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FOCUS: an Interactive Crystal Electric Field Parameter Fitting Package Using Neutron Scattering Data

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June 1995

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FOCUS

**An Interactive Crystal Electric Field
Parameter Fitting Package
Using Neutron Scattering Data**

Isis Science Division
Rutherford Appleton Laboratory

Peter Fabi
June 1995

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An overview on all FOCUS commands

Abbreviation	of HELP commands	page
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@ h	@focus help	20
@ h a	@focus help alter	20
@ h d	@focus help display	21
@ h h	@focus help help	20
@ h i	@focus help info	22
@ h m	@focus help montecarlo	22
@ h s	@focus help set	23

Abbreviation	of ALTER commands	page
@ a	@focus alter	25
@ a p	@focus alter parameter	25
@ a p b	@focus alter parameter bkq	25
@ a p v	@focus alter parameter vkq	25
@ a p x	@focus alter parameter xr	26

Abbreviation	of MONTECARLO commands	page
@ m	@focus montecarlo	46
@ m n	@focus montecarlo new	47
@ m d	@focus montecarlo display ...	48
@ m l	[n1] @focus montecarlo load	48
@ m p	[n1 n2-n3 ...] @focus montecarlo plot	49

Abbreviation	of DISPLAY commands	page
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Abbreviation	of INFO commands	page
@ i @focus info	30
@ i v @focus info version	30

Abbreviation	of SET commands	page
@ s	@focus set	27
@ s a	@focus set angles	27
@ s d	@focus set degeneration	28
@ s o	@focus set operator	29
@ s s	[n1 n2-n3 ...] @focus set shape	29

About FOCUS

The aim of FOCUS is to provide an easy-to-use program fitting package for crystal electric field parameter determination of rare earth containing materials. In general, neutron spectra of crystal electric field excitations are too complex to be run by batch jobs. FOCUS pays full attention to this fact and uses the interactive program shell of MULTI_FRILLS.

FOCUS has all rare earth ions R³⁺ implemented (excluding La³⁺ and Lu³⁺ which show no crystal electric field splitting) and supports all possible crystal electric field hamiltonians for the 32 different point symmetries of the crystal electric field. Additionally, FOCUS calculates the crystal electric field hamiltonian in two different ways; the first method uses Stevens' operator-equivalents whilst the second applies 3j-symbols. As both methods should exactly give the same result, the user has the possibility to check the calculations by switching between both kinds of methods.

FOCUS can handle three different kinds of crystal electric field parameter; the first ones are the so-called B_{kq} - parameters which are operating in front of the full Stevens' operator-equivalents $\hat{O}_{kq}(J)$. The second parameter scheme V_{kq} uses *normalised* full Stevens' operator-equivalents. The operator normalisation ensures that FOCUS varies parameters of equal size. The third scheme (x_i, R) is based on the normalised parameters mentioned above, and defines an overall crystal electric field splitting R and $n-1$ spherical parameters x_i if n is the number of fitting parameters. The overall splitting can take any real value (positive or negative) while the spherical parameters are limited to the range -1 to 1 , only. The user can switch between the different kinds of parameter schemes by using one only FOCUS command.

FOCUS also provides the possibility of a random selection of initial parameters with finite boundaries by Monte-Carlo simulation. This should help in all those cases where good starting parameters are not given by physical reasons.

How to get started

To start the FOCUS program package, you should have access to the ISISE-Network on the ISIS Facility of the Rutherford Appleton Laboratory. Before starting the FOCUS application set up the GENIE environment. If you are using a normal Decterm terminal it is sufficient to type `genie` only. A GKS icon will be created and the `>>` sign should appear on the original window. But if you are working on a PC which has a network node of `ndip09` and transfers its data via TCP/IP to the network, the following commands should define the required GENIE environment

```
ISISE> set display/create/node=ndip09/transfer=tcPIP
ISISE> genie/dev=motif
```

Calling the GENIE environment from your local PC.

Again a GKS icon and the `>>` sign should appear. If nothing happens, ask the computer support for help. In the next step you have to provide the neutron data you are interested in. FOCUS will expect a GENIE workspace.

```
>> read w1 het05388.cor 1
Reading block          1
>>
```

An example for loading the neutron data in a GENIE workspace `w1`.

