference between its new value and old value is displayed after its new value.</p> <p><i>After CAL STD has been clicked:</i></p> <p>After the parameters their standard deviation values are displayed according to the actual state of the fit.</p>

On the left of each parameter a colored rectangle or a colored circle is displayed. **Subspectra with rectangles** are non-shared subspectra that are present only in the actual spectrum. **Subspectra with circles** are shared subspectra that are present in two or more of the simultaneously fitted spectra. Shared subspectra have always the same structure in all of the simultaneously fitted spectra that they exist in. That is, if the interaction of a shared subspectrum is changed in the actual spectrum, then it will also change for all of the corresponding shared subspectra in all other simultaneously fitted spectra. In contrast, the interaction of unshared subspectra can be set independent from any other subspectra. Furthermore, shared subspectra can have shared parameters, while unshared ones cannot.

Click on a rectangle to choose one of the following tools:

Rename Subpectrum: #Subspectrum Name	To rename the selected subspectrum.
Add Subpectrum to all other spectra	The selected subspectrum will be added to all of the simultaneously fitted spectra, and all of them will be shared with the selected one.
Rejoin Subpectrum to existing sharing	The selected subspectrum will be joined to similar shared subspectra in other simultaneously fitted spectra. Use this option for subspectra that were unshared via " <i>Unshare Subpectrum in this spectrum only</i> ".
Delete subspectrum: #Subspectrum Name	To remove the selected subspectrum from the current model.
Join #Spectrum Name . #Subspectrum Name to:	To join the selected subspectrum to one of the similar subspectra (shared or yet unshared) in another simultaneously fitted spectrum.

Click on a circle to choose one of the following tools:

Rename Subpectrum: #Subspectrum Name	To rename the selected subspectrum.
Unshare Subpectrum in all of the spectra	The selected subspectrum, as well as all the subspectra that are shared with it in other spectra, will be disconnected from each other, so that they will be independent, with other word " <i>Unshared</i> ".
Unshare Subpectrum in this spectrum only	The selected subspectrum will get unshared in the current spectrum, so that it can be changed independently of the subspectra it was earlier shared with. (Use „ <i>Rejoin Subpectrum to existing sharing</i> ” to rejoin the selected subspectrum to the shared subspectra it was shared with.)
Delete subspectrum: #Subspectrum Name	To remove the selected subspectrum from the model of one or more simultaneously fitted spectra.
Share #Spectrum Name . #Subspectrum Name with:	To share the selected subspectrum with one of the similar (yet unshared) subspectra in another simultaneously fitted spectrum.

On the bottom of the Parameters Page there are the following boxes available.

DOWN / UP	To scroll the list of parameters on the Parameters Page by one parameter.
PAGE DOWN / PAGE UP	To scroll the list of parameters on the Parameters Page by one subspectrum.
CHI Weighted squared deviation (Chisquare) Simple squared deviation Absolute deviation Do not ignore zero points for current spectrum Ignore zero points for all fitted spectra	To select the fitness function that is minimized during the fitting process. To have the chi-square as fitness function, zero points must be ignored in all of the simultaneously fitted spectra. For the current spectrum zero points will be considered when the fitness function is calculated. For all of the simultaneously fitted spectra the zero valued data points will be ignored when the fitness function is calculated.
LINFIT	LMC to adjust the <i>amplitude type parameters of the current spectrum</i> to their optimal values. RMC to adjust the <i>amplitude type parameters of all the simultaneously fitted spectra</i> to their optimal values.
AREA / AMPLITUDE	To change between Area and Amplitude modes. For linear models these modes influence the meaning of the amplitude type parameters via influencing the calculation of individual absorption lines. For details see page 64.
TRANSMISSION / REFLECTION	To select the method used for the measurement. It determines whether the absorption lines of the calculated model are subtracted (transmission mode) or added (reflection mode) to the Background.
EXIT	LMC to leave the FIT menu and keep all distributions (if any). RMC to leave the FIT menu and does not keep any distributions.

Above these boxes the fitness function value is displayed, which value belongs to the group of the simultaneously fitted spectra as a whole. When the fitness function is the chi-square, then the meaning of the numbers is the following:

CHI: CHISQUARE (NORMALIZED CHISQUARE) [GOODNESS OF FIT]

27.8. Fixing and releasing parameters, the meaning of different parameter colors

To fix the value of a parameter, click on its name with the left mouse button. Its color will change to red. To release it, click with the left mouse button on its name again. Its color will change to darkgray again. The following table explains the meaning of various parameter colors.

Color of Parameter	Meaning
Darkgray	The parameter is free and it is fitted.
Red	The parameter is fixed, and it is not fitted.
Brown	The parameter is cross-referenced, or it is related to another parameter in some way. Click on its name to see how it depends on the other parameter(s).
Blue	The parameter shares a common value with corresponding parameters in other spectra. The common value is fitted. (To add a new spectrum to the current fit — in order to initiate simultaneous fitting of spectra — click on the ADD box and select NEW SPECTRUM TO FIT...)
Magenta	The parameter shares a common value with corresponding parameters in other spectra. The common value is fixed, not fitted.
White	The parameter is subjected to a distribution. This means that the corresponding subspectrum is a distribution in which the parameter in question serves as the distribution parameter. The corresponding distribution curve — whose X axis will display equally spaced values of the parameter in question, and whose Y axis will display the corresponding probabilities — can be made to become displayed on one of the Insight pages.

27.9. Simultaneous fitting of Mössbauer spectra

Simultaneous fitting of Mössbauer spectra provides the advantage that one can fit several Mössbauer spectra at once, with a common set of fitting parameters. Consequently, parameters of models (belonging to different spectra) that are related to each other — for some physical reason — does not need to be fitted independently, but they can be cross referenced to reduce the number of fitting parameters and to obtain a result that is better balanced in the rest of the parameters.

In MossWinn one has the possibility to cross-reference — or in general to relate — any two fitting parameters to each other. This can be done in the following way.

Select the parameter that should be related to another parameter that is, the value of the selected parameter should be influenced by the value of another parameter that is to be selected yet. (A parameter is THE SELECTED parameter, when it is selected in the Parameters List box on the Model Page.) Click on the **CONSTRAIN POPUP** box and select the type of relation (e.g. **:= #PARAMETER**). From the list of parameters, appearing on the left, select the parameter that should be the basis of the relation. If the required parameter is not among those listed, then select **MORE PARAMETERS...** that will bring you to a form where you can select any parameter of any of the subspectra in any of the simultaneously fitted spectra.

The procedure of defining all the necessary cross-references, however, may be time consuming in this way when numerous Mössbauer spectra are fitted simultaneously. Therefore a more powerful concept has also been adopted in MossWinn. This is **the concept of Shared and Unshared subspectra**.

Unshared subspectra are independent from any other subspectrum, and its parameters can be cross-referenced with other parameters only in the way described above.

In contrast, **Shared subspectra** are present in two or more spectra, always having the same structure (interaction, line shape etc.) in all of the spectra that they exist in. Shared subspectra, at the same time, provide a very simple way to cross-reference its parameters to the corresponding parameters of the corresponding subspectrum in all other spectra. The following cross-reference types are available.

Type of cross reference	How to ACTIVATE cross reference
The parameter should have the same value in all of the spectra in which the corresponding shared subspectrum exists. This value should be fitted.	Click on the name of the parameter with the right mouse button. When its color gets blue then the cross reference has been activated, and the corresponding parameter — if the corresponding subspectrum exists — gets blue in all other spectra as well.
The parameter should have the same value in all of the spectra in which the corresponding shared subspectrum exists, and this value should be fixed.	Perform the step above to make the parameter cross referenced, and its color to get blue. Then click on its name with the left mouse button and select: FIX THIS PARAMETER IN ALL OF THE SPECTRA

Type of cross reference	How to DEACTIVATE
The parameter should have the same value in all of the spectra in which the corresponding shared subspectrum exists. This value should be fitted.	Click on the name of the parameter with the right mouse button, and select one of the followings. Select UNSHARE PARAMETER IN THIS SPECTRUM ONLY to decouple the selected parameter from the others which will remain cross referenced. Select UNSHARE THIS PARAMETER IN ALL OF THE SPECTRA to completely eliminate the activated cross reference among the corresponding parameters.
The parameter should have the same value in all of the spectra in which the corresponding shared subspectrum exists, and this value should be fixed.	Click on the parameter with the left mouse button and select UNFIX THIS PARAMETER IN ALL OF THE SPECTRA (The parameters will remain cross referenced, but fixing will be lifted.)

In general, to change or lift a cross reference, click on the name of the cross-referenced parameter with the left or right mouse button, and select the required option.

To add an Unshared subspectrum to the current spectrum only, select ADD → NEW SUBSPECTRUM on the Model Page. To add a Shared subspectrum to all of the simultaneously fitted spectra, select ADD → NEW SHARED SUBSPECTRUM instead.

Shared and Unshared subspectra can be differentiated on the basis of the drawing before their parameters. Before the name of their parameters, UNSHARED subspectra are denoted by rectangles, and SHARED subspectra are denoted by circles. In each of the simultaneously fitted spectra the first subspectra after the background are the Shared subspectra in alphabetical order of their names. The Shared subspectra are then followed by the Unshared ones.

27.10. Fitness functions of the fit

One can choose from three different fitness functions in the **FIT** menu of MossWinn by the help of the CHI menu box (see page 55). During fitting the program searches then for the parameter vector which minimizes the selected fitness function.

CHISQUARE	<p>Mössbauer spectra encountered in practice suffer from nearly normally distributed statistical noise. In this case the maximum likelihood estimator of a fit is the chi-square quantity:</p> $\chi^2(\underline{y}) = \sum_{i=1}^h \frac{(W_i - f_i(\underline{y}))^2}{W_i}$ <p>Where W_i denotes the counts in the ith channel of the Mössbauer spectrum, h is the number of channels, and f_i is the value of the fitting function (e.g. sum of Lorentzians subtracted from the <i>Base Line</i>) corresponding to the ith channel of the spectrum. MossWinn also displays the quantities called NORMALIZED CHISQUARE, and GOODNESS OF FIT.</p> <p style="text-align: center;">Normalized Chisquare = Chisquare / Degree of freedom Degree of freedom = Fitted-channel number – Fitted-parameter number</p> <p>For GOODNESS OF FIT see: W.H.PRESS, B.P. FLANNERY, S.A. TEUKOLSKY, W.T. VETTERLING: <i>NUMERICAL RECIPES, THE ART OF SCIENTIFIC COMPUTING</i> CAMBRIDGE UNIVERSITY PRESS, CAMBRIDGE, NEW YORK (1990)</p>
SQUARED DEVIATION	$\text{Squared deviation}(\underline{y}) = \sum_{i=1}^h (W_i - f_i(\underline{y}))^2$ <p>Where W_i denotes the counts in the ith channel of the Mössbauer spectrum, h is the number of channels and f_i is the value of the fitting function corresponding to the ith channel of the spectrum.</p>
ABSOLUTE DEVIATION	$\text{Absolute deviation}(\underline{y}) = \sum_{i=1}^h W_i - f_i(\underline{y}) $ <p>Where W_i denotes the counts in the ith channel of the Mössbauer spectrum, h is the number of channels and f_i is the value of the fitting function corresponding to the ith channel of the spectrum.</p>

27.11. The Spectrum Page

In the right bottom corner of the FIT menu the **Spectrum Page** can be seen. The SPECTRUM TAB shows the current spectrum with the subspectra corresponding to the actual model. Click on the spectrum graph with the right mouse button to select another simultaneously fitted spectrum (if any). Press TAB / BACKSPACE on the keyboard to make the next / previous spectrum displayed — even during fitting. To make the residual displayed above the spectrum, press R or SHIFT+R on the keyboard. Click on the RESIDUAL TAB to make the spectrum and the residual to be displayed below each other. They are separated with a stripe that can be moved to resize the two windows. Additionally three Insight pages are available on the Spectrum page (Insight A, B, C). To change between the tabs in the Spectrum page during fitting, position the mouse pointer above the Spectrum page, and press space on the keyboard.

At the bottom of the spectrum page the fitness function value for the current spectrum is displayed. When the fitness function is the chi-square, then the meaning of the numbers is the following:

CHI: CHISQUARE (NORMALIZED CHISQUARE) [GOODNESS OF FIT]

Above the fitness function values there is a light-gray stripe that displays information on the current spectrum. Click on this stripe to change the type of the displayed information.

27.12. The Insight Pages

The INSIGHT PAGES (A, B, C, D, E) can be used to display any of the simultaneously fitted spectra, any distribution curves, and the dependence of any parameter of a shared subspectrum on another parameter of a shared subspectrum. All the five insight pages have equivalent functionality.

To set the parameter whose values should serve as the X axis of the graph on the current insight page, click on the popup box after the letters „X:”, and select one of the options. If a spectrum or a distribution is selected, then the content of the other axis will be set automatically. Otherwise, click on the popup box after the letters „Y:”, and select the parameter which should serve as the Y values of the function to be displayed.

A typical application of insight pages is to display the isomer shift of a shared subspectrum as a function of temperature for several simultaneously fitted spectra, which spectra were measured on the same material but at different temperatures.

If a single spectrum is fitted, then the only meaningful functionality of an insight page is to display a distribution curve belonging to one of the distribution subspectra of the fitted model.

27.13. The Functions Page

In the center of the **FIT** menu the FUNCTIONS PAGE can be seen with blue colored menus. The table below lists the functionality of the various boxes on the Functions Page.

GLOBAL	<p>Click on the GLOBAL box to perform an infinite global search for the optimum solution using Evolution Algorithm. During this global search the values of parameters will remain in the range determined by their relation list as displayed in the Relation List box on the Model Page. For simple models one can use global search to automatically set appropriate initial parameter values for the local search (fine tuning) procedure. For complicated models, however, it can be used to perform a long lasting search for a solution better than that already found. If it does not find a better solution, then with high probability there does not exist any better solution.</p> <p>Press the ESC key on the keyboard to finish the global search.</p>
FIT	<p>LMC Click with the left mouse button on the FIT box to initiate a local search (fine tuning) for the best set of fit parameters with high precision, using FITTING METHOD A. When the fit converges, the local search ends automatically. Press the ESC key on the keyboard to finish the local search any time before.</p> <p>RMC Click with the right mouse button on the FIT box to select one of the following options.</p> <p>FIT USING METHOD A – Equivalent to the LMC of the FIT box.</p> <p>FIT USING METHOD B – Method B performs a local search for the best parameter set just as Method A, but it displays interim results more frequently than Method A. Method B, at the same time, converges slower than Method A.</p> <p>LINEAR FIT AMPLITUDES – The optimal value of Amplitude type parameters will be set for the current spectrum.</p> <p>FIT CURRENT SPECTRUM ONLY – Fits only those fit parameters that belong to the current spectrum. (Uses Method A)</p> <p>FIT SPECTRA SEQUENTIALLY – Fits spectra one after the other, sequentially. (Uses Method A) Shared parameters are fitted only for one of the spectra.</p> <p>FIT ONLY AMPLITUDES – Fits only Amplitude type parameters. (Uses Method A)</p> <p>FIT ONLY POSITIONS – Fits only position type parameters. (Uses Method A)</p> <p>FIT ONLY LINE WIDTHS – Fits only Line Width type parameters. (Uses Method A)</p> <p>FIT ONLY EXTRA PARAMETERS – Fits only extra parameters. (Uses Method A)</p>
CAL STD	<p>LMC Click with the left mouse button on the Cal StD box to calculate the standard deviation of fit parameters via the inversion of the curvature matrix (being equal to one-half times the Hessian matrix) after a convergent fit was carried out. If the fit was not convergent, or the fit results are ambiguous, this routine will display a warning message. When weighted squared deviation (Chisquare) is selected as fitness function (see page 55), the program takes the variance of individual counts to be equal to the value of the counts. In other cases a uniform variance of the counts is estimated on the basis of a hypothetical normal distribution of the counts around the fit envelope curve.</p> <p>RMC Click with the right mouse button on the CAL STD box to select one of the following options.</p> <p>Copy correlation matrix to clipboard - Turn to this option in order to copy the correlation matrix of fit parameters into the clipboard. The correlation matrix becomes recalculated each time the StD of parameters is calculated via the inversion of the curvature matrix. As the output format of the correlation matrix the following options are available.</p> <p>As image (for all spectra) - The correlation matrix will be copied into the clipboard as a grayscale bitmap. All the fitted spectra are considered.</p> <p>As image (for current spectrum) - The correlation matrix will be copied into the clipboard as a grayscale bitmap. Only those fit parameters are considered, that belong to the fit model of the current spectrum.</p>