In the above example, GENIE reads workspace `w1` by a standard GENIE read command. A message like *Reading Block 1* signals that GENIE has found the specified workspace and that everything is working. After loading the neutron data in a GENIE workspace, type `@g:focus` to start up the FOCUS application. If `@g:focus` does not work try `@het$disk:[hetmgr.genie]focus`. FOCUS will ask you now for the workspace number of the neutron data you want to fit. The next input defines a workspace which can be used by FOCUS itself. Provide a workspace you do not need on your own.

```

>> @g:focus
>>
>> -----
>> |                               |
>> |           Start up command file for           |
>> | *****  ***   ***  *  *  ***             |
>> | *      *   *  *   *   *  *  *             |
>> | ***   *   *  *   *   *  *  ***           |
>> | *      *   *  *   *   *  *  *           |
>> | *      ***   ***   ***   ***             |
>> | An Interactive Crystal Electric Field       |
>> | Parameter Fitting Package using           |
>> | Neutron Scattering Data                   |
>> | Peter Fabi                                 |
>> | ISIS-Facility, Rutherford Appleton Laboratory |
>> | telephone: -44213544.5428                 |
>> | facsimile : -44213544.5383                 |
>> |-----|
>>
>> -----
>> | FOCUS Version for single workspace fit only |
>> |-----|
>> | Please give in first the workspace number where the crystal |
>> | electric field data are you want to fit (e.g. enter 1. for w1). |
>> | Then enter a workspace number for the FOCUS output.         |
>> |
>> | Enter the workspace number of neutron data : 1
>> | Enter the workspace number of FOCUS output : 2

```

Example for neutron data in workspace w1. The workspace w2 is used by FOCUS itself.

After typing in the workspace number of the FOCUS output (e.g. 2 for workspace w2) the *neutron data* workspace (in the above example this is workspace w1) is written by a GENIE write command to your scratch disk. The filename is *frills.in*. FOCUS will only be called if the GENIE transform command succeeded. Otherwise the control will be returned to GENIE. If you see the >> prompt, leave GENIE by typing **exit**, start GENIE, read in the workspace you want to fit and try to start up FOCUS again. If you fail again, ask the computer support for help.

Next, the user is asked for the point symmetry of the rare earth R³⁺ ion. Type in the symmetry number of the crystal electric field shown by the table.

POINT SYMMETRIES OF THE CRYSTAL FIELD AND SYMMETRY NUMBERS	
point symmetry of the crystal field	symmetry number
C _i C ₁	0
C ₂ C _s C _{2h}	1
C _{2v} D ₂ D _{2h}	2
C ₄ S ₄ C _{4h}	3
D ₄ C _{4v} D _{2d} D _{4h}	4
C ₃ S ₆	5
D ₃ C _{3v} D _{3d}	6
C ₆ C _{3h} C _{6h} D ₆ C _{6v} D _{3h} D _{6h}	7
T T _d T _h O O _h	8

How symmetry numbers are connected to the point symmetry of the crystal field of the R³⁺ ion.

What is the point symmetry of the rare earth ion ? Please type in the symmetry number, see table above (0-8) : 4

Example for a symmetry number of 4. The calculation of the crystal electric field will be valid for point symmetries of D_4 , C_{4v} , D_{2d} and D_{4h} .

The next input of FOCUS decides whether the rare earth moment is parallel to the +c-direction of the single crystal or not. The input defines the location of the quantization axis and has therefore no influence on the calculated transition energies, transition matrix elements and transition intensities. The only advantage is that it gives the easiest wavefunctions out.

If this question is answered by **yes** (or **y**) the calculation uses Stevens' operator-equivalents (stevens-operators) by default. The quantization axis will be +c.

What is the point symmetry of the rare earth ion ? Please type in the symmetry number, see table above (0-8) : 4

Shows the rare earth moment in the +c-direction [Y]? y

Example for a rare earth moment parallel to +c = [001].

In the case of no (or n) the user is asked for the Euler-angles α , β and γ . The Euler-angles determine the location of the rare earth moment relative to the crystallographic (single crystal) system with axes a b c. Now 3j-symbols are used by default for the calculation and the quantization axis is +z. The orientation of the axes x y z relative to a b c is defined by α , β and γ .

What is the point symmetry of the rare earth ion ? Please type in the symmetry number, see table above (0-8) : 4

Shows the rare earth moment in the +c-direction [Y]? n

Please give in now the Euler-angles (in units of degrees).

Euler-angle ALPHA [0=default]: 0

Euler-angle BETA [0=default]: -90

Euler-angle GAMMA [0=default]: -45

Example for a rare earth moment parallel to [110].

The following input asks (if possible) whether the real part or the

imaginary part of the crystal field parameter B_{kq} shall be chosen. Input a 0 for the real part or a 1 for the imaginary part.

```

Shows the rare earth moment in the +c-direction [Y]? y
-----
THE DEFINITION OF THE CRYSTAL FIELD HAMILTONIAN
-----

      \      ^      1 \      \      *      ^
H = > B  O (J) + --- > > B  O (J)
      /      k0  k0   2 /      /      kq  kq

-----
k=2,4,6          k=2,4,6  0>|q|>=0

-----
| S\B|2|0|2|1|22||40|41|42|43| 44||60|61|62|63|64|65|66||
|----|----|----|----|----|----|----|----|----|----|----|
| 4 |r| | ||r| | | |r||r| | | |r| | |
-----

B = Bkq-parameters and S = symmetry number
Used System : crystallographic system

A table which shows you which crystal field parameter is complex (c) or real(r)
for the given symmetry number of 4.

B(4,4) real (0) or imaginary (1) part [0=default]:
B(6,4) real (0) or imaginary (1) part [0=default]:

The CONTROL will now be given to MULT-FRILLS.

Type H <return> for a list of the available MULTI_FRILLS COMMANDS.
Type @ <return> for a list of the available FOCUS COMMANDS
Type D P <return> to DISPLAY the fitting parameters.
Type S P <return> to SET the fitting parameters.

Details of the fit are stored in SYSSCRATCH:FOCUS.LPT
Details of the crystal field are stored in SYSSCRATCH:FOCUS.CEF
Please wait ...

#
    
```

Example for a symmetry of 4. In both cases the real parts of the crystal field parameters are chosen.

The control of the program is then given to the program MULTI_FRILLS and after a short time the MULTI_FRILLS prompt # should appear. Type now **help** or **@focus** for a list of the available MULTI_FRILLS or FOCUS commands. Type **d p** to display the fitting parameters or **s p** if you want to set them. With **go** the calculation (fit) is started. FOCUS is finished by the **exit** command.

```
# d p
```

		Dataset 1		
		=====		
	Parameter set	P	Pmin	Pmax
1	0 Temperatur (Kelvin)	0.00000E+00		
2	0 Incoming Energy(meV)	0.00000E+00		
3	0 Detector angle	0.00000E+00		
4	0 Bkgd Constant	0.00000E+00		
5	0 Bkgd slope (meV-1)	0.00000E+00		
6	0 Elastic Intensity	0.00000E+00		
7	0 Elastic pos (meV)	0.00000E+00		
8	0 Elastic FWHM(meV)	0.00000E+00		
9	0 Inelastic FWHM (meV)	0.00000E+00		
10	0 Intensity factor	0.00000E+00		
11	0 B_ext(x) (Tesla)	0.00000E+00		
12	0 B_ext(y) (Tesla)	0.00000E+00		
13	0 B_ext(z) (Tesla)	0.00000E+00		
14	0 B_mol(x) (Tesla)	0.00000E+00		
15	0 B_mol(y) (Tesla)	0.00000E+00		
16	0 B_mol(z) (Tesla)	0.00000E+00		
17	0 Re B20 (meV)	0.00000E+00		
18	0 Re B40 (meV)	0.00000E+00		
19	0 Re B44 (meV)	0.00000E+00		
20	0 Re B60 (meV)	0.00000E+00		
21	0 Re B64 (meV)	0.00000E+00		

```
#
```

The fit parameters for a symmetry number of 4. The fitting parameters 1 to 16 do not depend on the selected symmetry number.

FOCUS Commands

This chapter describes all FOCUS commands which are available in the program package of Version 1.0. As is the case for MULTI_FRILLS, every command or keyword may be abbreviated by its first letter, optional parameters are surrounded by square brackets. Numerical values may be separated by spaces or commas. All FOCUS commands start with **@focus**. Each command is finished by the *<return>* key.

Help commands provided by FOCUS

<u>Command</u>	: @focus
<u>Abbreviation</u>	: @
<u>Action</u>	: Provides a help and the entry to all defined FOCUS commands. A user of FOCUS has either to know @focus or @ to have full access to all possible FOCUS commands.

```
# @focus
Possible FOCUS commands are:
@ Alter          - Alter Parameter
@ Display        - Display Angles, Cef symmetry, Degeneration, Excitations,
                  IOn R3+, INTensities, Level scheme, MAtrix elements,
                  MOment of R3+, Operator, Shape of excitations,
                  Wavefunctions
@ Help           - Help Alter, Display, Help, Info, Montecarlo, Set
@ Info           - Info Version
@ Montecarlo     - Monte-Carlo
@ Set            - Set Angles(Euler), Degeneration, Operator, Shape of line
Capital letters sign the minimal abbreviation.
Type @ HELP HELP for further informations.
#
```

For example, type **@ i v** to get an information about the version of FOCUS you are using now or type **@ a** to have an entry to all alter commands. In all cases there is a guide to help you through the FOCUS command language.

Command : **@focus help** or **help @focus**
Abbreviation : **@ h** or **h @**
Action : Both commands have the same action as **@focus**. The first command does what it says, it will give you a help on all defined FOCUS commands. Additionally, the second command shows more the fact that **@focus** is actually an additional MULTI_FRILLS command which has to be provided by a help.

Command : **@focus help help**
Abbreviation : **@ h h**
Action : This command prints out a help on the help command. It will show you how the help command should be used to get a help on the different FOCUS commands.

```
# @focus help help
@ HELP is possible on the following COMMANDS:
@ Help Alter      - Help provided on the ALTER  command
@ Help Display    - Help provided on the DISPLAY command
@ Help Help       - Help provided on the HELP   command
@ Help Info       - Help provided on the INFO   command
@ Help Montecarlo - Help provided on the MONTE  command
@ Help Set        - Help provided on the SET    command
Capital letters sign the minimal abbreviation.
#
```

For example, if you want to know what action the **@focus display** command has, type **@focus help display** or use the abbreviation **@ h d**.