	<p>As image (value limited, for all spectra) - The correlation matrix will be copied into the clipboard as a grayscale bitmap. Only those fit parameters are considered that display correlation values higher than or equal to the value set by the user on the appearing dialog box.</p> <p>As text (for all spectra) - The correlation matrix will be copied into the clipboard as a table given as comma delimited text. All the fitted spectra are considered.</p> <p>As text (for current spectrum) - The correlation matrix will be copied into the clipboard as a table given as comma delimited text. Only those fit parameters are considered, that belong to the fit model of the current spectrum.</p> <p>As text (value limited, for all spectra) - The correlation matrix will be copied into the clipboard as a table given as comma delimited text. Only those fit parameters are considered that display correlation values higher than or equal to the value set by the user on the appearing dialog box.</p> <p>Save correlation matrix - Turn to this option in order to save the correlation matrix of fit parameters as a GIF image file that is optimal for being inspected by the help of web browsers. As the output format of the correlation matrix the following options are available.</p> <p>As GIF image (for all spectra) - The GIF image of the correlation matrix is saved by considering all the fitted spectra.</p> <p>As GIF image (for current spectrum) - The GIF image of the correlation matrix is saved by considering only those fit parameters that belong to the fit model of the current spectrum.</p> <p>As GIF image (value limited, for all spectra) - The GIF image of the correlation matrix is saved by considering only those fit parameters that display correlation values higher than or equal to the value set by the user.</p> <p>CALCULATE STD OF PARAMETERS VIA MATRIX INVERSION – Equivalent to the LMC of the CAL STD box.</p> <p>APPROXIMATE STD VIA MONTE CARLO ITERATIONS – Standard deviation values will be estimated using Monte Carlo iterations. This procedure can be time consuming, but it provides one with the well balanced standard deviation values of any of the fitting parameters. The number of iterations to be taken can be selected in the appearing popup. To finish calculations, press ESC on the keyboard. This method calculates the reliability of distributions as well.</p> <p>APPROXIMATE RELIABILITY OF DISTRIBUTIONS – Assuming all the fitting parameters to be fixed to their actual value, this method calculates the reliability of distributions (if any) using a Monte Carlo procedure. It generates model spectra from the envelope of the current fit by simulating normal statistical noise, and adding it to the envelope. Then for the resulted model spectrum the distributions will be calculated. On any of the insight pages displaying a distribution one red and one blue curve will appear beside the black one. At any points of the distribution the red curve denotes the maximum probability value encountered by fitting the model spectra, while the blue curve denotes the minimum probability value encountered. The blue curve is the more informative one. In the points where the blue curve displays zero probability, there could as well be zero probability in the original distribution curve if the measurement would be repeated. So that in all that points either the non-zero value of the distribution curve, or the position of the corresponding peak can not be taken seriously. In this way you can avoid to interpret small peaks in the distribution curve, which peaks are only a consequence of the normal noise present in any measured Mössbauer spectrum. Note, that this method does not take into account the uncertainty in the fit parameters, as they are kept fixed during the calculations. On the other side, this method provides a valuable result in a short time. To calculate the blue and red curves more precisely, the APPROXIMATE STD VIA MONTE CARLO ITERATIONS method can be used.</p> <p>RESET DISTRIBUTION GRAPHS – Select this option to remove the red and blue curves from the distributions.</p>
ACCEPT	<p>Click on the ACCEPT box with the left mouse button in order to save the actual state of the fit of the spectra to the spectrum files. Accepting of the fit is important, as MossWinn will try to extract the fit results from the spectrum files in various situations. Such a situation can be for example the creation of a table of the fit results in the TBL menu , or the refitting of the spectrum later on. When the fit is accepted, fits that were accepted earlier for the same spectrum, will be overwritten.</p>

PRINT	<p>Press on the PRINT menu box with the left mouse button in order to carry out the default print operation assigned to the PRINT menu box in the corresponding submenu of the SET menu box. Press on the PRINT menu box with the right mouse button in order to access one of the following options.</p> <p>Print fit results as text - Select this option in order to print the textual fit report associated with one or more of the fitted spectra to the default printer. If a parameter (submenu item) is selected, then the individual fit reports will follow each other in order according to the value of the selected parameter.</p> <p>Print current spectrum - Select this option in order to print the graph of the current spectrum to the printer set as default in the SET menu.</p> <p>Print current spectrum + distributions - Select this option in order to print the graph of the current spectrum and those of the fitted distributions (if any) to the printer set as default in the SET menu. The graphs are all printed on the same page.</p> <p>Print fit results + spectrum + distributions - Select this option in order to print to the default printer the textual fit report(s), and then on separate page (pages) the graph (graphs) of the spectrum (spectra) and fitted distributions (if any). If a parameter (submenu item) is selected, then the individual fit reports will follow each other in order according to the value of the selected parameter.</p> <p>Print all spectra - Select this option in order to print to the default printer the graph of all the simultaneously fitted spectra, on a single page. If a parameter (submenu item) is selected, then the spectrum graphs will be arranged according to the value of the selected parameter.</p> <p>Copy to clipboard as text - Select this option in order to copy the textual fit report associated with the current spectrum to the clipboard of Windows.</p> <p>Copy all to clipboard as text - Select this option in order to copy the textual fit report of all the simultaneously fitted spectra to the clipboard of Windows. If a parameter (submenu item) is selected, then the individual fit reports will follow each other in order according to the value of the selected parameter.</p> <p>Copy to clipboard as table for graphics - Select this option in order to copy the fit results to the clipboard as comma-delimited text forming a table in which the parameters characterizing a particular spectrum are all listed in a single row, whereas each parameter - as well as each StD value - has its own column. This arrangement is especially useful for drawing the value of some parameter (e.g. isomer shift) as a function of another one (e.g. temperature) by the help of an external grapher program. If a parameter (submenu item) is selected, then the created table will be in order according to the value of the selected parameter.</p> <p>Copy to clipboard as table for presentation - Select this option in order to copy the fit results to the clipboard as comma-delimited text forming a table in which the parameters characterizing a particular spectrum are all listed in a single column, whereas each parameter has its own row. This arrangement is considered to be useful when creating tables for a presentation. If a parameter (submenu item) is selected, then the created table will be in order according to the value of the selected parameter.</p> <p>Copy current spectrum to clipboard - Select this option in order to copy the graph of the current spectrum to the clipboard of Windows according to the default settings attributed to Clipboard - single spectrum on the Printer Setup Dialog.</p> <p>Copy current spectrum + distributions to clipboard - Select this option in order to copy the graph of the current spectrum and those of the fitted distributions (if any) to the clipboard of Windows.</p> <p>Copy all Insight Pages to clipboard - Select this option in order to copy the graphical content of non-empty insight pages (if any) to the clipboard of Windows.</p> <p>Copy all spectra to clipboard - Select this option in order to copy the graph of all the simultaneously fitted spectra to the clipboard of Windows. If a parameter (submenu item) is selected, then the spectrum graphs will be arranged according to the value of the selected parameter.</p> <p>Save as simple text - Select this option in order to save the fit report of the current spectrum as text file.</p> <p>Save all as simple text - Select this option in order to save the fit report of all the simultaneously fitted spectra in the same text file one after the other. If a parameter (submenu item) is selected, then the individual fit reports will follow each other in order according to the value of the selected parameter.</p> <p>Save as table for graphics - Select this option in order to save the fit results as comma-delimited text into a text file forming a table in which the parameters characterizing a particular spectrum are all listed in a single row, whereas each parameter - as well as each standard deviation value - has its own column. This arrangement is especially useful for drawing the value of some parameter (e.g. isomer shift) as a function of another one (e.g. temperature) by the help of an external grapher program. If a parameter (submenu item) is selected, then the created table will be in order according to the value of the selected parameter.</p> <p>Save as table for presentation - Select this option in order to save the fit results as comma-delimited text into a text file forming a table in which the parameters characterizing a particular spectrum are all listed in a single column, whereas each parameter has its own row. This arrangement is considered to be useful when creating tables for a presentation. If a parameter (submenu item) is selected, then the created table will be in order according to the value of the selected parameter.</p>
--------------	--

SET	<p>Click with the left mouse button on the Set box to select one of the following options.</p> <p>SPECTRUM PARAMETERS - Select this option in order to set/modify spectrum parameters associated with the current spectrum.</p> <p>ISOMER SHIFT REFERENCE - Select this option in order to set/modify the isomer shift of the isomer shift reference material (associated with the current source nuclide) relative to the corresponding standard IS reference material. The value given here is considered when the fitness of MIDB records is evaluated (with respect to the current spectrum) for example when the FIND AND APPLY BEST MATCH submenu option of the DB menu is selected.</p> <p>LINE WIDTHS...</p> <p>CONSTRAIN ALL TO BE THE SAME - All Lorentzian line width parameters in the model of the current spectrum will be cross-referenced to be always the same.</p> <p>SET ALL TO BE INDEPENDENT - Cross references that relate line width type parameters to each other will be removed.</p> <p>PARAMETER BOUNDARIES...</p> <p>SHARE FOR THE SELECTED PARAMETER - Parameter boundaries set for the actually selected parameter will be transferred to the corresponding parameter (if it exists) in all other spectra that are fitted simultaneously.</p> <p>SHARE FOR POSITION AND WIDTH PARAMETERS - Parameter boundaries set for position and width type parameters <i>in the actually selected subspectrum</i> will be transferred to the corresponding parameters (if they exist) in all other spectra that are fitted simultaneously.</p> <p>SHARE FOR ALL POSITION AND WIDTH PARAMETERS - Parameter boundaries set for position and width type parameters <i>in the model of the actually selected spectrum</i> will be transferred to the corresponding parameters (if they exist) in all other spectra that are fitted simultaneously.</p> <p>STRETCH TO MAKE CURRENT PARAMETER VALUES VALID - Parameter boundaries, that do not contain the actual value of the corresponding parameter, will be extended so that all actual parameter values will be valid.</p> <p>TRY PARAMETERS OF CURRENT SOLUTION FOR ALL OTHER SPECTRA - Parameter values of shared subspectra in the current spectrum will be tried for another spectra. If a better fit is obtained, the corresponding parameter values will be transferred from the current spectrum to the other simultaneously fitted spectra.</p> <p>IF LORENTZIAN WITH DISPERSION IS SELECTED AS LINE SHAPE...</p> <p>SET IT ONLY FOR THE SELECTED SUBSPECTRUM - When the user selects "Lorentzian with dispersion" as the line shape for a subspectrum, then only the subspectrum in question will be altered.</p> <p>SET IT FOR ALL THE SUBSPECTRA - When the user selects "Lorentzian with dispersion" as the line shape for a subspectrum, then this line shape will be set for all the existing subspectra (recommended option).</p> <p>DISABLE SUBSPECTRUM CALCULATION FOR TRANSMISSION INTEGRAL - In Transmission Integral mode formal subspectra are calculated. Select this option to disable the calculation of these formal subspectra, and speed up the calculation process.</p> <p>DETERMINE PARAMETER VALUES WITH A RELATIVE PRECISION OF - In the appearing popup select the relative precision required for the fitted parameters. When during a fit the relative change in the fit parameters is less than this set value, then the fit terminates.</p> <p>ENABLE NEGATIVE AMPLITUDE/AREA VALUES - Set this option to enable the setting of negative area and amplitude values.</p> <p>ENABLE NEGATIVE LINE WIDTH VALUES - Set this option to enable the setting of negative line width values.</p> <p>REMOVE CALIBRATION OF THE CURRENT SPECTRUM - Set this option to discard the calibration of the current spectrum. After that the X axis of the spectrum will display channel numbers rather than velocity values.</p> <p>LEFT MOUSE CLICK ON THE PRINT BOX SHOULD... - Several options are available for the default function of the PRINT box for the case when it is clicked with the left mouse button.</p>
------------	--

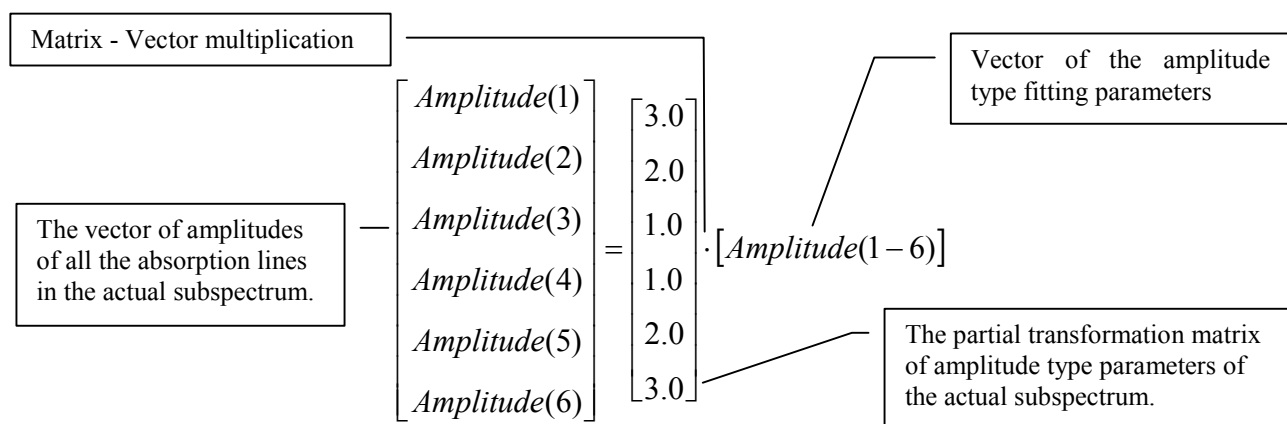
27.14. The Details Page

Click on the **DETAILS** box on the MODEL PAGE to invoke the **DETAILS** page. This page can be used to fine tune linear models. Models based on Hamiltonian calculations can not be modified in this way.

In the top of the **DETAILS** page there is a Subspectrum popup in which the actual subspectrum can be selected. Below this popup there are three list boxes. The first one is a **PARAMETERS** list box in which the parameters of the actual subspectrum are displayed, and the actual parameter can be selected. Right beside there is the **AFFECTED LINES** list box which lists all the absorption lines belonging to the actual subspectrum. The absorption lines that are influenced by the actual parameter are selected blue; those not influenced by the actual parameter are not selected. Further on the right there is the **MATRIX** list box that displays the matrix elements belonging to the partial transformation matrix of the actual parameter in the actual subspectrum. To each of the parameter types (Amplitude type, Position Type, Line Width type) there is an independent partial transformation matrix maintained. Whenever a zero value occurs among the matrix elements, the corresponding line will be deselected, as it is not influenced by the actual parameter.

In the actual subspectrum, the amplitudes of all the constituent absorption lines are calculated on the basis of the amplitude type parameters in the **PARAMETERS** list box. How this is done is explained in the followings.

To each of the amplitude type parameters belongs exactly one column in the partial transformation matrix of the Amplitude type parameters in the actual subspectrum. The elements of this column can be seen in the **MATRIX** list box when the parameter is selected in the **PARAMETERS** list box. For the case of a sextet described by one amplitude type parameter for example, the partial transformation matrix has only one column, and the amplitudes of the absorption lines are calculated in the following way.



For the case of a sextet described by two amplitude type parameters (for single crystal) the multiplication looks like this:

$$\begin{bmatrix} \textit{Amplitude}(1) \\ \textit{Amplitude}(2) \\ \textit{Amplitude}(3) \\ \textit{Amplitude}(4) \\ \textit{Amplitude}(5) \\ \textit{Amplitude}(6) \end{bmatrix} = \begin{bmatrix} 3.0 & 0.0 \\ 0.0 & 1.0 \\ 1.0 & 0.0 \\ 1.0 & 0.0 \\ 0.0 & 1.0 \\ 3.0 & 0.0 \end{bmatrix} \cdot \begin{bmatrix} \textit{Amplitude}(1,3,4,6) \\ \textit{Amplitude}(2,5) \end{bmatrix} = \begin{bmatrix} 3.0 \cdot \textit{Amplitude}(1,3,4,6) \\ 1.0 \cdot \textit{Amplitude}(2,5) \\ 1.0 \cdot \textit{Amplitude}(1,3,4,6) \\ 1.0 \cdot \textit{Amplitude}(1,3,4,6) \\ 1.0 \cdot \textit{Amplitude}(2,5) \\ 3.0 \cdot \textit{Amplitude}(1,3,4,6) \end{bmatrix}$$

In this latter case the ratio of the lines (1,6) and (3,4) is fixed to 3:1, and the amplitude of the lines (2,5) is independent from the amplitude of the lines (1,3,4,6).

The same works for position and line width type parameters as follows. For a sextet described with three different line width type parameters the partial transformation matrix and the corresponding multiplication looks like this:

Matrix - Vector multiplication

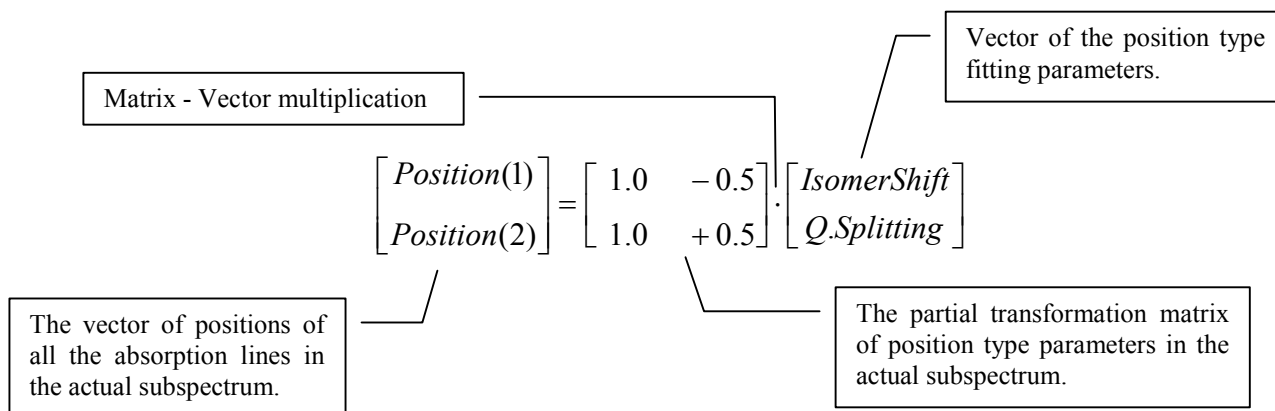
$$\begin{bmatrix} \textit{LineWidth}(1) \\ \textit{LineWidth}(2) \\ \textit{LineWidth}(3) \\ \textit{LineWidth}(4) \\ \textit{LineWidth}(5) \\ \textit{LineWidth}(6) \end{bmatrix} = \begin{bmatrix} 1.0 & 0.0 & 0.0 \\ 0.0 & 1.0 & 0.0 \\ 0.0 & 0.0 & 1.0 \\ 0.0 & 0.0 & 1.0 \\ 0.0 & 1.0 & 0.0 \\ 1.0 & 0.0 & 0.0 \end{bmatrix} \cdot \begin{bmatrix} \textit{LineWidth}(1,6) \\ \textit{LineWidth}(2,5) \\ \textit{LineWidth}(3,4) \end{bmatrix}$$

Vector of the line width type fitting parameters.