Command : **@focus help alter**
Abbreviation : **@ h a**
Action : Provides a help on the **alter** command.

```
# @focus help alter
@ Alter Parameter [Bkq] - use the Bkq-parameter for fitting
                   [Vkq] - use the Vkq-parameter for fitting
                   [Xr] - use n-dimensional sphere parameter
Capital letters sign the minimal abbreviation.
#
```

If you want to alter from the Bkq-parameter scheme to the more sophisticated Vkq-parameter scheme which uses normalised operators for fitting then the command @ a p v will do this.

Command : @focus help display
Abbreviation : @ h d
Action : Provides a help on the display command.

```
# @focus help display
@ Display  Angles..... - list the Euler-angles of the R3+ moment
                   -> use @ s a to set the Euler-angles
          Cef symmetry..... - list the CEF point symmetry the calculation is for
          Degeneration..... - list if the degeneration flag is ON (degenerated
                   energy levels are combined) or OFF (degenerated
                   energy levels are NOT combined)
                   -> use @ s d to change the degeneration flag
          Excitations..... - list the calculated crystal field excitations
          IO..... - list the R3+ ion the calculation is for
          INTensities..... - list the CEF transition intensities between
                   CEF energy levels
          Level scheme..... - list the CEF level scheme (CEF transition
                   energies and CEF transition matrix elements for
                   a powdered sample)
          MAtrix elements.. - list the CEF transition matrix elements
          Moment R3+..... - list the calculated magnetic moment of R3+
          Operator..... - list if the calculation uses steven-operators (ON)
                   or 3j-symbols (OFF)
                   -> use @ s o to change the operator flag
          Shape..... - list the lineshape of a special excitation
                   -> use @ s s to change the lineshape
          Wavefunctions..... list the wave function of the R3+ ion
Capital letters sign the minimal abbreviation.
#
```

If you want to know what the excitations are then type @ display excitations or @ d e for short.

Command : @focus help info
Abbreviation : @ h i
Action : Provides a help on the info command.

```
# @focus help info
@ Info Version .....- prints out which version of FOCUS you have
Capital letters sign the minimal abbreviation.
#
```

Type @ i v to find out which FOCUS version is released to you.

Command : @focus help montecarlo
Abbreviation : @ h m
Action : Provides a help on the montecarlo command.

```
# @focus help montecarlo
@ Montecarlo [New] - Monte-Carlo on all parameters with finite boundaries.
[Display chi**2] - display all chi**2 values found by @ m n.
[Plot parameters] [n1 n2-n3 n4 ... ] - plot parameter sets defined
by @ m n over the neutron
data. n1, n2, ... are the
positions of the Chi**2
values in the Chi**2 list.
--> See @ m d.
[Load parameters] [n1] - load in a selected parameter set which
has been defined by @ m n. n1 is the
position of a Chi**2 value in the Chi**2
list.
--> See @ m d.
Capital letters sign the minimal abbreviation.
#
```

Type @ m n to start the Monte-Carlo simulation, type @ m d to display all found Chi**2 values lower than or equal to a given maximum of Chi**2, and for example to plot the calculated excitations of the first 20 parameter sets one after the other over the experimental neutron data type @ m p 1-20.

Command : @focus help set
Abbreviation : @ h s
Action : Provides a help on the set command.

```
# @focus help set
@ Set Angles          - set the Euler-angles alpha, beta and gamma
  Degeneration [OFF] - degenerated energy levels are't combined (default)
                  [ON] - degenerated energy levels are combined
  Operator   [OFF] - calculation uses 3j-symbols
                  [ON] - calculation uses steven-operators
  Shape [n1 n2-n3 n4 ...] - set a specified lineshape for a
                           specific excitation. n1, n2, ... are
                           numbers of excitations. See: @ d s
Capital letters sign the minimal abbreviation.
#
```

If you want to use 3j-symbols instead of Stevens' operator-equivalents for the crystal electric field calculation then type @ set operator off or use the abbreviation @ s o of. If you want to combine degenerated energy levels then use the command @ s d on. If you want to set the third and the tenth up to fifteenth excitation to another lineshape then input @ s s 3 10-15.

Alter command provided by FOCUS

Command : @focus alter
Abbreviation : @ a
Action : The entry to all alter commands.

```
# @focus alter
Alter what? Implemented are:
Parameter: p
Alter parameter to what? Implemented are:
Bkq, Vkq, Xr : v
#
```

The user is asked for an input. For altering the fitting parameters to the normalised Vkq-parameter, first type in p and then v .

Command : @focus alter parameter bkq
Abbreviation : @ a p b
Action : Alters the fitting parameters to the Bkq-parameter. You can check the kind of fitting parameters you are using by typing $d p$.

```
# @focus alter parameter bkq
#
```

To alter the fitting parameter to the Bkq-parameter scheme.