The vector of line widths of all the absorption lines in the actual subspectrum.

The partial transformation matrix of line width type parameters of the actual subspectrum.

The position of the lines in a quadrupole doublet is calculated from the position type parameters and the partial transformation matrix of position type parameters in the following way.



Readers familiar with the Transformation Matrix system of MossWinn version 2.0i may have already recognized that the system of partial transformation matrices works exactly like that of the Transformation matrix, but unlike Transformation matrices that describe a whole fit model with all of its subspectra, the sphere of operation of a partial transformation matrix is a certain type (amplitude, position or width) of parameters in a single subspectrum.

The elements of the partial transformation matrix can be changed in the **MATRIX** list box. To connect the amplitude of a certain absorption line to a certain amplitude type parameter, do the followings. Select the parameter in question in the **PARAMETERS** list box. The absorption line whose amplitude should be determined by the selected parameter is not selected yet in the **AFFECTED LINES** list box. To make the connection, click on the name of the absorption line in question with the left mouse button in the **AFFECTED LINES** box. As a result it will get selected blue, and at the same time it will be disconnected from the parameter that determined its amplitude earlier. The amplitude of the selected absorption line is now determined by the actual amplitude type parameter. The very same procedure works for line width type parameters. MossWinn will change the name of parameters, and remove or add parameters automatically when it is required during these procedures.

To make an absorption line disconnected from a certain amplitude type / line width type parameter, click on its selected name in the **AFFECTED LINES** box. As a result a new amplitude type / line width type parameter will be added to the parameter list, which parameter will determine the amplitude / line width of the absorption line disconnected from the other parameter.

On the bottom of the **DETAILS PAGE** there are three boxes with the following options.

HIDE	To hide the DETAILS PAGE . It can be invoked again by a LMC on the DETAILS box on the MODEL PAGE .
TOOLS	Further necessary tools to fine-tune linear models.
ADD POSITION TYPE PARAMETER	To add a new position type parameter to the actual subspectrum. For example, to create the subspectrum of a doublet from the subspectrum of a singlet, one could add one absorption line to the subspectrum first, then add a new position type parameter (Q. Splitting) to the resulted subspectrum. After that the matrix elements belonging to the new position type parameter should be set to their correct values (-0.5 and +0.5 for the first and second lines, respectively).
REMOVE POSITION TYPE PARAMETER	To remove a position type parameter from the actual subspectrum.
ADD ABSORPTION LINE	To add a new absorption line to the actual subspectrum.
REMOVE ABSORPTION LINE	To remove an absorption line from the actual subspectrum.
SHOW MATRIX ELEMENTS	These three options determine the content of the DETAILS PAGE . To show the AFFECTED LINES and MATRIX list boxes.
SHOW ENABLED INTERVALS	To show the enabled intervals for the actual parameter. Here one can check how MossWinn compiled the relations defined for the actual parameter in the RELATIONS list box on the MODEL PAGE .
SHOW INTERNAL VALUES	To show the values of internal variables belonging to the actual subspectrum. It is intended to help the author to monitor the working of the program. Some notations are listed here, while others are not documented. N - the number of the actual parameter in the actual subspectrum. AN - The number of amplitude type parameters in the actual subspectrum. PN - The number of position type parameters in the actual subspectrum. WN - The number of width type parameters in the actual subspectrum. EN - The number of extra parameters in the actual subspectrum. DP - The serial number of the parameter that serves as the basis of a distribution. P_LLW - The serial number of the extra parameter that determines the Lorentzian line width for PSEUDO-VOIGT line shapes. P_VANGLE - The serial number of the extra parameter that determines the Visual Angle for LORENTZIAN WITH COSINE SMEARING line shapes. CODE - Each subspectrum should have a different code number. SHARED CODE - Subspectra with the same — nonzero — shared code are shared subspectra that are connected to each other.

27.15. Fitting of hyperfine field distributions

MossWinn is able to fit distributions of any position type parameter, of any subspectrum. Subspectra of distributions and subspectra of crystalline sites can be combined arbitrarily. The maximum number of distribution subspectra in one spectrum is 5. The maximum number of distribution data points altogether for five distributions is 180.

To fit a magnetic field distribution, for example, add a new subspectrum to the actual model. Then select the corresponding interaction — e.g. MAGNETIC (POWDER) in this case — in the **INTERACTIONS** popup box on the **MODEL PAGE**. Select the parameter named MAGNETIC FIELD [T] in the **PARAMETERS LIST** box on the **MODEL PAGE**. Then click on the popup box with the text **CONSTRAIN**, and select **DISTRIBUTION / POSITIVE, ZERO LEFT & RIGHT BOUNDARIES (PZLRB)**. As a result, a magnetic field distribution becomes activated with an isomer shift independent from the magnetic field.

To activate correlations, select any of the position type parameters — in our case the **ISOMER SHIFT** parameter — in the **PARAMETERS LIST** box on the **MODEL PAGE**. Click again on the **CONSTRAIN** popup box, and go to the item **:= #PARAMETER * CONST1 + CONST2**, and select the parameter **MAGNETIC (1) . MAGNETIC FIELD [T]** from the appearing list of parameters. As a result, the **ISOMER SHIFT** parameter will depend linearly on the **MAGNETIC FIELD [T]** parameter, so that a distribution with linear correlation has been activated. The linear correlation coefficients are now added to the parameter list of the distribution subspectrum.

To see the distribution curve itself, go to one of the Insight pages, e.g. **INSIGHT D**, and select the activated distribution by clicking on the popup box after the **Y:** letters. The actual state of the distribution curve will be displayed on the **INSIGHT PAGE D**. The displayed distribution curve will change continuously when the corresponding parameter values are changed.

The value of the distribution parameter — in our case **MAGNETIC FIELD [T]** — will be always equal to the weighted average of the corresponding distribution curve. For the parameters correlated with the distribution parameter a value will be displayed that is based on this weighted average of the distribution parameter.

When a model contains one or more distributions, and some of the subspectra are constrained by a percentage parameter, but there is at least one distribution that is not constrained by a percentage parameter, then MossWinn will add the parameter **TOTAL AREA MULTIPLIER** to the parameter list of the Background. The value of this parameter is used to derive the correct value of the total area under the spectrum from the total area estimated on the basis of the spectrum data points. This parameter can be fitted, but in normal situations its value should remain higher and close to 1.0. MossWinn estimates the total spectrum area in the following way in this case:

$$\text{Total Spectrum Area} = \text{Total Area Multiplier} * (\text{Spectrum area estimated on the basis of the measured data points})$$

MossWinn calculates the distributions on the basis of a slightly modified version of the method of Hesse and Rübartsch^{*}. This modification makes it possible to fit the **SMOOTHING FACTOR** when a strictly positive valued distribution is fitted. In the case of **UNRESTRICTED** distributions, which are derived exactly via the original method of Hesse and Rübartsch, the **SMOOTHING FACTOR** can not be fitted.

^{*}J. HESSE, A. RÜBARTSCH: J. PHYS. E :SCI. INSTR. 7 (1974) 526.

27.16. How to complement MossWinn with user programmed functions

One can add any function on the subspectrum level to the list of theories built into MossWinn by default. Thus, MossWinn's capabilities are not restricted to the built in theories, linear and Hamiltonian models, but it can fit any fitting function programmed and compiled by the user.

27.16.1. How to compile a user written model function

To complement MossWinn with a custom model function, the source code of the function has to be written, and compiled to a library, by the user. It is recommended to use Borland/Inprise/CodeGear Delphi 2.0 or later 32 bit compilers to compile the written source code.

If the source code is written as outlined in this chapter, then the compiler will compile it as a Dynamic Link Library (DLL). This DLL should have a name corresponding to the mask **SUB*.DLL**. When the compilation was successful, place the corresponding DLL library file in the folder `..\MOSSWINN 4.0\DLLs\`. In order to access the functions of the new library, restart MossWinn or turn to the menu option **SET** → **Enable/disable libraries**.

One can fit a spectrum according to a model function included in a DLL by selecting the corresponding DLL function under the **EXTERNAL LIBRARIES** menu option of the **INTERACTIONS** popup box, on the **MODEL** page of the **FIT** menu. MossWinn identifies DLL code libraries on the basis of their file name. Consequently, if the code of a DLL with a given name is changed, models that contained a subspectrum taken from the old DLL will be changed as well.

Below an example is given for a library source code that can be compiled for example with Delphi 2007. The bold characters are in the file — named `SUB_DLL1.PAS` — itself, comments with non-bold characters are there only to explain the functionality of the procedures, they should not be included in the source file. The name of the procedures can start with **DLL1** (as below) or, alternatively, with **DLL2**, **DLL3** or simply **DLL**. It is important to use the variable type **ShortString** instead of string throughout the library.

```
library SUB_DLL1;
uses SysUtils,Classes;
{$R *.res}

procedure DLL1_SET_INTERACTION_NAME(var s:ShortString;source:ShortString);export;
begin
  s:='Custom DLL';
end;
```

The headline of the library.

This is the first procedure in the library. Its job is to define the short name of the physical interaction, and to put it into the variable `s`. The name of the interaction can depend on the value of the `source` string variable, which contains the source string actually selected in MossWinn. It can have one of the following values:

```
57FE 119SN 151EU 125TE 121SB 129I 197AU 161DY 141PR 237NP M1/E1 M1+E2 E2
```

This procedure has the job to define a longer description for the interaction. It takes the `source` string as parameter, and returns the longer name of the interaction in the string `s`.

```
procedure DLL1_SET_DESCRIPTION(var s:ShortString;source:ShortString);export;
var
  s2:ShortString;
begin
  DLL1_SET_INTERACTION_NAME(s2,source);
  s:='DLL(1) - 1 SINGLET'+(''+s2+'');
end;
```

This procedure has the job to set the following internal values of the subspectrum:

AN = Number of the amplitude type parameters.
PN = Number of the position type parameters.
WN = Number of the line width type parameters.
NAME = A descriptive name of the subspectrum.

Again, this procedure takes the **source** parameter, and the action taken may depend on it. Also a **p** pointer is passed to this routine, but this pointer should not be referenced, as in the present version its value is set to **NIL**.

```
procedure DLL1_SET_SUBSPECTRUM_INTERNAL_VALUES (var AN,PN,WN:byte;var Name:ShortString;
Source:ShortString;p:pointer);export;
begin
  AN:=1;
  PN:=1;
  WN:=1;
  Name:='DLL Singlet (1)';
end;
```

This procedure has the job to initialize parameters of the subspectrum. Its action again may depend on the value of the **source** passed to it. The **p** pointer should not be referenced; its value is **NIL**. The procedure takes the following input parameters:

n = The serial number of the parameter that should be initialized.
Cmin = The absolute minimum of the spectrum.
Cmax = The absolute maximum of the spectrum.
Vmin = The minimum of the velocity axis.
Vmax = The maximum of the velocity axis.

The procedure has to set the value of four variables:

Name = The name of the parameter.
Minimum_Value = A value which the parameter should exceed.
Maximum_Value = A value which the parameter should not exceed.
Initial_Value = A valid value for the parameter.

```
procedure DLL1_SET_PARAMETERS_INTERNAL_VALUES (n:longint;Cmin,Cmax,Vmin,Vmax:double;
var Name:ShortString;
var Minimum_Value,Maximum_Value,
Initial_Value:double;
Source:ShortString; p:pointer);export;
begin
  Case n of
    1:begin
      Name:='Amplitude';
      Minimum_Value:=0.0;
      Maximum_Value:=abs(Cmax-Cmin)+2.0*sqrt(abs(Cmax));
      Initial_Value:=abs(Cmax-Cmin);
    end;
    2:begin
      Name:='Isomer Shift';
      Minimum_Value:=Vmin;
      Maximum_Value:=Vmax;
      Initial_Value:=(Vmin+Vmax)/2.0;
    end;
    3:begin
      Name:='Line Width';
      Minimum_Value:=0.2;
      Maximum_Value:=0.6;
      Initial_Value:=0.2;
    end;
  end;
end;
```

This procedure has the job to calculate the subspectrum. Its action again may depend on the value of the **source** string passed to it. The **p** pointer should not be referenced; its value is **NIL**.

The procedure takes the following input parameters:

AreaMode = TRUE if the actual mode in MossWinn is the AREA mode. FALSE if the actual mode in MossWinn is the AMPLITUDE mode. The calculations may — and should — depend on the value of this Boolean variable.

n = The number of channels in the spectrum. The subspectrum has to be calculated for all the **n** channels.

pPARAMETERS = Pointer that points to the start address of a vector of floating point numbers of the type **DOUBLE**. Reference it as in the example below. It contains the values of the subspectrum parameters one after the other.

pDATA = Pointer that points to the start address of a vector of exactly **n** floating point numbers of the type **DOUBLE**. This is the data array, where the results of the calculations should be — not placed but — added. The subspectrum should be calculated and added with the absorption peaks pointing ‘upwards’, that is in positive direction. Do not change the content of this vector in any other way, because it may already contain the contribution of other subspectra.

pVELOCITY = Pointer that points to the start address of a vector of exactly **n** floating point numbers of the type **DOUBLE**. This is the data array that lists the velocity value for each channel one after the other.

```
procedure DLL1_SET_SUBSPECTRUM(n:longint;
                               pPARAMETERS,pDATA,pVELOCITY:pointer;
                               AreaMode:boolean;Source:ShortString;p:pointer);export;
```

Type

```
TARRAY = ARRAY[1..8191] of DOUBLE;
var
  PARAMETERS,DATA,VELOCITY:^TARRAY;
  i:longint;
  x,y,v,A,ISH,LW:double;
begin
  PARAMETERS:=pPARAMETERS;DATA:=pDATA;VELOCITY:=pVELOCITY;

  A:=PARAMETERS^[1];if A<0.0 then A:=0.0;

  ISH:=PARAMETERS^[2];

  LW:=PARAMETERS^[3];if LW<=0.0 then LW:=0.001;

  y:=LW*LW/4.0;

  if AreaMode then
    begin
      for i:=1 to n do
        begin
          v:=Velocity^[i];
          x:=(v-ISH)*(v-ISH)+y;
          DATA^[i]:=DATA^[i]+(LW/(Pi+Pi))*A/x;
        end;
      end
    else
      begin
        for i:=1 to n do
          begin
            v:=Velocity^[i];
            x:=(v-ISH)*(v-ISH)+y;
            DATA^[i]:=DATA^[i]+y*A/x;
          end;
        end;
      end;
end;
```

This procedure has the job to calculate the area of the subspectrum solely on the basis of the subspectrum parameters. Its action again may depend on the value of the **source** string passed to it. The **p** pointer should not be referenced; its value is **NIL**. The procedure takes the following input parameters:

AreaMode = TRUE if the actual mode in MossWinn is the AREA mode. FALSE if the actual mode in MossWinn is the AMPLITUDE mode. The calculations may — and should — depend on the value of this boolean variable.

pPARAMETERS = Pointer that points to the start address of a vector of floating point numbers of the type **DOUBLE**. Reference it as in the example below. It contains the values of the subspectrum parameters one after the other.

The procedure should set the value of the following variables:

AREA = This should be set equal to the subspectrum area that was calculated.

CanDO = Set it to TRUE if you can do the calculation of the subspectrum area on the basis of the subspectrum parameters. Set it to FALSE, and proceed like in the alternative solution below, if you can not calculate the area of the subspectrum. The latter solution is much simpler, but results in a slower execution, because in this case MossWinn will calculate the subspectrum area by numerical integration.

```
procedure DLL1_SET_AREA_OF_SUBSPECTRUM( var AREA:double;
                                         var CanDO:boolean;
                                         pPARAMETERS:pointer;
                                         AreaMode:boolean;Source:ShortString;
                                         p:pointer) ;export;
```

Type

```
TARRAY = ARRAY[1..8191] of DOUBLE;
```

var

```
PARAMETERS:^TARRAY;
```

```
A,LW:double;
```

begin

```
PARAMETERS:=pPARAMETERS;
```

```
CanDO:=True;
```

```
A:=PARAMETERS^[1];if A<0.0 then A:=0.0;
```

```
LW:=PARAMETERS^[3];if LW<=0.0 then LW:=0.001;
```

```
if AreaMode then AREA:=A else AREA:=A*LW*Pi/2.0
```

end;

{An alternative solution:

```
procedure DLL1_SET_AREA_OF_SUBSPECTRUM( var AREA:double;
                                         var CanDO:boolean;
                                         pPARAMETERS:pointer;
                                         AreaMode:boolean;Source:ShortString;
                                         p:pointer) ;export;
```

begin

```
CanDo:=False;
```

end;

}

The library should end like this.

exports

```
DLL1_SET_INTERACTION_NAME,
DLL1_SET_DESCRIPTION,
DLL1_SET_SUBSPECTRUM_INTERNAL_VALUES,
DLL1_SET_PARAMETERS_INTERNAL_VALUES,
DLL1_SET_SUBSPECTRUM,
DLL1_SET_AREA_OF_SUBSPECTRUM;
```

begin

end.