Command : @focus alter parameter vkq
Abbreviation : @ a p v
Action : Alters the fitting parameters to the normalised Vkq-parameter. See *The transformation to a normalised parameter scheme* in the Appendix to get a proper definition what is meant by this. Again, you can check the kind of fitting parameters you are actually using by typing $d p$.

```
# @focus alter parameter vkq
#
```

To alter the fitting parameter to the Vkq-parameter scheme.

Command : @focus alter parameter xr
Abbreviation : @ a p x
Action : Alters the fitting parameters to the (x,R)-parameter scheme. See *The n-dimensional spherical parameters* in the Appendix for a proper definition. The transformation affects only those parameters which have a parameter number greater or equal 11 and are not fixed. See page 17 for the definition of the parameter 1 to 10. Type **d p** to see which parameter will be transformed. In general, these are all magnetic field parameter (external and molecular) and all crystal electric field parameter. The transformation to the (x,R)-scheme will be successful if there is at least one free fitting parameter with a parameter number greater or equal 11. Otherwise an error message will be given out. The reason why only magnetic and crystal field parameter are affected by the spherical transformation is the following. All other parameters either mirror experimental conditions, are dictated by the resolution function or at least are found quickly and therefore will be fixed afterwards. In contrast to this, the work of FOCUS really lies in determining the magnetic and the crystal electric field parameters. Again, the kind of the actual fitting parameters might be checked by typing **d p**.

```
# @focus alter parameter xr
#
```

To alter the fitting parameter to the (x,R)-parameter scheme.

Set commands provided by FOCUS

Command : @focus set
Abbreviation : @ s
Action : The entry to all set commands.

```
# @focus set
Set what? Implemented are:
Angles(Euler), Degeneration, Operator, Shape of line : s
```

The user is asked for an input. For example, to set special lineshapes to specific excitations type *shape of line* or *s* only. If the message *ERROR: Excitation spectrum not yet determined* appears, fix all parameters (to make sure that they are not varied) and define the excitation spectrum by typing *go*.

Command : @focus set angles
Abbreviation : @ s a
Action : Sets the Euler-angles α , β and γ . The Euler-angles define how the crystal electric field and the external magnetic field will be rotated after the next *go* command. The molecular magnetic field is per definition parallel to the rare earth moment and therefore not influenced by the rotation defined above. The rotation operator and details of both rotations are listed in the Appendix.

```
# @focus set angles
The R3+ moment is canted compared to the crystal system (a,b,c)
by the Euler-angles.
Please give in now the Euler-angles (in units of degrees).
<return>-key only: old value will not be changed.
Euler-angle ALPHA : 0
Euler-angle BETA : -90
Euler-angle GAMMA : -45
```

The user is asked for the Euler-angles α , β and γ . Example for a rare earth moment parallel to [110].

Command : **@focus set degeneration on**
Abbreviation : **@ s d on**
Action : This flag influences the output of the energy levels, transition matrix elements, transition intensities and wavefunctions. All energy levels which are closer than 0.005 meV are assumed to be degenerated and are labeled by a degeneration index. The status of the degeneration flag can be checked by the command **@focus display degeneration** or by **@ d d**.

```
# @focus set degeneration on
#
```

To combine degenerated energy levels.

Command : **@focus set degeneration off**
Abbreviation : **@ s d of**
Action : This flag influences the output of the energy levels, transition matrix elements, transition intensities and wavefunctions. All energy levels which are closer than 0.005 meV are *not* assumed to be degenerated and are *not* labeled by a degeneration index. The status of the degeneration flag can be checked by the command **@focus display degeneration** or by **@ d d**.

```
# @focus set degeneration off
#
```

Do not combine degenerated energy levels.

Command : **@focus set operator on**
Abbreviation : **@ s o on**
Action : The crystal electric field is calculated by Stevens' operator-equivalents after the next **go** command. The status of the operator flag can be checked by the command **@focus display operator** or by **@ d o**.

```
# @focus set operator on
#
```

Choose Stevens' operator-equivalents for the next calculation.

Command : **@focus set operator off**
Abbreviation : **@ s o of**
Action : The crystal electric field is calculated by 3j-symbols operators after the next **go** command. The status of the operator flag can be checked by the command **@focus display operator** or by **@ d o**.

```
# @focus set operator on
#
```

Choose stevens-operators for the next calculation.

Command : **@focus set shape**
Abbreviation : **@ s s**
Action : Sets a lineshape to *all* positive excitations. The lineshape of a negative excitation is defined by the positive one. By default the lineshape of the quasi elastic line is **lorentzian*bosefactor** with the bosefactor $E*(1+n(E))$. E means energy transfer and $n(E)$ is the occupation factor of the bose statistic for a given temperature T, i.e. $n(E) = (e^{-E/T} - 1)^{-1}$. All other excitations (including the elastic line) have gaussian lineshape by default. Type **@focus display shape** or **@ d s** to see what the lineshapes of all positive excitations are. If a message **ERROR:**

Excitation spectrum not yet determined appears, fix all parameters and type **go**. **Remark:** also possible is e.g. **@ s s 1-3 5** to set the lineshape of specific excitations only (e.g. 1-3 and 5).

```
# @focus set shape 0-1
ERROR: Excitation spectrum not yet determined
# go
Do you wish to restore the old parameters [N]?
# @focus set shape 0-1
Give the excitation value. For its definition see: @ d s
INPUT BELOW is expected as follows:
  <return> : old value is not changed
  1 <return> : to choose GAUSSIAN shape
  2 <return> : to choose LORENTZIAN shape
  3 <return> : to choose LORENTZIAN*BOSEFACTOR shape
  0 : elastic line Gauss : 2
  1 : 0.00 meV 24.66 barn Lorentz*Bosefactor : 2
#
```

The lineshape of the elastic and quasi elastic line is set to lorentzian shape.

Info commands provided by FOCUS

Command : **@focus info**
Abbreviation : **@ i**
Action : The entry to all **info** commands.

```
# @focus info
Info what? Implemented are:
Version : v
You have FOCUS version: 1.0
#
```

The user is asked for an input. For example, if you want to show the version of FOCUS which is released to you, type *v*.

Display commands provided by FOCUS

Command : @focus display
Abbreviation : @ d
Action : The entry to all **display** commands.

```
# @focus display
Display what? Implemented are:
Angles, Cef symmetry, Degeneration, Excitations,
INtensities, IOn R3+, Level scheme, Operator, MAtrix elements,
MOment of R3+, Shape of lines, Wavefunctions : ma
```

The user is asked for an input. For example, to display the calculated matrix elements the user should type in *matrix elements* or *ma* only. If the message *ERROR: excitation spectrum not yet determined* appears, type **go**.

Command : @focus display angles
Abbreviation : @ d a
Action : Print out to the screen the values of the Euler-angles which are used in the calculation. Use **@focus set angles** to change the values.

```
# @focus display angles

The R3+ moment is canted compared to the crystal system (a,b,c)
by the following Euler-angles:
alpha   (Euler) =    0.00  degrees
beta    (Euler) =    0.00  degrees
gamma   (Euler) =    0.00  degrees

#
```

Output if all Euler-angles are zero.

Command : @focus display cef symmetry
Abbreviation : @ d c
Action : prints the point symmetry of the crystal electric field to the screen.

```
# @focus display cef symmetry  
  
point symmetry of crystal field | symmetry number  
D4 C4v D2d D4h ----- 4 -----  
  
#
```

Output for a symmetry number of 4.

Command : @focus display degeneration
Abbreviation : @ d d
Action : Shows the status of the degeneration flag.

```
# @focus display degeneration  
The degeneration flag is OFF.  
Degenerated energy levels are not combined!  
Use @ s d to change the degeneration flag.  
  
#
```

Output if the degeneration flag is off.

```
# @focus display degeneration  
The degeneration flag is ON.  
Degenerated energy levels are combined!  
Use @ s d to change the degeneration flag.  
  
#
```

Output if the degeneration flag on.

Command : @focus display excitations
Abbreviation : @ d e
Action : Shows all the calculated crystal electric field excitations. The excitations are ordered by increasing intensities. If a message *ERROR: Excitation spectrum not yet determined* appears, type **go**.

```
# @focus display ion

The calculation is for rare earth ion : Er3+

# @focus display cef symmetry

point symmetry of crystal field | symmetry number
D4 C4v D2d D4h ----- 4 -----

#
```

The calculation of the excitation spectrum will be for the rare earth ion Er3+ and for a point symmetry with symmetry number 4.

```
# display parameter
Dataset 1
=====
Parameter set          P          Pmin          Pmax
1 0 Temperatur (Kelvin) 4.5000          Fixed
2 0 Incoming Energy(meV) 15.000          Fixed
3 0 Detector angle      20.000          Fixed
4 0 Bkgd Constant       0.10000         Fixed
5 0 Bkgd slope (meV-1)  0.00000E+00     Fixed
6 0 Elastic Intensity    51.910          Fixed
7 0 Elastic pos (meV)    0.10000E-01     Fixed
8 0 Elastic FWHM(meV)   0.43270         Fixed
9 0 Inelastic FWHM (meV) 0.43270         Bound to parameter 8
10 0 Intensity factor    1.7309          Fixed
11 0 B_ext(x) (Tesla)    0.00000E+00     Fixed
12 0 B_ext(y) (Tesla)    0.00000E+00     Fixed
13 0 B_ext(z) (Tesla)    0.00000E+00     Fixed
```

Continued on next page.