27.16.2. How to complement MossWinn with an arbitrary cross-reference function

There is a possibility to complement the four cross-reference options available in MossWinn with an arbitrary function programmed by the user. With the help of this option arbitrary functional dependence can be defined between parameters. That is, one parameter can be made to depend on one or more parameters via an arbitrary function. To define this custom functional dependence, the source file DEP_DLL1.PAS has to be modified and compiled by using a Borland/Inprise/CodeGear Delphi 2.0 or later 32 bit compiler. The resulted new file (named DEP_DLL1.DLL) should replace then the old DEP_DLL1.DLL. The default content of DEP_DLL1.PAS is listed below with notes explaining the job of the procedures. The source code below can be compiled, e.g., with Delphi 2007.

```
library DEP_DLL1;
```

```
uses SysUtils, Classes;
```

```
{$R *.res}
```

This procedure has the job to define a short name for the function.

```
Procedure DEPDLL1_SET_SHORT_NAME(var s:ShortString);export;
begin
  s:='Cubic';
end;
```

This procedure has the job to define a longer name for the function.

```
Procedure DEPDLL1_SET_LONG_NAME(var s:ShortString);export;
begin
  s:=':= User Programmed Function [ Cubic ]';
end;
```

This procedure has the job to define the number of extra parameters that are necessary to add to the list of parameters to make the function work.

```
Procedure DEPDLL1_SET_NUMBER_OF_EXTRA_PARAMETERS(var n:longint);export;
begin
  n:=4;
end;
```

This procedure has the job to define a short name for each of the extra parameters. The serial number of the extra parameter whose name should be put into the string **s** is given by the variable **n**.

```
Procedure DEPDLL1_SET_PARAMETER_NAME(var s:ShortString;n:longint);export;
begin
  Case n of
    1:s:='Constant';
    2:s:='Linear';
    3:s:='Quadratic';
    4:s:='Cubic';
  end;
end;
```

This procedure has the job to initialize each of the extra parameters, and to define their minimum and maximum values. The serial number of the extra parameter that should be initialized is given by the variable **n**.

```

Procedure DEPDLL1_INITIALIZE_PARAMETER(var value,min,max:double;n:longint);export;
begin
  Case n of
    1:begin
      Value:=0.0;
      min:=0.0;
      max:=1.0;
      end;
    2:begin
      Value:=0.0;
      min:=-1.0;
      max:=1.0;
      end;
    3:begin
      Value:=0.0;
      min:=0.0;
      max:=1.0;
      end;
    4:begin
      Value:=0.0;
      min:=0.0;
      max:=1.0;
      end;
  end;
end;
end;

```

This procedure has the job to calculate the value of the parameter for which the cross reference was activated in MossWinn.

pPARAMETERS = pointer that points to the start address of (n+1) floating point numbers of the type **DOUBLE**, where n equals to the number of the extra parameters that was set by the procedure **DEPDLL1_SET_NUMBER_OF_EXTRA_PARAMETERS**. The (n+1)th parameter is the parameter that serves as the base of the cross reference (this is the parameter that was selected from the appearing subpop list of the **CONSTRAIN** popup).

The calculated value should be placed in the variable **x**.

```

Procedure DEPDLL1_SET_PARAMETER_VALUE(var x:double;pPARAMETERS:pointer);export;
Type
  TARRAY = ARRAY[1..8191] of DOUBLE;
var
  PARAMETERS:^TARRAY;
begin
  PARAMETERS:=pPARAMETERS;
  x:=PARAMETERS^[1]+PARAMETERS^[5]*(PARAMETERS^[2]+PARAMETERS^[5]*(PARAMETERS^[3]+Parameters^[5]*Parameters^[4]))
end;

```

The library should end like this.

```

exports
  DEPDLL1_SET_SHORT_NAME,
  DEPDLL1_SET_LONG_NAME,
  DEPDLL1_SET_NUMBER_OF_EXTRA_PARAMETERS,
  DEPDLL1_SET_PARAMETER_NAME,
  DEPDLL1_INITIALIZE_PARAMETER,
  DEPDLL1_SET_PARAMETER_VALUE;

begin
end.

```

28. The Mössbauer Line Sharpening menu

The precise constraints required in the model-dependent analysis of Mössbauer spectra are often not known. In some case we may not even be able to determine the number of the resonance lines. However, a model-independent analysis can be performed based on the knowledge that in thin absorber approximation the spectrum, $y(\nu)$, can be considered to be the convolution of the distribution function of hyperfine energies, $p(\nu)$, with a Lorentzian curve, $l(\nu)$:

$$y(\nu) = \int_{-\infty}^{+\infty} p(w) \cdot l(\nu - w) \cdot dw$$

The relevant information about the spectrum is contained in $p(\nu)$ which, obviously, consists of sharper peaks than $y(\nu)$ does. In principle, if we have a small number of well-defined environments of the resonant nucleus in the sample, $p(\nu)$ is the sum of delta-functions. Therefore, in the case of overlapped Mössbauer spectra, the knowledge of such a $p(\nu)$ can effectively help the spectrum decomposition by the recognition of individual spectral lines. This can help establish the appropriate model. In the ideal case, $p(\nu)$ can be easily obtained by deconvolution using Fourier transformation.

According to the previous equation $y(\nu)$ is a convolution of $p(\nu)$ and $l(\nu)$. Hence

$$p(\nu) = \mathbf{F}^{-1} \frac{\mathbf{F}y(\nu)}{\mathbf{F}l(\nu)} = \mathbf{F}^{-1} \frac{Y(k)}{L(k)}$$

$$\mathbf{F}y(\nu) = Y(k) = (2\pi)^{-1/2} \int_{-\infty}^{+\infty} y(\nu) \cdot e^{ik\nu} \cdot d\nu$$

$$\mathbf{F}^{-1}Y(k) = y(\nu) = (2\pi)^{-1/2} \int_{-\infty}^{+\infty} Y(k) \cdot e^{-ik\nu} dk$$

Where \mathbf{F} denotes the Fourier transformation operation, while $Y(k)$ and $L(k)$ are the Fourier transforms of $y(\nu)$ and $l(\nu)$ respectively. The described model-independent spectrum transformation is the **line sharpening** method. In applications of the Fourier transform methods for deconvolution, a *filter function* is needed to eliminate unwanted statistical noise. The choice of the filter function is crucial from the point of view of the results obtained. In the case of Mössbauer spectroscopy different filter functions, $D(k)$, have been tried in order to reduce the high-frequency oscillations in $p(\nu)$ arising from statistical noise. In principle, every spectrum would require its own unique filter function.

The Mössbauer Line Sharpening (**MLS**) menu allows the deconvolution of a Lorentzian line shape with a given line width from the normalized Mössbauer spectrum. The resulting sharpened spectrum can help to recognize the peak patterns underlying of / contributing to spectra with broad absorption / reflection peaks, which in turn may help to identify the correct fit model that needs to be invoked to fit the spectrum.

In this menu the following windows can be seen on the screen.

- 1, The original spectrum after normalization (Left Upper corner).
- 2, The filtered power spectrum of the normalized spectrum (Right Upper corner).
- 3, The filtered power spectrum of the deconvoluted spectrum (Center).
- 4, The deconvoluted spectrum. (Left Bottom corner).

The functions of the various visual elements are as follows.

The original spectrum - This spectrum window shows either the original spectrum that was in the red-framed window when the MLS menu was entered, or its normalized version. (If the red-framed spectrum is not normalized when the MLS menu is entered, then the program offers to carry out normalization of the spectrum.) The MLS menu works properly only if this original spectrum has a baseline equal or close to zero.

The filtered power spectrum - This window shows the power spectrum (under which we mean the absolute value of the Fourier spectrum) of the original spectrum filtered according to one of the built in

filter functions as selected by the user. If there is not any filter function selected, then the content of the window simply shows the power spectrum of the original spectrum. (Manual filtering does not affect the content of this window: this is because manual filtering is applied *after* the deconvolution process.)

The power spectrum after deconvolution - This window shows the power spectrum of the original spectrum after noise filtering via one of the built in filter functions (if selected), the deconvolution of the Lorentzian line shape, as well as manual filtering (if any) has taken place. The window also shows the shape of the selected filter function by red line provided that the show filter check box is checked. Move the mouse over this window in order to carry out manual filtering: press the left mouse button in order to increase / decrease the amplitude of a selected frequency component, or press the right mouse button to limit the amplitude of the power spectrum right hand side of the cross (which follows the movement of the mouse) according to the actual height of the cross.

The spectrum after deconvolution - This window shows the resulted, sharpened counterpart of the original spectrum, after noise filtering and deconvolution of the Lorentzian peak shape has taken place. It is calculated as the inverse Fourier transform of the frequency domain function underlying the deconvoluted power spectrum shown in the middle of the menu screen. This is the result that is preserved when the menu is left via pressing the **EXIT** menu box.

The filter selector popup - Press on this box to select one of the built in filter functions from the appearing list. The shape of the filter functions may depend on the cutoff frequency and - in the case of the Fermi-Dirac filter - Lorentz width parameters. It is also possible to use a custom filter function loaded from the data window that was the green-framed one when the MLS menu was entered. Selecting a built in filter function will undo any manual filtering carried out previously.

Show filter check box - Check / uncheck this check box in order to show / hide the selected built in filter function overlaid by red line on the graph of the deconvoluted power spectrum. The filter function corresponding to the effects of manual filtering (if any) is not included in the curve.

Filter cutoff frequency - This is the frequency (as measured on the frequency scale of the power spectrum after deconvolution) beyond which built in filter functions strongly suppress frequency components. The actual meaning of the cutoff frequency depends on the type of the built in filter function selected. Click on the number part of this box in order to set the cutoff frequency value. If the value is set higher than the maximum value achievable by the filter cutoff frequency slide, then the latter maximum will be extended such that the newly set value will be set as the new maximum value. Set here a negative value for the filter cutoff frequency in order to set the maximum of the cutoff frequency slide (to the corresponding absolute value) irrespective of whether the newly set value is higher or lower than the former maximum.

Filter cutoff frequency slide - Press on this slide to change the filter cutoff frequency continuously with the movement of the mouse. The filtered power spectrum and the sharpened end result will be updated continuously, too. In order to set the maximum cutoff frequency achievable by this slide, turn to the edit box of the cutoff frequency.

Lorentz width - This is the width (FWHM) of the Lorentzian peak shape that is deconvoluted from the original normalized spectrum. This is usually set to the minimum experimental line width value (e.g. 0.28 mm/s) achievable via the applied radioactive source and experimental setup. As a result of deconvolution high frequency statistical noise becomes intensified as an exponential function of the product of frequency and line width, such that the application of higher line widths will generally require the setting of a lower filter cutoff frequency. Click on the number part of the box in order to edit the Lorentzian width value. If the value is set higher than the maximum value achievable by the Lorentzian width slide, then the latter maximum will be extended such that the newly set value will be set as the new maximum value. Set here a negative value for the Lorentzian width in order to set the maximum of the Lorentzian width slide (to the corresponding absolute value) irrespective of whether the newly set value is higher or lower than the former maximum.

Lorentzian width slide - Press on this slide to change the Lorentzian width continuously with the movement of the mouse. The filtered power spectrum and the sharpened end result will be updated continuously, too. In order to set the maximum Lorentzian width achievable by this slide, turn to the Lorentz width edit box.

Reset all - Press on this box to undo all filter operations.

Adjust Y scale - Press on this box to recalibrate the Y axis of the deconvoluted power spectrum shown in the middle of the menu screen. This is useful when the maximum of the deconvoluted power spectrum is reduced by manual filtering, because in such a case the Y-axis range is not adjusted automatically.

Exit & Keep - to leave the MLS menu by previously selecting the set of windows (e.g. the applied filter function) that is preserved as result.

Exit - to leave the MLS menu instantly by preserving only the sharpened spectrum as result.

Cancel - to leave the MLS menu instantly without preserving any result.

References

D.L.NAGY, U. RÖHLICH: HYPERFINE INTERACTIONS **66** (1991) 105.

29. The noise FiLTerIng menu

With the help of the **FLT** menu statistical noise can be filtered out from data files. The windows in this menu have similar functionality to those described in the previous section in the case of the **MLS** menu. The only difference is that in the **FLT** menu the step of the deconvolution of the Lorentzian line shape is omitted. The following windows can be seen on the screen in this menu.

- 1, The original spectrum after normalization (Left Upper corner).
- 2, The power spectrum of the normalized spectrum (Right Upper corner).
- 3, The filtered power spectrum (Center).
- 4, The filtered spectrum. (Left Bottom corner).

The functions of the various visual elements are as follows.

The original spectrum - This spectrum window shows either the original spectrum that was in the red-framed window when the FLT menu was entered, or its normalized version. (If the red-framed spectrum is not normalized when the FLT menu is entered, then the program offers to carry out normalization of the spectrum.) The FLT menu works properly only if this original spectrum has a baseline equal or close to zero.

The power spectrum - This window shows the power spectrum (under which we mean the absolute value of the Fourier spectrum) of the original spectrum.

The filtered power spectrum - This window shows the power spectrum of the original spectrum after noise filtering via one of the built in filter functions (if selected) and manual filtering (if any) has taken place. The window also shows the shape of the selected filter function by red line provided that the show filter check box is checked. Move the mouse over this window in order to carry out manual filtering: press the left mouse button in order to increase / decrease the amplitude of a selected frequency component, or press the right mouse button to limit the amplitude of the power spectrum right hand side of the cross (which follows the movement of the mouse) according to the actual height of the cross.

The filtered spectrum - This window shows the resulted, filtered counterpart of the original spectrum, after noise filtering has taken place. It is calculated as the inverse Fourier transform of the frequency domain function underlying the filtered power spectrum shown in the middle of the menu screen. This is the result that is preserved when the menu is left via pressing the **EXIT** menu box.

The filter selector popup - Press on this box to select one of the built in filter functions from the appearing list. The shape of the filter functions may depend on the cutoff frequency and - in the case of the Fermi-Dirac filter - steepness parameters. It is also possible to use a custom filter function loaded from the data window that was the green-framed one when the FLT menu was entered. Selecting a built in filter function will undo any manual filtering carried out previously.

Show filter check box - Check / uncheck this check box in order to show / hide the selected built in filter function overlaid by red line on the graph of the filtered power spectrum. The filter function corresponding to the effects of manual filtering (if any) is not included in the curve.

Filter cutoff frequency - This is the frequency (as measured on the frequency scale of the filtered power spectrum) beyond which built in filter functions strongly suppress frequency components. The actual meaning of the cutoff frequency depends on the type of the built in filter function selected. Click on the number part of this box in order to set the cutoff frequency value. If the value is set higher than the maximum value achievable by the filter cutoff frequency slide, then the latter maximum will be extended such that the newly set value will be set as the new maximum value. Set here a negative value for the filter cutoff frequency in order to set the maximum of the cutoff frequency slide (to the corresponding absolute value) irrespective of whether the newly set value is higher or lower than the former maximum.

Filter cutoff frequency slide - Press on this slide to change the filter cutoff frequency continuously with the movement of the mouse. The filtered power spectrum and the filtered end result will be updated continuously, too. In order to set the maximum cutoff frequency achievable by this slide, turn to the edit box of the cutoff frequency.

Steepness - This parameter determines the steepness of the Fermi-Dirac filter function. Click on the number part of the box in order to edit the steepness value. If the value is set higher than the maximum value achievable by the steepness slide, then the latter maximum will be extended such that the newly set value will be set as the new maximum value. Set here a negative value for the steepness in order to set the maximum of the steepness slide (to the corresponding absolute value) irrespective of whether the newly set value is higher or lower than the former maximum. The steepness edit box is shown only when the Fermi-Dirac function is selected as filter.

Steepness slide - Press on this slide to change the steepness of the Fermi-Dirac filter continuously with the movement of the mouse. The filtered power spectrum and the filtered end result will be updated continuously, too. In order to set the maximum steepness achievable by this slide, turn to the steepness edit box. The steepness slide is shown only when the Fermi-Dirac function is selected as filter.

Reset all - Press on this box to undo all filter operations.

Adjust Y scale - Press on this box to recalibrate the Y axis of the filtered power spectrum shown in the middle of the menu screen. This is useful when the maximum of the filtered power spectrum is reduced by manual filtering, because in such a case the Y-axis range is not adjusted automatically.

Exit & Keep - to leave the FLT menu by previously selecting the set of windows (e.g. the applied filter function) that is preserved as result.

Exit - to leave the FLT menu instantly by preserving only the filtered spectrum as result.

Cancel - to leave the FLT menu instantly without preserving any result.