14	0	B_mol(x)	(Tesla)	0.00000E+00	Fixed
15	0	B_mol(y)	(Tesla)	0.00000E+00	Fixed
16	0	B_mol(z)	(Tesla)	0.00000E+00	Fixed
17	0	Re B20	(meV)	-0.14000E-01	Fixed
18	0	Re B40	(meV)	-0.12000E-03	Fixed
19	0	Re B44	(meV)	0.31000E-03	Fixed
20	0	Re B60	(meV)	0.59000E-06	Fixed
21	0	Re B64	(meV)	0.29000E-04	Fixed
#					

The above fit parameters are used for the calculation below.

```
# @focus display excitations
ERROR: Excitation spectrum not yet determined
# go
Do you wish to restore the old parameters [N]?
# @focus display excitations

The sample temperature is : 4.50 Kelvin
Energy levels which are closer than 0.06 Kelvin are assumed to be degenerated.
Only those excitations are printed out whose intensities are greater or
equal 0.01 barn. The excitations are ordered by decreasing intensities.

1 : 0.00 meV 24.66 barn Lorentz*Bosefactor
2 : 2.83 meV 11.87 barn Gauss
3 : 0.41 meV 7.59 barn Gauss
4 : 3.92 meV 3.88 barn Gauss
5 : -0.41 meV 2.66 barn Gauss
6 : 9.46 meV 1.52 barn Gauss
7 : 7.22 meV 1.42 barn Gauss
8 : 10.83 meV 0.60 barn Gauss
9 : 9.05 meV 0.53 barn Gauss
10 : 3.51 meV 0.44 barn Gauss
11 : 8.17 meV 0.23 barn Gauss
12 : 2.42 meV 0.21 barn Gauss
13 : 10.43 meV 0.02 barn Gauss
14 : 7.76 meV 0.02 barn Gauss

#
```

The calculated excitation spectrum of Er³⁺ at a temperature of 4.5 Kelvin for the parameter settings given above.

Command : @focus display intensities
Abbreviation : @ d in
Action : Shows for a given temperature the energy levels of the crystal electric field and the transition matrix elements for a powdered sample. Whether the degenerated energy levels of the crystal field are combined or not depends on the status of the degeneration flag. Type @ d d to display the status of the degeneration flag. Use @ s d to change it. If a message *ERROR: Excitation spectrum not yet determined* appears, type go.

```
# @focus set degeneration on
# @focus display intensities
```

THE CALCULATED ENERGY LEVELS

```
1 :      0.00 meV Degeneration : 2-fold
2 :      0.41 meV Degeneration : 2-fold
3 :      2.83 meV Degeneration : 2-fold
4 :      3.92 meV Degeneration : 2-fold
5 :      7.63 meV Degeneration : 2-fold
6 :      8.17 meV Degeneration : 2-fold
7 :      9.46 meV Degeneration : 2-fold
8 :     10.83 meV Degeneration : 2-fold
```

FOR POWDER MEASUREMENTS

The transition intensities $I(i \rightarrow k)$ in barn.
temperature : 4.50 Kelvin.

	1	2	3	4	5	6	7	8	
1	15.53	7.59	11.87	3.88	0.00	0.23	1.52	0.60	41.24
2	2.66	9.12	0.21	0.44	1.42	0.02	0.53	0.02	14.42
3	0.01	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.03
4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Continued on next page.

6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

With $\text{const} := 4\pi \cdot (1/2 \cdot r_0 \cdot g_j)^2$ we may write :

$$I(i-k) = \text{const} \cdot \exp(-E(i)/T) / Z(T) \cdot |\langle i | j | t | k \rangle|^2.$$

For each row the sum of the columns is equal to:

$$2/3 \cdot j \cdot (j+1) \cdot \text{const} \cdot \exp(E(i)/T) / Z(T).$$

Summing additionally over all rows, we get the total scattered magnetic intensity to :

$$2/3 \cdot \text{const} \cdot j \cdot (j+1): 55.70 \text{ barn.}$$

#

The calculated crystal electric field energy levels and transition intensities of Er³⁺ at a temperature of 4.5 Kelvin. The parameter settings are described in the command explanation of **@focus display excitation**.

Command : **@focus display ion r3+**

Abbreviation : **@ d io**

Action : Displays for which rare earth ion R³⁺ the crystal electric field calculation is for.

@focus display ion r3+

The calculation is for rare earth ion : Er³⁺

#

The calculation is for Er³⁺.