30. The TaBLe Maker menu

The TBL menu provides the possibility to create tables of fit parameters participating in the fit accepted previously in the FIT menu for the red-framed spectrum. While the names of possible fit parameters are extracted exclusively from the file associated with the red-framed window, values of the fit parameters are extracted from all (or some, depending on the choice of the user) of the files associated with the spectrum windows on the current project desk. The extracted parameter names are shown in the **ITEMS FOUND** box: a parameter will be included in the table if the corresponding check box is checked. In the table to be created parameters appear with shorter names which are displayed in the **NAME IN TABLE** box. The box entitled **FORMAT** displays whether the value of a parameter is to be treated as a numeric value or as a string. The extracted parameter values will appear in the table with the number of decimals shown in the **DEC** box. The title of the table will be displayed in the upper left corner cell of the table. The table will be ordered according to the value of the **master item**.

Tables can be created with two different arrangements: either with the parameters or with the file names listed downwards. Press on the corresponding grid shown on the right side of the screen in order to choose between the two options.

The functions of the various visual elements are as follows.

Items found (list of parameter items) - The items found box contains the names of parameters extracted from fits accepted previously for the red-framed spectrum. Check the check box before those parameters

that should be present in the table to be built. Press on the magenta colored headline of the box in order to select/deselect more parameters at once. If there are more parameters than the box allows to see, scroll down/up the parameter list either by using the mouse wheel, or by pressing on the lower/upper part of the box. In order to select the master parameter, i.e. the parameter according to which the table should be ordered, press with the right mouse button on the corresponding check box. The master parameter will be shown by red color, and its name will also appear in the **MASTER ITEM (X)** info box. To add a new, custom parameter to the list, press on the **ADD NEW ITEM** box.

Name in table - This box displays the names by which the selected parameters will appear in the table to be built. Press on the names in order to edit them.

Format - This box displays the way parameter values are handled when the table is built. Whereas for numeric values only a single number will be present in the table, in string values any character (e.g. %) as well as multiple numbers can be present. Press on the magenta colored headline of the box in order to set whether standard deviation values should be included in the table or not.

DEC - This box displays the maximum number of decimals that the parameter values can have when they appear in the table. Click on the numbers to edit them one by one, or press on the magenta colored headline of the box in order to limit the number of decimals for all the selected parameters. The limit set here will also influence the appearance of numbers inside string values.

Title of Table - The string set here will appear in the upper left corner cell of the table.

Master item (X) - This box displays the master item on the basis of which the table will be ordered. In the **ITEMS FOUND** box press on a check box with the right mouse button in order to make the corresponding parameter to be the master item. The master item/parameter also provides the abscissa (x) values of tables saved as X,Y[x] data.

Include files - Press on this box in order to set which spectrum files should participate in the table among those being on the current project desk.

Add new item - Press on this box in order to add a custom parameter item to the list of items extracted from the file of the red-framed spectrum window. If the newly added parameter item can be found in the remaining spectra on the current project desk, then the corresponding parameter values will appear in the table to be created.

Save - Press on this box to save the table as a comma-delimited text file.

Copy - Press on this box to copy the table to the Windows clipboard as comma-delimited text.

Print table - Press on this box to print the table to the default printer.

Print to file - Press on this box to print the table to a bitmap image file.

X,Y[x] - Press on this box to save the table to file as X,Y[x] data intended for grapher programs.

Exit - to leave the TBL menu.

31. The MTX menu

In MossWinn 2.0i, and in earlier versions as well, the so-called transformation matrices served as models to fit Mössbauer spectra. Such transformation matrices can be managed in the **MTX** menu. However, beginning with the version of MossWinn 3.0, a new system has been used for the description of Mössbauer models (this new system can be managed in the **FIT** menu itself), and the system based on transformation matrices can be considered as obsolete. To preserve compatibility with earlier versions, in MossWinn 4.0Pre the transformation matrices remained applicable. However, whenever a transformation matrix is selected as fit model and the fit menu is entered, MossWinn will compile the transformation matrix to a model of the new system.

The menu of MTX allows to load, modify and build together existing transformation matrices being in the Transformation Matrix Directory (`.. \MOSSWINN 4.0 \USERS \PUBLIC \TMATRIX \`) and having the extension: **.MAT**. Transformation Matrices describe linear fit models. How this is done, is described in the followings.

31.1. The job of the Transformation Matrix

An individual Lorentzian line can be described by 3 parameters: Amplitude, Position, and Line Width. A spectrum containing only one Lorentzian can be described by 4 parameters: Base Line + The parameters describing the Lorentzian line itself. If we have, however, a symmetrical quadrupole doublet (consisting of two Lorentzians with the same amplitude) to fit, then we won't need $1+3+3 = 7$ parameters to describe the two lines because the amplitudes of them are the same. How to tell an information like this to the fitting program? This is what a Transformation Matrix can do.

A Transformation Matrix is a matrix of dimension $N \times M$ (N rows, M columns). N is always equal to **$3L + \text{The number of parameters describing the Background}$** (usually only the Base Line parameter, but slope and curvature parameters are also possible), where L denotes the number of Lorentzians being present in the spectrum. M is equal to the number of parameters actually fitted in the **FIT** menu. The transformation matrix has always a block diagonal form in the case of the MossWinn program.

If **V** denotes the vector built from the parameters describing the background and the Lorentzian lines (usually **V** has $3L+1 = N$ elements) and **W** denotes the vector built from the independent parameters actually fitted (**W** has M elements) and **T** denotes the Transformation Matrix then

$$\mathbf{V} = \mathbf{T} \cdot \mathbf{W}$$

In the case of fitting only one Lorentzian line the matrix **T** is diagonal and the multiplication above has the rather trivial form:

$$\begin{bmatrix} \text{BASELINE} \\ \text{AMPLITUDE} \\ \text{POSITION} \\ \text{LINEWIDTH} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \times \begin{bmatrix} \text{BASELINE} \\ \text{AMPLITUDE} \\ \text{ISOMERSHIFT} \\ \text{LINEWIDTH} \end{bmatrix}$$

In the case of the fitting of a symmetrical quadrupole doublet, the multiplication can be written in the following form:

$$\begin{bmatrix} \textit{BASELINE} \\ \textit{AMPLITUDE} - (1) \\ \textit{AMPLITUDE} - (2) \\ \textit{POSITION} - (1) \\ \textit{POSITION} - (2) \\ \textit{LINEWIDTH} - (1) \\ \textit{LINEWIDTH} - (2) \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & +0.5 & 0 \\ 0 & 0 & 1 & -0.5 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} \times \begin{bmatrix} \textit{BASELINE} \\ \textit{AMPLITUDE} \\ \textit{ISOMERSHIFT} \\ \textit{Q.SPLITTING} \\ \textit{LINEWIDTH} \end{bmatrix}$$

If the Lorentzians of the quadrupole doublet do not have necessarily the same line width then the multiplication looks like this:

$$\begin{bmatrix} \textit{BASELINE} \\ \textit{AMPLITUDE} - (1) \\ \textit{AMPLITUDE} - (2) \\ \textit{POSITION} - (1) \\ \textit{POSITION} - (2) \\ \textit{LINEWIDTH} - (1) \\ \textit{LINEWIDTH} - (2) \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & +0.5 & 0 & 0 \\ 0 & 0 & 1 & -0.5 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \times \begin{bmatrix} \textit{BASELINE} \\ \textit{AMPLITUDE} \\ \textit{ISOMERSHIFT} \\ \textit{Q.SPLITTING} \\ \textit{LINEWIDTH} - (1) \\ \textit{LINEWIDTH} - (2) \end{bmatrix}$$

31.2. Examples for transformation matrices stored as text files

The MossWinn program uses the following coding system to store transformation matrices in the form of text files on the hard disk. Transformation matrices are stored in the form of text files thus they can be edited with any text editor program. A matrix of **one singlet** should look like this (characters between the signs {} are not in the file.)

```

1      {The first row of the text file. The number of Lorentzians ( L )}
0      {The number of curvature type parameters.([0,1])}
0      {The number of slope type parameters.([0,1])}
1      {The number of base line parameters. (Always 1)}
1      {The number of Amplitude type parameters }
1      {The number of Position type parameters (IS,QS,MS)}
1      {The number of Width type parameters }
[1 Singlet] {Name of the matrix}
BASE LINE: {Name of the Base Line type parameter}
1      { T[1,1] }
AMPLITUDE: {Name of the Amplitude type parameter}
1      { T[2,2] }
ISOMER SHIFT: {Name of the Position type parameter}
1      { T[3,3] }
LINE WIDTH: {Name of the Width type parameter}
1      { T[4,4] }
ETM    {Indicates the end of the matrix definition}

```

A text file of a matrix describing a **symmetrical quadrupole doublet** is the following.

```

2      {The first row of the text file. The number of Lorentzians ( L )}
0      {The number of curvature type parameters.([0,1])}
0      {The number of slope type parameters.([0,1])}
1      {The number of base line parameters. (Always 1)}
1      {The number of Amplitude type parameters }
2      {The number of Position type parameters (IS,QS,MS)}
1      {The number of Width type parameters }
[1 Doublet] {Name of the matrix}
BASE LINE: {Name of the Base Line type parameter}
1      { T[1,1] }
AMPLITUDE: {Name of the Amplitude type parameter}
1      { T[2,2] }
1      { T[3,2] }
ISOMER SHIFT: {Name of the first Position type parameter}
1      { T[4,3] }
1      { T[5,3] }
Q.SPLITTING: {Name of the second Position type parameter}
+0.5   { T[4,4] }
-0.5   { T[5,4] }
LINE WIDTH: {Name of the Width type parameter}
1      { T[6,5] }
1      { T[7,5] }
ETM    {Indicates the end of the matrix definition}

```

A text file of a matrix describing **1 doublet + 1 singlet** can be the following:

```

3      {The first row of the text file. The Number of Lorentzians ( L )}
0      {The number of curvature type parameters.([0,1])}
0      {The number of slope type parameters.([0,1])}
1      {The number of base line parameters. (Always 1)}
2      {The number of Amplitude type parameters }
3      {The number of Position type parameters (IS,QS,MS)}
2      {The number of Width type parameters }
[1 D + 1 S] {Name of the matrix}
BASE LINE: {Name of the Base Line type parameter}
1      { T[1,1] }
A (Doublet): {Name of the first Amplitude type parameter}
1      { T[2,2] }
1      { T[3,2] }
0      { T[4,2] }
A (Singlet): {Name of the second Amplitude type parameter}
0      { T[2,3] }
0      { T[3,3] }
1      { T[4,3] }
IS (Doublet): {Name of the first Position type parameter}
1      { T[5,4] }
1      { T[6,4] }
0      { T[7,4] }
Q.S.(D): {Name of the second Position type parameter}
+0.5   { T[5,5] }
-0.5   { T[6,5] }
0.0    { T[7,5] }
IS (Singlet): {Name of the third Position type parameter}
0      { T[5,6] }
0      { T[6,6] }
1      { T[7,6] }
LW (Doublet): {Name of the first Width type parameter}
1      { T[8,7] }
1      { T[9,7] }
0      { T[10,7] }
LW (Singlet): {Name of the second Width type parameter}
0      { T[8,8] }
0      { T[9,8] }
1      { T[10,8] }
ETM    {Indicates the end of the matrix definition}

```

The next matrix-file can be used to analyze an **α -iron calibration** spectrum.

```

6
0
0
1
3
2
1
IRON CALIBRATION (SIX LINES ; 3 AMPLITUDES ; EQUAL LINE WIDTHS)
BASE LINE:
1
AMPLITUDE (1-6):
1
0
0
0
0
1
AMPLITUDE (2-5):
0
1
0
0
1
0
AMPLITUDE (3-4):
0
0
1
1
0
0
CENTER:
1
1
1
1
1
1
REC.CAL.FACT.:
-5.32128 {Position of the 1st line of the  $\alpha$ -Fe sextet relative to its center.}
-3.08079 {Position of the 2nd line of the  $\alpha$ -Fe sextet relative to its center.}
-0.84029 {Position of the 3rd line of the  $\alpha$ -Fe sextet relative to its center.}
0.84029 {Position of the 4th line of the  $\alpha$ -Fe sextet relative to its center.}
3.08079 {Position of the 5th line of the  $\alpha$ -Fe sextet relative to its center.}
5.32128 {Position of the 6th line of the  $\alpha$ -Fe sextet relative to its center.}
LINE WIDTHS:
1
1
1
1
1
1
1
ETM

```

31.3. Options available in the MTX menu

In the menu of **MTX** there is the possibility to modify existing Transformation Matrices and to build new Transformation Matrices by merging existing matrices together. The functions of the various visual elements are as follows.

Transformation matrices found - This box lists the transformation matrices (with extension MAT) found in the transformation matrix directory of MossWinn. A transformation matrix can be selected for modifications by pressing with the right mouse button on the check box before its name. As a result, the name of the matrix will become red (it will be the **red-selected matrix**) and the parameters included in the corresponding fit model will appear in the PARAMETERS FOUND box. In order to build together existing transformation matrices (for example with the aim to create the model of [1 singlet + 1 doublet] from the individual models of [1 singlet] and [1 doublet]) select them by pressing with the left mouse button on the check box before their name. If there are more matrices than the box allows to see, scroll down/up the matrix list either by using the mouse wheel, or by pressing on the lower/upper part of the box. Press on the magenta colored headline of the box in order to edit the file name or the headline of the red-selected matrix.

Parameters found - This box displays the fit parameters included in the fit model represented by the red-selected matrix (if any being highlighted in the TRANSFORMATION MATRICES FOUND box). Press on the name of one of the fit parameters with the right mouse button in order to select it (its name will be highlighted in red color). The matrix elements associated with the selected parameter will be shown in the ELEMENTS box. In order to edit a parameter name, press on it with the left mouse button. Whether in this box a parameter is selected or not influences the effect of the ADD, DEL, INSERT, UNGROUP and GROUP menu boxes.

Elements - This box displays the matrix elements belonging to the parameter selected in the PARAMETERS FOUND box. In order to edit the displayed matrix elements, press on them with the mouse. There will be as many matrix elements (i.e. as many rows in the box) as the number of Lorentzians (or in general: absorption peaks) contributing to the corresponding fit model. A given amplitude-, position- or width-type fit parameter can influence the amplitude/position/width of a Lorentzian peak only if it has a nonzero matrix element in the row associated with the peak in question. If there are more than 6 rows/Lorentzians, use the mouse wheel or press on the magenta colored top/bottom edges of the box to scroll the elements up or down.

Add - This menu box has multiple functions depending on whether a parameter in the Parameters found box is selected or not:

If a parameter is selected, then press on the ADD menu box in order to set the minimum and maximum of the selected fit parameter, which information is automatically loaded when the corresponding transformation matrix is invoked for fitting.

If there is not any parameter selected, then press on the ADD menu box to add a new parameter to the parameter list, or to add a new Lorentzian/peak to the fit model corresponding to the red-selected matrix.

Del - This menu box has multiple functions depending on whether a parameter in the Parameters found box is selected or not:

If a parameter is selected, then press on the DEL menu box in order to delete the selected parameter from the fit model corresponding to the red-selected transformation matrix.

If there is not any parameter selected, then press on the DEL menu box to delete the last Lorentzian/peak from the fit model corresponding to the red-selected transformation matrix.

Insert - By the help of this menu box one can reorder the parameters in the PARAMETERS FOUND box. First select one of the parameters, then press on this box to have the text INSERT become highlighted in yellow. Then press on one of the parameters by the left mouse button in order to insert the selected parameter before or after the parameter that was pressed on.

Ungroup - This menu box can be used to ungroup the Lorentzians/peaks from the viewpoint of the selected parameter. First select one of the parameters in the PARAMETERS FOUND box, then press on this

menu box. If the selected parameter has influenced the amplitude/position/width of more than one Lorentzians/peaks, then new parameters of the same type will be created and added to the list in order to have each of the associated parameters influence only one of the Lorentzians/peaks. The effect of this menu box can be undone by the application of the GROUP menu box in conjunction with the newly created parameters.

Group - This menu box can be used to group together the Lorentzians/peaks influenced by two parameters of the same (amplitude/position/width) type. First select one of the parameters, then press on this box to have the text GROUP become highlighted in yellow, then press on one of the remaining parameters with the left mouse button. As a result, the two parameters will be merged into a single parameter that influences all the Lorentzians/peaks influenced earlier by the two independent parameters.

Build - This menu box can be used to merge the selected/checked (blue-colored) matrices. The result is a new transformation matrix that includes all the subspectra and associated parameters that take place in the selected matrices that were built together. The newly created matrix will appear in the TRANSFORMATION MATRICES FOUND box if it is saved with the extension MAT.

Exit - Press on this box to leave the MTX menu and load in the red-selected transformation matrix (if any).

32. The Mössbauer Project Desks menu

The Mössbauer Project Desks (**MPD**) menu serves for the organization of Mössbauer spectra in different project desks. Projects are organized in project groups. To add a spectrum to the actually selected project, simply load the spectrum via the **LOAD** menu. The program updates the content of the project desks automatically when the program is exited. Any project and all the spectra belonging to it can then be reloaded easily any time later on. LMC the MPD box to access the following options.

- **List of project groups and associated projects** - click to display the selected project desk on the screen.
- **Add new Project...** - to create a new project desk either in one of the existing project groups or in a newly created project group. MossWinn can handle around 800 project desks distributed in around 25 project groups.
- **Import Project...** - to import a project desk - or a whole project group with multiple project desks - from a *.TPF file (Transfer Project File), that was exported previously via the EXPORT CURRENT PROJECT... or EXPORT PROJECT GROUP.... menu options. The imported project(s) will be added to the project structure of MossWinn: they will contain all the spectrum- and text windows that were present on the corresponding project desks when the latter were exported. The imported windows will refer to newly created physical data files. Exporting/importing transfer project files is the recommended way to exchange data between different copies of MossWinn, as well as to archive projects/project groups.
- **Export Current Project...** - to export the current project desk with all of its associated data and text windows into a standalone transfer project file (*.TPF) that can be imported via the IMPORT PROJECT... menu option. **This is the best way to exchange data with another researcher using MossWinn.**
- **Export Project Group...** - to export the selected project group with all of its project desks and associated data and text windows into a standalone transfer project file (*.TPF) that can be imported via the IMPORT PROJECT... menu option. **This is the best way to archive the corresponding data.**
- **Update Current Project** - to update the current project desk according to its actual state. Normally, active project desks become updated when the program is closed. (Entering the ORGANIZE MOSSBAUER PROJECTS menu will cause the active project desks to become updated, too.)
- **Rename Current Project** - to change the name of the current project.
- **Rename Project Group...** - to change the name of the selected project group.
- **Organize Projects...** - to enter the ORGANIZE MOSSBAUER PROJECTS menu (equivalent to the action of the right mouse button).

32.1. How to organize Mössbauer Projects

To organize existing Mössbauer projects, RMC the **MPD** box. On the appearing form the screen is divided into two equivalent sides, one on the left, and one on the right of the screen.

In this menu there is the possibility

1. TO EXPORT A PROJECT OR A WHOLE PROJECT GROUP TO A STANDALONE FILE.

To export a whole project group:

- Select the project group in the left or right cyan colored popup box.
- Click on **EXPORT PROJECT GROUP** on the corresponding side (left or right) and follow the instructions.

To export a project:

- Select the project group that contains the required project.
- Select the required project in the corresponding list box.
- Click on **EXPORT PROJECT** on the corresponding side (left or right) and follow the instructions.

2. TO MOVE OR COPY PROJECTS BETWEEN PROJECT GROUPS.

To copy a project to an another project group:

- Select the source project group in the popup box on the left side.
- Select the project to be copied in the list box on the left side.
- Select the target project group in the popup box on the right side.
- Click on the **COPY PROJECT** box on the left side.

To move a project to an another project group:

- Select the source project group in the popup box on the left side.
- Select the target project group in the popup box on the right side.
- DRAG AND DROP the required project from the list box on the left to the list box on the right.

3. TO MOVE OR COPY SPECTRA BETWEEN PROJECTS.

To copy a spectrum to an another project:

- Select the source project in the list box on the left side.
- Select the spectrum to be copied in the list box on the left side.
- Select the target project in the list box on the right side.
- Click on the **COPY FILE** box on the left side.

To move a spectrum to an another project:

- Select the source project in the list box on the left side.
- Select the target project in the list box on the right side.
- DRAG AND DROP the required spectrum file from the list box on the left to the list box on the right.

4. TO REMOVE PROJECTS OR WHOLE PROJECT GROUPS FROM THE PROJECT DESK SYSTEM.

- Select the project to be removed on the left side.
- Click on the **DELETE PROJECT** box on the left side.
- To remove a project group remove all of its projects.

5. TO REMOVE SPECTRA FROM PROJECTS.

- Select the spectrum to be removed in the list box on the left side.
- Click on the **REMOVE FILE** box on the left side. (The spectrum file on the hard disk won't be altered.)

33. The DaTA operations menu

The DTA menu provides the possibility to edit measured spectrum data, delete selected subspectrum envelopes, copy data series (e.g. subspectra) from one spectrum window to the other, as well as to examine and edit parameters associated with the spectrum data. Although these functions can also be invoked by other means in MossWinn (spectrum data can be edited in the SRE menu, subspectra can be deleted and grouped/ungrouped via the DEL menu and the PLT menu, respectively, and finally spectrum parameters can be edited via the EDT menu), the DTA menu provides a useful and convenient collection of them. The menu screen is divided into two panels of equivalent function, one on the left and one on the right side. Any of the data windows being present on the actual project desk can be selected for processing via the data window list popup box, one being situated on the top of each panel. The functions of the various visual elements are as follows.

Data window list - Press on this popup box to select the spectrum window whose data are to be displayed in the corresponding panel.

Data series list - This list box shows the data series (measured data, fit envelope and subspectra - if any) of the data window selected for the corresponding panel. Click on the items to select/deselect one or more of them. Selected items will be displayed by white background color, and they will vanish from the graph of the spectrum. Press on the DELETE SELECTED menu box in the corresponding panel in order to delete the selected subspectrum items. In order to add one of the displayed data series to those of the spectrum window displayed in the right panel, drag & drop the corresponding item either to the data series list or to the spectrum window of the right panel.

Velocities - X data - This list box shows the velocities attributed to the channels of the spectrum displayed in the corresponding panel. The corresponding measured data can be seen/edited in the list box beside it. The velocities themselves can not be edited. Use the mouse wheel or press on the arrows to scroll the data up or down.

Measured data series - Y data - This list box shows the measured data of the spectrum displayed in the corresponding panel. Press on the list box to edit the data. Use the mouse wheel or press on the arrows to scroll the data up or down.

Delete selected - Press on this box to delete the selected data series (subspectra or the envelope) from the spectrum window shown in the corresponding panel. The data series belonging to the measured data can not be deleted. Press on the UPDATE box to finalize the operation by updating the physical file associated with the spectrum window.

Update - Press on this box to update the physical file associated with the spectrum window of the corresponding panel according to the actual state of the window. When the spectrum parameters are edited, the update procedure is carried out automatically.

Spectrum window - This is the spectrum window selected via the DATA WINDOW LIST in the corresponding panel. In order to add a subspectrum to the corresponding data, drag & drop to this window one of the data series shown in the other panel.

Spectrum parameters - Press on this box to edit the shown spectrum parameters. Use the mouse wheel or press on the arrows to scroll the parameter list up or down. When the spectrum parameters are edited, the corresponding spectrum window becomes automatically updated.

34. The menu of Hard Disk Operations

LMC the **HDO** box to access the following options.

- **Rename red window** - to rename the file associated with the red-framed window.
- **Update red window** - to update the content of the file associated with the red-framed window according to the actual state of the window. If the window does not have an associated file (i.e. it has not been saved yet), then it will be saved as a temporary file.
- **Update all windows** - to update all windows (i.e. the files associated with them) on the current project desk according to their actual state. Windows that have not been saved yet will be saved as a temporary file.
- **Update current project** - to update the current project desk according to its actual state. Normally active project desks are automatically updated when MossWinn is closed.
- **Save all shown temporary files into a single folder** - to save all temporary files (shown as gray-framed windows) associated with the current project desk into a single folder to be created or entered on the appearing dialog form. The program also offers the option to make the current project refer to the newly saved files. This option can be used, e.g., to convert hyperfine field distributions — derived in the FIT menu as temporary files — to normal (i.e. not temporary) files.
- **Save all files of the project into a single folder** - to save a copy of all files associated with the current project desk into a single folder to be created or entered on the appearing dialog form. The program also offers the option to make the current project refer to the newly saved files. This option can be used, e.g., to store a project based on files loaded from removable media on a local fixed disk, or to duplicate the files referenced by the current project.
- **Save all files of the project group into a single folder** - to save a copy of all files associated with the projects of the selected project group into subfolders of a single folder to be created or entered on the appearing dialog form. The subfolders store the files and bear the name associated with the individual projects of the project group. The program also offers the option to make the projects of the selected project group refer to the newly saved files. This option can also be used to duplicate the files associated with the selected project group.
- **Reload red window** - to reload the content of the red-framed window from the file associated with it.
- **Reload current project** - to reload the current project desk. Changes applied to the project desk (e.g. new windows created or loaded) since its last update will be abandoned.
- **Create new directory...** - to display the file explorer dialog of MossWinn in *create new directory* mode, which allows the creation of a new directory on a storage medium.

35. PRiNting graphics

- **Save RED as...** - to save the graphical content of the red-framed window (via the file explorer dialog) as an image having the selected format: **GIF image**, **JPEG image**, **Color bitmap** or **B&W bitmap**. If an attempt is made to save the image file with a file name that already exists, then - without prompting - the program will save the image file with a name that differs from the given name (e.g. IMAGE.JPG) by numbering: IMAGE_(1).JPG. (The attributed number is increased until a file name is reached that does not exist yet.) The created image will obey the options set as default for CLIPBOARD - SINGLE SPECTRUM on the PRINTER SETUP DIALOG.
- **Save ALL as...** - to save the graphical content (i.e. all the windows) of the current project desk (via the file explorer dialog) as an image having the selected format: GIF image, JPEG image, Color bitmap or B&W bitmap. The created image will obey the options set as default for CLIPBOARD - MULTIPLE SPECTRA on the PRINTER SETUP DIALOG.

- **Print RED (ctrl-p)** - to print the graphical content of the red-framed window to the default printer. (Equivalent to the keystroke CTRL-P.) The default printer can be selected in the SET menu.
- **Print ALL (ctrlshift-p)** - to print the graphical content (i.e. all the windows) of the current project desk to the default printer. (Equivalent to the keystroke CTRL+SHIFT-P.)
- **Copy RED to clipboard (ctrl-c)** - to copy the graphical content of the red-framed window to the clipboard of Windows. (Equivalent to the keystroke CTRL-C.) The options influencing the appearance of the resulting image can be set on the PRINTER SETUP DIALOG.
- **Copy ALL to clipboard (ctrlshift-c)** - to copy the graphical content (i.e. all the windows) of the current project desk to the clipboard of Windows. (Equivalent to the keystroke CTRL+SHIFT-C.) The options influencing the appearance of the resulting image can be set on the PRINTER SETUP DIALOG.
- **Print / Copy / Set defaults...** - to display the **PRINTER SETUP DIALOG** that allows the setting of options influencing the appearance of spectrum images printed to printer, copied into the clipboard or saved to a file.

35.1. The printer setup dialog

The printer setup dialog provides the possibility to set the default attributes of the graphs printed / copied by MossWinn. For the different available printers default attributes can be defined independently. From this point of view *copy to clipboard* functions are also formally treated here as printers (CLIPBOARD - SINGLE SPECTRUM and CLIPBOARD - MULTIPLE SPECTRA). The menu can also be used to print / copy graphs with attributes different from the default ones. The functions of the various visual elements are as follows.

File name (popup box) - This popup box enables the selection of the red-framed spectrum window directly on the printer setup dialog. The red-framed window is the one whose parameters are displayed in the spectrum parameters list box, and whose content becomes printed / copied when the PRINT RED or COPY RED TO CLIPBOARD buttons are pressed.

Show Caption (check box) - Put a check on this box in order to have the caption - shown on the right - to be displayed on the bottom of the spectrum graph printed / copied. By default, the caption is equal to the headline of the red-framed spectrum.

Caption (edit box) - This is the (editable) caption that is displayed on the bottom of the printed / copied spectrum graph provided that the corresponding check box is checked. Note that the caption is set equal to the headline of the red-framed spectrum whenever the latter is changed.

Set X Axis Decimals (check box) - Put a check on this box in order to enforce the number of decimals displayed by the numeric labels of the X axis of the printed / copied graph. If the box is checked, then the number of decimals is determined by the number in the edit box on the right. Otherwise, the applied number of decimals is determined automatically.

Set X Axis Decimals (edit box) - This is the decimal number of the numeric labels of the X axis that is enforced if the corresponding check box is checked.

Set Y Axis Decimals (check box) - Put a check on this box in order to enforce the number of decimals displayed by the numeric labels of the Y axis of the printed / copied graph. If the box is checked, then the number of decimals is determined by the number in the edit box on the right. Otherwise, the applied number of decimals is determined automatically.

Set Y Axis Decimals (edit box) - This is the decimal number of the numeric labels of the Y axis that is enforced if the corresponding check box is checked.

Set Font Size (check box) - Put a check on this box in order to enforce the font size of the numeric / textual labels of the graph printed / copied. If the box is checked, then the font size is determined by the number in the edit box on the right. Otherwise, it is determined automatically.

Set Font Size (edit box) - This is the font size of the labels of the printed / copied graph that is enforced if the corresponding check box is checked. The possible values are 1 (small), 2 (medium) and 3 (big).

Left Margin (edit box) - This is the left margin applied to the printed graph, i.e. on the printed page the

graph is shifted to the right by an amount of points given by this value. (One full page is usually equivalent to a few thousands of image points.) Graphs copied to the clipboard are not affected by this parameter.

Top Margin (edit box) - This is the top margin applied to the printed graph, i.e. on the printed page the graph is shifted downwards by an amount of points given by this value. (One full page is usually equivalent to a few thousands of image points.) Graphs copied to the clipboard are not affected by this parameter.

Horizontal size (edit box) - This is the horizontal resolution (i.e. resolution in the direction of the X axis) of the printed / copied image in pixels. (Depending on the resolution of the applied printer, one pixel can be equivalent to several printed image points.)

Vertical size (edit box) - This is the vertical resolution (i.e. resolution in the direction of the Y axis) of the printed / copied image in pixels. (Depending on the resolution of the applied printer, one pixel can be equivalent to several printed image points.)

Point size (check boxes) - These check boxes enable the selection of the size of the individual data points on the printed / copied image. For high resolution printout or for low amounts of data BIG, whereas for lower resolutions or for higher amounts of data MEDIUM or SMALL data point size is recommended.

YL (Y label) (check box) - If this check box is checked, then all the printed / copied spectrum graphs will display the text on the right as Y-axis title label. Otherwise the Y-axis title label is set individually for each spectrum according to the Y-AXIS TITLE spectrum parameter (see the EDT menu).

YL (Y label) (edit box) - This is the text that is displayed as Y-axis title label for each of the printed / copied spectrum graphs provided that the corresponding check box is checked.

XL (X label) (check box) - If this check box is checked, then all the printed / copied spectrum graphs will display the text on the right as X-axis title label. Otherwise the X-axis title label is set individually for each spectrum according to the X-AXIS TITLE spectrum parameter (see the EDT menu).

XL (X label) (edit box) - This is the text that is displayed as X-axis title label for each of the printed / copied spectrum graphs provided that the corresponding check box is checked.

Show Value of (special parameters) (list box) - The value of special spectrum parameters (see the EDT menu) selected in this list box will be displayed on the top of the printed / copied spectrum data.

Show Residual (check box) - Put a check on this box in order to have the residual displayed above the spectrum data on the printed / copied spectrum graph.

Print in color (check box) - Uncheck this box in order to have the spectrum graph printed / copied in grayscale instead of in color.

Econo Mode (check box) - Put a check on this box in order to have the spectrum graph printed / copied in econo mode, i.e. with lighter colors that consume less ink when printed.

Connect (check box) - Put a check on this box in order to have the neighboring spectrum data points connected by a straight line on the printed / copied spectrum graph.

Portrait (check box) - Put a check on this box in order to set printout orientation to Portrait, and to reload the default settings for the portrait mode of the current printer. For a given printer different default settings can be attributed to the portrait and landscape modes. This option does not affect clipboard functions.

Landscape (check box) - Put a check on this box in order to set printout orientation to Landscape, and to reload the default settings for the landscape mode of the current printer. For a given printer different default settings can be attributed to the portrait and landscape modes. This option does not affect clipboard functions.

Print Red (button) - Press on this box in order to print the red-framed spectrum to the currently selected printer. If the currently selected printer is one of the clipboard functions (Clipboard - single spectrum or Clipboard - multiple spectra), then the graph is printed to the default printer (see the SET menu). Printing is performed by considering the currently set attributes.

Print All (button) - Press on this box in order to print all spectra on the current desk to the currently selected printer. If the currently selected printer is one of the clipboard functions (Clipboard - single spectrum or Clipboard - multiple spectra), then the graph is printed to the default printer (see the SET menu). Printing is performed by considering the currently set attributes.

Copy Red To Clipboard (button) - Press on this box in order to copy the graph of the red-framed spectrum to the clipboard of Windows by considering the current attributes set on the printer setup dialog.

Copy All To Clipboard (button) - Press on this box in order to copy the graph of all the spectra on the current desk to the clipboard of Windows by considering the current attributes set on the printer setup dialog.

Printer (popup box) - Press on this popup box in order to select another available printer / clipboard function, and to reload the default attributes of the newly selected printer / function.

Load Defaults (button) - Press on this box in order to reload the default attributes of the currently selected printer / clipboard function.

Save as default (button) - Press on this box in order to save the currently set printing attributes as the default attributes of the currently selected printer / clipboard function.

Spectrum parameters (list box) - This box shows the parameters of the red-framed spectrum window.

Quit - Press on this box in order to close the Printer Setup dialog.

36. The EXEcute menu

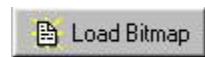
Press with the left mouse button on the EXE box in order to access the following options:

- **List of user-selected executables** - to execute the selected program (*.EXE) or the program associated with the selected file (e.g. the PDF reader for *.PDF files).
- **Add new executable...** - to display the file explorer dialog of MossWinn in *file selection* mode, in order to add a new file entry to the user-selected list of executables.
- **Remove from the list of executables** - to remove the selected file entry from the list of executables.
- **Select Editor Program...** - to display the file explorer dialog of MossWinn in *file selection* mode, in order to select the text editor program invoked by MossWinn when configuration files are to be edited (via the SET menu), or when the file belonging to the red-framed window needs to be edited (on pressing key 'E').
- **Run SCANFIT.EXE** - to execute the SCANFIT.EXE program that allows the creation of ASCII spectrum data from bitmap images of Mossbauer spectra. This program is located inside the directory `.. \MOSSWINN 4.0 \EXES \`

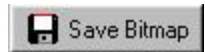
Press with the right mouse button on the EXE box in order to execute the program in the list of executables, that has the code word RMC written after its path+name in the configuration file **execute.cfg** (see section 8). Turn to the option EDIT CONFIGURATION FILE... in the menu list of the SET menu in order to add the code word after the file name of one of the executables.

37. The ScanFit.exe program

The ScanFit program can be started from the EXE menu of MossWinn. With the aid of ScanFit one can create ASCII data from bitmap images of Mössbauer spectra. Next follows the description of the available menus of the ScanFit program.



- To load the Bitmap containing the picture of the Mössbauer spectrum. In the latest version this item can be found in the File menu.



- To save the Bitmap in its actual state. In the latest version this item can be found in the File menu.



- Click to zoom in or out the Bitmap image on the screen.



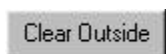
- Set GREY LIMIT to a lower value to make noisy gray background to appear as white. Any Bitmap point that is lighter than the given value will be treated as white. (255 = White , 0 = Black)



The area of the Bitmap picture *outside* of the selected rectangle will be *cut away*.



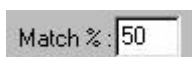
The area *inside* the selected rectangle will be filled with white.



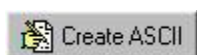
The area *outside* of the selected rectangle will be filled with white.



To create the ASCII data from the Bitmap image one has to select an area of the Bitmap that will serve as the unit of the identification procedure. In the case of Mössbauer spectra the unit should be one point of the spectrum (cross-, rectangle-, circle-, triangle-, or another type). The program does not require that all the points are exactly the same as the unit, but the unit should bear a basic resemblance to other points, at least considering its approximate size. To set the unit, select a single spectrum point on the Bitmap, and press the “Set as Unit” button. Before selection, zoom in the picture if necessary. A large unit with a large number of pixels (>100) may result in slower execution. In such a case reduce the number of pixels (via “Reduce Size”, see later) if necessary.



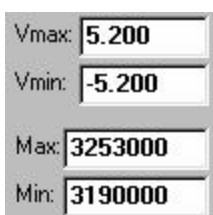
If the match between a specific area of the Bitmap and the selected Unit exceeds the given value, then that area will be identified as a spectrum point. Set it to a lower value if ScanFit did not identify all the Mössbauer data points.



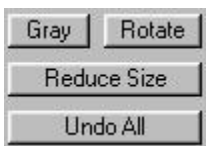
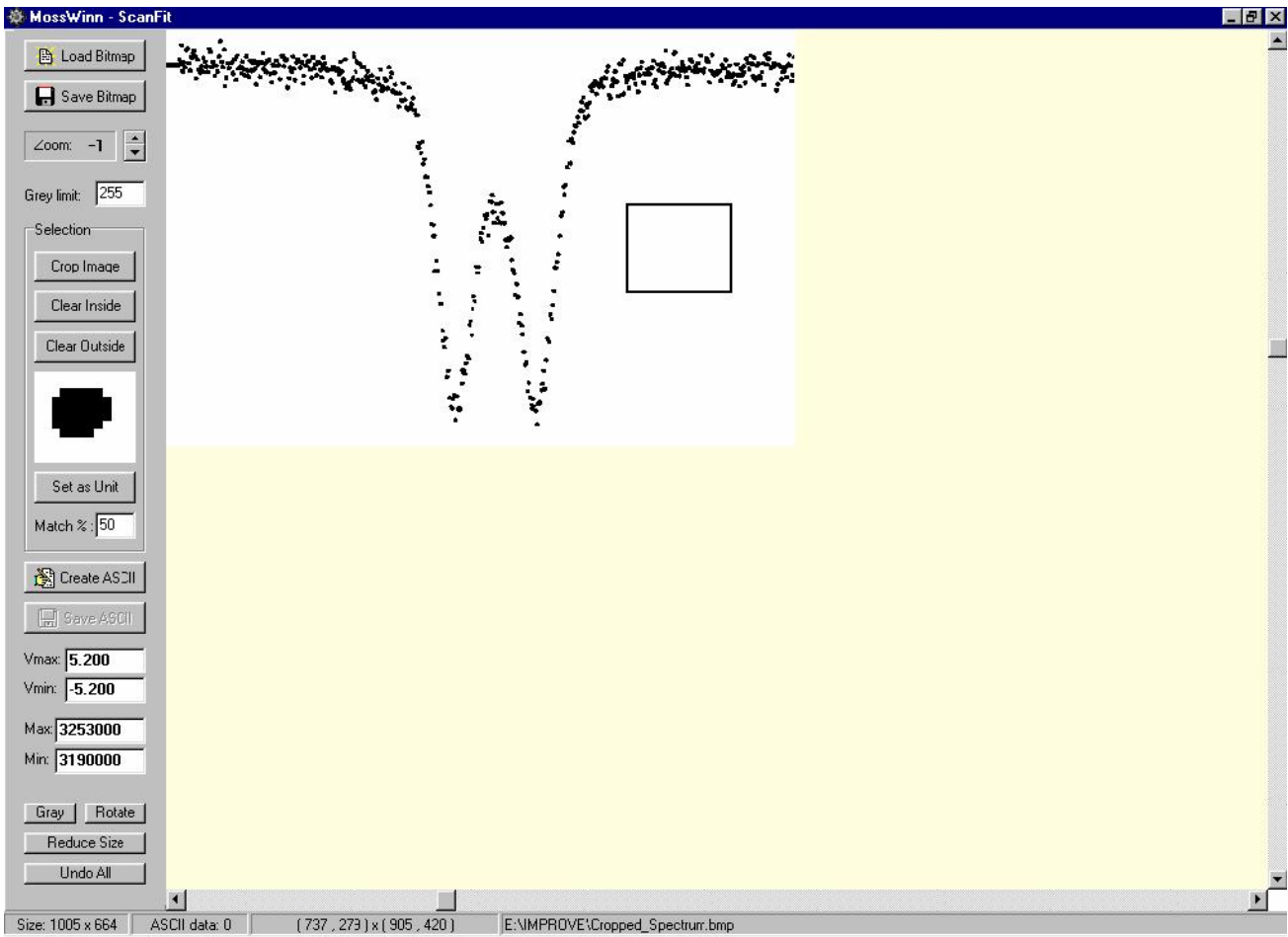
Click this button to start the ASCII data creation procedure.



Click the “Save ASCII” button to save the ASCII data that was created by the CREATE ASCII procedure. In the latest version this item can be found in the File menu.



Before starting the CREATE ASCII process, in order to create the correct ASCII data, set the minimum and maximum of the velocity axis — approximated on the basis of the Bitmap picture of the Mössbauer spectrum. The minimum and maximum of the spectrum — also approximated on the basis of the Bitmap image — can be set here as well. **These values will be attributed to the leftmost (Vmin), rightmost (Vmax), bottommost (Min) and topmost (Max) pixel of the Bitmap image when the ASCII data are created.** Therefore, before pressing “Create ASCII”, use the “Crop Image” button to make the Bitmap look like it is illustrated on the next page, that is, the bitmap should contain only the spectrum data without the axes.



In the latest version these items can be found in the Edit menu.

- Click the “Gray” button to turn color images into grayscale. (Discard color information)
- Click the “Rotate” button to rotate the Bitmap image in order to make the velocity axis to be horizontal on the screen. This procedure introduces a slight distortion into the image therefore the number of rotations applied should be kept at a minimum.
- Click the “Reduce Size” button to reduce the number of pixels the Bitmap image consists of. Turn to this option if the image is too big to handle appropriately by your computer.
- Click on the “Undo All” button to restore the Bitmap image to the form it had when it was loaded.

The ASCII data file created and saved by the ScanFit program will have the appropriate form to get loaded and fitted by MossWinn.

38. The HELP menu

Press on the HELP menu box with the left mouse button in order to access the following options.

- **Request MIDB database subscription for the attached key...** – to request / renew subscription to the MossWinn Internet Database for the attached hardware key by opening a subscription request E-mail in the default E-mail client.
- **Read release notes on the web...** - to open the web page displaying the release notes associated with the released MossWinn versions.
- **Check for updates of MossWinn executables...** - to download and install the latest version of the MossWinn program from the web.
- **Download and install latest help from the web** - to update the local help files to the latest version published on the web.
- **Help on the main menu** - to bring up the html help of MossWinn.
- **Help on the left side menus...** - to bring up the help information as included in the html help concerning the selected left side menu box.
- **Help on the right side menus...** - to bring up the help information as included in the html help concerning the selected right side menu box.
- **Help on the MossWinn Internet Database (MIDB)** - to bring up the help information as included in the html help concerning the MossWinn Internet Database.
- **Turn help mode ON/OFF** - to turn MossWinn's help mode ON/OFF. Equivalent to the function of the right mouse button.

Press on the HELP menu box with the right mouse button in order to turn MossWinn's help mode ON/OFF. If help mode is ON, then a mouse click on the menu boxes will bring up the corresponding help information in the html help. Help mode is ON if the HELP menu text is highlighted in red color.

39. The EXIT menu

LMC the EXIT box to leave the MossWinn program. The project desks loaded into the program will get updated automatically. If the number of windows decreased on a desk then MossWinn will ask for confirmation. An exception is the GENERAL DESK in the GENERAL PROJECTS project group, which desk gets updated automatically even if it is empty.

40. Keystrokes applicable in MossWinn

- **F1** - Set application window size to 640 × 350.
- **F2** - Set application window size to 1280 × 700.
- **F3** - Set application window size to 1920 × 1050.
- **F4** - Toggle between full screen and windowed modes.
- **F5** - Toggle between *always on top* and normal window modes.
- **F12** - Invoke the html help.
- **TAB** - Go to the next active project desk.
- **Backspace** - Go to the previous active project desk.
- **E** - Edit the text file associated with the red-framed window by executing the user-defined editor program (see the EXE menu).
- **ESC** - Show/hide the blue side menus. (Rearranges the spectrum windows.)
- **ctrl-C** - Copy image of the red-framed spectrum into the clipboard of Windows.
- **ctrl+shift-C** - Copy image of all the spectra on the screen into the clipboard of Windows.
- **ctrl-P** - Print image of the red-framed spectrum to the default Windows printer.
- **ctrl+shift-P** - Print image of all the spectra on the screen to the default Windows printer.
- **J** - Save image of the red-framed spectrum as a JPEG image file.
- **shift-J** - Save image of all the spectra on the screen as a JPEG image file.
- **C** - Save image of the red-framed spectrum as a 24 bit color bitmap.
- **shift-C** - Save image of all the spectra on the screen as a 24 bit color bitmap.
- **B** - Save image of the red-framed spectrum as a 1 bit B&W bitmap.
- **shift-B** - Save image of all the spectra on the screen as a 1 bit B&W bitmap.
- **R** - to show/hide the residual for the red-framed spectrum window.
- **shift-R** - to show/hide the residual for all the spectrum windows.
- **shift-M** - Display the amount of physical memory available to MossWinn.
- **shift-A** - Display the 'About' page of MossWinn.

41. Nuclear constants as used in MossWinn 4.0Pre

In practice it may happen to be necessary to analyze Mössbauer spectra using nuclear constants different from those used in the MossWinn program by default. Nuclear data default in MossWinn are based on the following references (note that some of the nuclear constants default in the MossWinn 4.0 series are very different from the corresponding constants default in the 3.0 series):

E.R. COHEN, B.N. TAYLOR: REV. MOD. PHYS. **59** (1987) 1121.

P. RAGHAVAN: ATOMIC DATA AND NUCLEAR DATA TABLES **42** (1989) 189.

* P. DUFEK, P. BLAHA, K. SCHWARZ: PHYS. REV. LETT. **75** (1995) 3545.

**A.A. MOOLENAAR: A ¹⁴¹Pr MÖSSBAUER STUDY OF PRASEODYMIUM COMPOUNDS, PhD THESIS (1994), INTERFACULTY REACTOR INSTITUTE, DELFT UNIVERSITY OF TECHNOLOGY, ISBN 90-73861-20-9

AA. MOOLENAAR, P.C.M. GUBBENS, J.J. VAN LOEF, M.J.V. MENKEN, A.A. MENOVSKY: PHYSICA C **267 (1996) 279.

P. PYYKKÖ: MOLECULAR PHYSICS **99** (2001) 1617.

P. PYYKKÖ: MOLECULAR PHYSICS **106** (2008) 1965.

NUDAT2: [HTTP://WWW.NNDC.BNL.GOV/NUDAT2/](http://www.nndc.bnl.gov/NUDAT2/)

In order to override the default nuclear constants of MossWinn, create a text file named **nuclear.cfg**, and place it inside the directory: `.. \MOSSWINN 4.0 \USERS \PUBLIC \STATUS \`

In the file **nuclear.cfg** the new values of nuclear constants can be defined as it is illustrated in the following table.

SYNTAX (In the file NUCLEAR.CFG)	EXAMPLE (Default in MossWinn)	MEANING
gFe32: <i>newvalue</i>	gFe32: -0.103267	Gyromagnetic factor of the excited state of ⁵⁷ Fe
gFe12: <i>newvalue</i>	gFe12: +0.18088	Gyromagnetic factor of the ground state of ⁵⁷ Fe
QFe32: <i>newvalue</i>	QFe32: +0.16E-28 {m2}	Quadrupole moment of the excited state of ⁵⁷ Fe *
EgammaFe: <i>newvalue</i>	EgammaFe: 14.4129 {keV}	Energy of the gamma ray of the ⁵⁷ Fe Mössbauer transition
gSn32: <i>newvalue</i>	gSn32: +0.422	Gyromagnetic factor of the excited state of ¹¹⁹ Sn
gSn12: <i>newvalue</i>	gSn12: -2.09456	Gyromagnetic factor of the ground state of ¹¹⁹ Sn
QSn32: <i>newvalue</i>	QSn32: -0.132E-28 {m2}	Quadrupole moment of the excited state of ¹¹⁹ Sn
EgammaSn: <i>newvalue</i>	EgammaSn: 23.871 {keV}	Energy of the gamma ray of the ¹¹⁹ Sn Mössbauer transition
gTe32: <i>newvalue</i>	gTe32: +0.403333	Gyromagnetic factor of the excited state of ¹²⁵ Te
gTe12: <i>newvalue</i>	gTe12: -1.77702	Gyromagnetic factor of the ground state of ¹²⁵ Te
QTe32: <i>newvalue</i>	QTe32: -0.31E-28 {m2}	Quadrupole moment of the excited state of ¹²⁵ Te
EgammaTe: <i>newvalue</i>	EgammaTe: 35.4919 {keV}	Energy of the gamma ray of the ¹²⁵ Te Mössbauer transition
gEu72: <i>newvalue</i>	gEu72: +0.740286	Gyromagnetic factor of the excited state of ¹⁵¹ Eu
gEu52: <i>newvalue</i>	gEu52: +1.38868	Gyromagnetic factor of the ground state of ¹⁵¹ Eu
QEu72: <i>newvalue</i>	QEu72: +1.28E-28 {m2}	Quadrupole moment of the excited state of ¹⁵¹ Eu
QEu52: <i>newvalue</i>	QEu52: +0.903E-28 {m2}	Quadrupole moment of the ground state of ¹⁵¹ Eu
EgammaEu: <i>newvalue</i>	EgammaEu: 21.541 {keV}	Energy of the gamma ray of the ¹⁵¹ Eu Mössbauer transition
gSb72: <i>newvalue</i>	gSb72: +0.7194286	Gyromagnetic factor of the excited state of ¹²¹ Sb
gSb52: <i>newvalue</i>	gSb52: +1.34536	Gyromagnetic factor of the ground state of ¹²¹ Sb
QSb72: <i>newvalue</i>	QSb72: -0.728E-28 {m2}	Quadrupole moment of the excited state of ¹²¹ Sb
QSb52: <i>newvalue</i>	QSb52: -0.543E-28 {m2}	Quadrupole moment of the ground state of ¹²¹ Sb
EgammaSb: <i>newvalue</i>	EgammaSb: 37.133 {keV}	Energy of the gamma ray of the ¹²¹ Sb Mössbauer transition
gPr72: <i>newvalue</i>	gPr72: +0.8	Gyromagnetic factor of the excited state of ¹⁴¹ Pr **
gPr52: <i>newvalue</i>	gPr52: +1.71016	Gyromagnetic factor of the ground state of ¹⁴¹ Pr **
QPr72: <i>newvalue</i>	QPr72: +0.28E-28 {m2}	Quadrupole moment of the excited state of ¹⁴¹ Pr **
QPr52: <i>newvalue</i>	QPr52: -0.0589E-28 {m2}	Quadrupole moment of the ground state of ¹⁴¹ Pr **
EgammaPr: <i>newvalue</i>	EgammaPr: 145.44 {keV}	Energy of the gamma ray of the ¹⁴¹ Pr Mössbauer transition **

SYNTAX (In the file NUCLEAR.CFG)	EXAMPLE (Default in MossWinn)	MEANING
g129I72: <i>newvalue</i>	g129I72: +0.748857	Gyromagnetic factor of the ground state of ^{129}I
g129I52: <i>newvalue</i>	g129I52: +1.1218	Gyromagnetic factor of the excited state of ^{129}I
Q129I72: <i>newvalue</i>	Q129I72: -0.498E-28 {m2}	Quadrupole moment of the ground state of ^{129}I
Q129I52: <i>newvalue</i>	Q129I52: -0.604E-28 {m2}	Quadrupole moment of the excited state of ^{129}I
Egamma129I: <i>newvalue</i>	Egamma129I: 27.8 {keV}	Energy of the gamma ray of the ^{129}I Mössbauer transition
gNp52g: <i>newvalue</i>	gNp52g: +1.256	Gyromagnetic factor of the ground state of ^{237}Np
gNp52e: <i>newvalue</i>	gNp52e: +0.672	Gyromagnetic factor of the excited state of ^{237}Np
QNp52g: <i>newvalue</i>	QNp52g: +3.886E-28 {m2}	Quadrupole moment of the ground state of ^{237}Np
QNp52e: <i>newvalue</i>	QNp52e: +3.85E-28 {m2}	Quadrupole moment of the excited state of ^{237}Np
EgammaNp: <i>newvalue</i>	EgammaNp: 59.541 {keV}	Energy of the gamma ray of the ^{237}Np Mössbauer transition
gAu32: <i>newvalue</i>	gAu32: +0.097167	Gyromagnetic factor of the ground state of ^{197}Au
gAu12: <i>newvalue</i>	gAu12: +0.84	Gyromagnetic factor of the excited state of ^{197}Au
QAu32: <i>newvalue</i>	QAu32: +0.547E-28 {m2}	Quadrupole moment of the ground state of ^{197}Au
AE2pM1AU: <i>newvalue</i>	AE2pM1AU: +0.3317	AMPLITUDE (δ) of the E2/M1 mixing ratio in the Mössbauer transition of ^{197}Au .
PE2pM1AU: <i>newvalue</i>	PE2pM1AU: 180.0 {deg}	PHASE difference between the E2 and M1 radiations in the Mössbauer transition of ^{197}Au . MEASURED IN DEGREES. ($180 \cdot \frac{\zeta}{\pi}$ where ζ appears as $\delta \cdot e^{i\zeta}$)
EgammaAu: <i>newvalue</i>	EgammaAu: 77.351 {keV}	Energy of the gamma ray of the ^{197}Au Mössbauer transition
g161Dy52g: <i>newvalue</i>	g161Dy52g: -0.19212	Gyromagnetic factor of the ground state of ^{161}Dy
g161Dy52e: <i>newvalue</i>	g161Dy52e: +0.2376	Gyromagnetic factor of the 5/2- excited state of ^{161}Dy
Q161Dy52g: <i>newvalue</i>	Q161Dy52g: +2.507E-28 {m2}	Quadrupole moment of the ground state of ^{161}Dy
Q161Dy52e: <i>newvalue</i>	Q161Dy52e: +2.506E-28 {m2}	Quadrupole moment of the 5/2- excited state of ^{161}Dy
Egamma161Dy52: <i>newvalue</i>	Egamma161Dy52: 25.6514 {keV}	Energy of the gamma ray of the ^{161}Dy [excited 5/2-] → [ground 5/2+] Mössbauer transition

To check whether the override of the above nuclear parameters is in effect in MossWinn, examine the file STARTUP.TXT that informs about any parameter override that took place when MossWinn started. The override of any parameter is in effect only if there is a clear indication in the file STARTUP.TXT about.

The following table informs about the value of further important physical constants used in MossWinn:

<i>Constant and its value as used in MossWinn</i>	<i>Explanation</i>
$c = 2.99792458 \times 10^8$ m/s	Speed of light in vacuum
$e = 1.60217653 \times 10^{-19}$ C	Elementary charge
$k_B = 1.3806505 \times 10^{-23}$ J/K	Boltzmann constant
$h/2\pi = 1.05457168 \times 10^{-34}$ Js	Planck constant / 2π
$\mu_N = 5.05078343 \times 10^{-27}$ J/T	Nuclear magneton
IS (SNP) = -0.26 mm/s	Isomer shift of Sodium Nitroprusside relative to α -Iron
IS (Fe(Cr)) = -0.154 mm/s	Isomer shift of Fe in Chromium matrix relative to α -Iron
IS (SS) = -0.09 mm/s	Isomer shift of Stainless Steel relative to α -Iron
IS (α -Fe) = 0.0 mm/s	Isomer shift of α -Iron (reference)
IS (Fe(Rh)) = +0.114 mm/s	Isomer shift of Fe in Rhodium matrix relative to α -Iron
IS (Fe(Pd)) = +0.177 mm/s	Isomer shift of Fe in Palladium matrix relative to α -Iron

NLW (^{57}Fe) = 0.194 mm/s	(Experimental) Natural line width of ^{57}Fe (3/2 \rightarrow 1/2)
NLW (^{119}Sn) = 0.646 mm/s	(Experimental) Natural line width of ^{119}Sn (3/2 \rightarrow 1/2)
NLW (^{125}Te) = 5.209 mm/s	(Experimental) Natural line width of ^{125}Te (3/2 \rightarrow 1/2)
NLW (^{151}Eu) = 1.31 mm/s	(Experimental) Natural line width of ^{151}Eu (7/2 \rightarrow 5/2)
NLW (^{121}Sb) = 2.10 mm/s	(Experimental) Natural line width of ^{121}Sb (7/2 \rightarrow 5/2)
NLW (^{141}Pr) = 1.017 mm/s	(Experimental) Natural line width of ^{141}Pr (7/2 \rightarrow 5/2)
NLW (^{129}I) = 0.586 mm/s	(Experimental) Natural line width of ^{129}I (5/2 \rightarrow 7/2)
NLW (^{237}Np) = 0.06727 mm/s	(Experimental) Natural line width of ^{237}Np (5/2 \rightarrow 5/2)
NLW (^{197}Au) = 1.882 mm/s	(Experimental) Natural line width of ^{197}Au (1/2 \rightarrow 3/2)
NLW (^{161}Dy) = 0.378 mm/s	(Experimental) Natural line width of ^{161}Dy (5/2 \rightarrow 5/2)

42. Quadrupole splitting conversion constants

The following table can be used to derive the value of $eQ_{\text{ground}}V_{zz}$ in units of mm/s and MHz from the value of V_{zz} measured in units of 10^{21} V/m² as displayed in MossWinn.

For example, if $V_{zz} = +3.0$ [10^{21} V/m²] for ^{151}Eu , then $eQ_{\text{ground}}V_{zz}$ [mm/s] can be obtained by multiplying 3.0 by 1.257(14), the end result being 3.77(4) mm/s, where the numbers in parentheses refer to the uncertainties in the last digits of the preceding values.

The constants in the table below were calculated by assuming the validity of the built in nuclear constants of MossWinn (see previous chapter). If the user has overridden the corresponding nuclear constants, then the conversion constants below are not valid anymore (in such a case use the corresponding constants **QSCe** and **QSCg** written on the fit reports – see section 4).

For some of the nuclear transitions, the electric quadrupole moment of the ground state equals to zero. In those cases (^{57}Fe , ^{119}Sn , ^{125}Te) Q_{excited} is used instead of Q_{ground} .

In general 1 mm/s is equivalent to $0.806554486 \times (E_{\gamma} / \text{keV})$ MHz, where E_{γ} is the energy of the Mossbauer transition.

Nuclear transition	In order to obtain $eQ_{\text{ground}}V_{zz}$ [mm/s], V_{zz} [10^{21} V/m ²] should be multiplied by:	In order to obtain $eQ_{\text{ground}}V_{zz}$ [MHz], V_{zz} [10^{21} V/m ²] should be multiplied by:
^{57}Fe (3/2 \rightarrow 1/2) ($eQ_{\text{excited}}V_{zz}$)	+0.333(2)	+3.87(2)
^{119}Sn (3/2 \rightarrow 1/2) ($eQ_{\text{excited}}V_{zz}$)	-0.166(1)	-3.19(2)
^{125}Te (3/2 \rightarrow 1/2) ($eQ_{\text{excited}}V_{zz}$)	-0.262(17)	-7.5(5)
^{151}Eu (7/2 \rightarrow 5/2)	+1.257(14)	+21.83(24)
^{121}Sb (7/2 \rightarrow 5/2)	-0.438(9)	-13.13(27)
^{141}Pr (7/2 \rightarrow 5/2)	-0.0121(8)	-1.42(10)
^{129}I (5/2 \rightarrow 7/2)	-0.537(8)	-12.04(17)
^{237}Np (5/2 \rightarrow 5/2)	+1.957(3)	+93.96(15)
^{161}Dy (5/2 \rightarrow 5/2)	+2.930(23)	+60.62(48)
^{197}Au (1/2 \rightarrow 3/2)	+0.212(6)	+13.23(39)

43. References

J.M. Blatt, V.F. Weisskopf:

THEORETISCHE KERNPHYSIK, Teubner verlag, Leipzig (1959)

S.Margulies, J.R.Ehrman:

Nuclear Instruments and Methods **12** (1961) 131.

S.Margulies, P.Debrunner, H.Frauenfelder:

Nuclear Instruments and Methods **21** (1963) 217.

O.C. Kistner:

Phys. Rev. **144** (1966) 1022.

W. Kündig:

Nuclear Instruments and Methods **48** (1967) 219.

M. Blume, J.A. Tjon:

Phys. Rev. **165** (1968) 446.

J.A. Tjon, M. Blume:

Phys. Rev. **165** (1968) 456.

R.M. Housley, R.W. Grant, U. Gonser:

Phys. Rev. **178** (1969) 514.

F.E. Wagner, B.D. Dunlap, G.M. Kalvius, H. Schaller, R. Felscher, H. Spieler:

Phys. Rev. Lett. **28** (1972) 530.

H.-D. Pfannes, U. Gonser:

Appl. Phys. **1** (1973) 93.

D.J. Erickson, M.W.J. Prins, L.D. Roberts:

Phys. Rev. C **8** (1973) 1916.

G.K. Shenoy, J.M. Friedt, H. Maletta, S.L. Ruby: CURVE FITTING AND THE TRANSMISSION INTEGRAL: WARNINGS AND SUGGESTIONS, in *Mössbauer Effect Methodology*, Volume 9, (Edited by I.J. Gruverman, C.W. Seidel, D.K. Dieterly) (1974) pp. 277.

J. Hesse, A. Rübartsch:

J. Phys. E :Sci. Instr. **7** (1974) 526.

J.G. Stevens, V.E. Stevens (eds):

Mössbauer Effect Data Index covering the 1975 literature, IFI/PLENUM (1975)

R.W. Grant: MÖSSBAUER SPECTROSCOPY IN MAGNETISM: CHARACTERIZATION OF MAGNETICALLY-ORDERED COMPOUNDS, IN *MÖSSBAUER SPECTROSCOPY*, ED. U. GONSER, SPRINGER-VERLAG, **5** (1975) PP. 97.

G.K. Shenoy, J.M. Friedt:

Nuclear Instruments and Methods **136** (1976) 569.

R. H. Herber:

Chemical Mössbauer Spectroscopy, Plenum Press, New York & London, (1984)

N. Blaes, H. Fischer, U. Gonser:

Nuclear Instruments and Methods in Physics research B **9** (1985) 201.

D. Crespo, J. Parellada:

Hyp. Int. **29** (1986) 1539.

W. I. F. David:

J. Appl. Cryst. **19** (1986) 63.

E.R. Cohen, B.N. Taylor:

Rev. Mod. Phys. **59** (1987) 1121.

P. Raghavan:

Atomic Data and Nuclear Data Tables **42** (1989) 189.

A.Vértes, D.L.Nagy (Eds.):

Mössbauer Spectroscopy of Frozen Solutions, Akadémiai Kiadó, Budapest (1990) p34.

W.H.Press, B.P. Flannery, S.A. Teukolsky, W.T. Vetterling:

Numerical Recipes, The Art of Scientific Computing, Cambridge University Press, Cambridge, New York (1990)

D.L.Nagy, U. Röhlich:

Hyperfine Interactions **66** (1991) 105.

J. Lindén, J. Hietaniemi, E. Ikonen, M. Lippmaa, I. Tittonen, T. Katila, T. Karlemo, M. Karppinen, L. Niinistö, K. Ullakko:

Phys. Rev. B **46** (1992) 8534.

Z. Michalewicz:

Genetic Algorithms+Data Structures=Evolution Programs, Springer - Berlin, New York (1992)

A.A. Moolenaar:

PhD Thesis (1994), Interfaculty Reactor Institute, Delft University of Technology, ISBN 90-73861-20-9

P. Dufek, P. Blaha, K. Schwarz:

Phys. Rev. Lett. **75** (1995) 3545.

A.A. Moolenaar, P.C.M. Gubbens, J.J. van Loef, M.J.V. Menken, A.A. Menovsky:

Physica C **267** (1996) 279.

Z. Klencsár, E. Kuzmann, A. Vértes:

Journal of Radioanalytical and Nuclear Chemistry **210** (1996) 105.

Z. Klencsár:

Nuclear Instruments and Methods in Physics research B **129** (1997) 527.

P. Pyykkö:

Molecular Physics **99** (2001) 1617.

P. Pyykkö:

Molecular Physics **106** (2008) 1965.

<hr/>	
A	
Abbreviations.....	5
Absolute deviation.....	56
Absorber material.....	29
Accept	
Calibration fit.....	30
Fit results.....	59
Add	
New spectrum to the fit.....	31
New subspectrum.....	31
NEW SUBSPECTRUM GROUP.....	31
ARR.....	20
ASCII data formats.....	13
ASP.....	23
<hr/>	
B	
Blaes's expression.....	44
<hr/>	
C	
CAF.....	5
Cal StD.....	58
Calibration	
Transfer to uncalibrated spectra.....	22
Using the ASP menu.....	23
Using the CAL menu.....	22
Chi-square.....	53
Color of parameters.....	54
CONSTRAINS.....	33
Copy to clipboard	
Fit results.....	60
<hr/>	
D	
Delete	
Absorption line.....	65
Fit model.....	32
Fit parameter.....	32
Position type parameter.....	65
Project.....	85
Spectrum from project.....	85
Subspectrum from model.....	32
Dispersion Amplitude.....	48
Distribution.....	66
DN.....	5
DOF.....	5
<hr/>	
E	
Enabled intervals.....	65
Export project.....	85
<hr/>	
F	
Fit	
Red window as the green one.....	30
Spectrum series.....	27
Fixing parameters.....	54
FoLD.....	22
<hr/>	
G	
GKE.....	5
Global fit.....	58
How to stop.....	58
Goldanskii-Karyagin Effect.....	43
Green window.....	19
GROUP FILES.....	18
<hr/>	
H	
Hamiltonian.....	40
Headline.....	19
Hyperfine field distribution.....	66
<hr/>	
I	
Insight pages.....	57
Installation.....	6
Isomer shift reference.....	29
<hr/>	
L	
Line shapes	
Lorentzian.....	48
Lorentzian with cosine smearing.....	49
Lorentzian with dispersion.....	48
Pseudo-Voigt.....	48
LinFit.....	53
LMC.....	5
<hr/>	
M	
Mixed transition M1+E2.....	39, 42
Mosaic sample.....	41
Mouse issues	
Functionality of the right mouse button.....	20
MSD.....	5
<hr/>	
N	
Nuclides	
⁵⁷ Fe, ¹¹⁹ Sn, ¹²⁵ Te, ¹⁵¹ Eu, ¹²¹ Sb, ¹²⁹ I, ¹⁴¹ Pr, ²³⁷ Np, ¹⁹⁷ Au, ¹⁶¹ Dy, M1, E1, E2, M1+E2.....	36
<hr/>	
O	
Overflows.....	21
<hr/>	
P	
PAS.....	5

Percentage constrained	34
Powder sample.....	41
Precision	61
Print	
Fit results	60
Printer issues	
Network printer.....	25, 26
Orientation	25, 26
Set resolution	25, 26

R

Red window.....	19
Reflection mode.....	53
RELATIVE AMPLITUDE.....	33
Relaxation	
Magnetic	45
Quadrupole	46
Remove	
Absorption line	65
Fit model.....	32
Position type parameter	65
Project.....	85
Spectrum from fit.....	32
Spectrum from project	85
Subspectrum from model.....	32
Rename	
Spectrum file.....	87
Subspectrum	52
Residual	57
REVerse.....	22
RMC	5

S

SAVE	
Fit results	60
SUBSPECTRUM GROUP.....	32
ScanFit.....	91

Shared subspectra	55
Simultaneous fitting.....	54
Single crystal.....	41
Sinusoid	29
Smoothing factor.....	66
SO	5
Source matrix	29
Special parameter types	25, 26
Squared deviation	56
SRE	21
Standard deviation	58
SUB_DLL1.DLL	7, 67

T

Total Area Multiplier	66
Transmission integral.....	50
Triangle.....	29
TSA.....	5

U

Unshared subspectra	55
---------------------------	----

V

Visual angle	49
--------------------	----

X

X,Y[X].....	17, 18
-------------	--------

Z

ZDN	5
ZVC	5