Command : @focus display level scheme
Abbreviation : @ d l
Action : Shows for a given temperature the energy levels of the crystal electric field and the transition matrix elements for a *powdered* sample. Whether the degenerated energy levels of the crystal field are combined or not depends on the status of the degeneration flag. Type @ d d to display the status of the degeneration flag. Use @ s d to change it. If a message *ERROR: Excitation spectrum not yet determined* appears, type go.

```
# @focus set degeneration on
# @focus display level scheme
```

THE CALCULATED ENERGY LEVELS

```
1:      0.00 meV Degeneration : 2-fold
2:      0.41 meV Degeneration : 2-fold
3:      2.83 meV Degeneration : 2-fold
4:      3.92 meV Degeneration : 2-fold
5:      7.63 meV Degeneration : 2-fold
6:      8.17 meV Degeneration : 2-fold
7:      9.46 meV Degeneration : 2-fold
8:     10.83 meV Degeneration : 2-fold
```

FOR POWDER MEASUREMENTS

The transition matrix elements $|<ij|t|k>|^2$

	1	2	3	4	5	6	7	8	
1	32.01	15.65	24.46	8.00	0.01	0.48	3.14	1.25	85.00
2	15.65	53.74	1.24	2.59	8.39	0.11	3.14	0.14	85.00
3	24.46	1.24	14.68	23.81	3.24	14.73	0.50	2.33	85.00
4	8.00	2.59	23.81	29.66	5.07	4.26	8.46	3.14	85.00
5	0.01	8.39	3.24	5.07	24.83	24.75	19.74	2.97	85.00
6	0.48	0.11	14.73	4.26	24.75	24.21	2.51	17.94	85.00
7	3.14	3.14	0.50	8.46	19.74	2.51	22.33	25.19	85.00

Continued on next page.

```
8 1.25 0.14 2.33 3.14 2.97 17.94 25.19 32.06 85.00
```

The sum of each row I is : $2/3*j*(j+1)*n_i$
 n_i is the degeneration of the energy level i
 which belongs to the row I. See above : THE
 CALCULATED ENERGY LEVELS for the
 convention of labeling of the energy levels.

```
#
```

The calculated crystal electric field energy levels and transition matrix elements for a powdered sample of Er³⁺ at a temperature of 4.5 Kelvin. The parameter settings are described in the command explanation **@focus display excitation**.

Command : **@focus display matrix elements**

Abbreviation : **@ d ma**

Action : Shows for a given temperature the energy levels of the crystal electric field and the transition matrix elements for a *single crystal* and a *powdered* sample. Whether the degenerated energy levels of the crystal field are combined or not depends on the status of the degeneration flag. Type **@ d d** to display the status of the degeneration flag. Use **@ s d** to change it. If a message *ERROR: Excitation spectrum not yet determined* appears, type **go**.

```
# @focus set degeneration on
# @focus display matrix elements
```

```
-----
THE CALCULATED ENERGY LEVELS
-----
```

```
1 :      0.00 meV Degeneration : 2-fold
2 :      0.41 meV Degeneration : 2-fold
3 :      2.83 meV Degeneration : 2-fold
4 :      3.92 meV Degeneration : 2-fold
5 :      7.63 meV Degeneration : 2-fold
```

Continued on next page.

6: 8.17 meV Degeneration : 2-fold
 7: 9.46 meV Degeneration : 2-fold
 8: 10.83 meV Degeneration : 2-fold

FOR SINGLE CRYSTAL MEASUREMENTS

The transition matrix elements $|\langle ijx|k\rangle|^{**2}$

	1	2	3	4	5	6	7	8	
1	15.59	11.74	7.12	6.00	0.01	0.09	2.35	0.20	43.10
2	11.74	0.00	0.93	0.02	6.20	0.08	0.28	0.10	19.36
3	7.12	0.93	10.40	17.86	2.43	1.86	0.37	1.44	42.41
4	6.00	0.02	17.86	22.11	2.28	3.20	5.36	2.36	59.20
5	0.01	6.20	2.43	2.28	2.34	15.56	13.44	2.23	44.49
6	0.09	0.08	1.86	3.20	15.56	15.60	1.88	1.57	39.85
7	2.35	0.28	0.37	5.36	13.44	1.88	0.37	18.89	42.94
8	0.20	0.10	1.44	2.36	2.23	1.57	18.89	21.84	48.63

The transition matrix elements $|\langle iljy|k\rangle|^{**2}$

	1	2	3	4	5	6	7	8	
1	15.59	11.74	7.12	6.00	0.01	0.09	2.35	0.20	43.10
2	11.74	0.00	0.93	0.02	6.20	0.08	0.28	0.10	19.36
3	7.12	0.93	10.40	17.86	2.43	1.86	0.37	1.44	42.41
4	6.00	0.02	17.86	22.11	2.28	3.20	5.36	2.36	59.20
5	0.01	6.20	2.43	2.28	2.34	15.56	13.44	2.23	44.49
6	0.09	0.08	1.86	3.20	15.56	15.60	1.88	1.57	39.85
7	2.35	0.28	0.37	5.36	13.44	1.88	0.37	18.89	42.94
8	0.20	0.10	1.44	2.36	2.23	1.57	18.89	21.84	48.63

The transition matrix elements $|\langle iljz|k\rangle|^{**2}$

	1	2	3	4	5	6	7	8	
1	16.84	0.00	22.46	0.00	0.00	0.53	0.00	1.47	41.29
2	0.00	80.61	0.00	3.83	0.17	0.00	4.15	0.00	88.77
3	22.46	0.00	1.23	0.00	0.00	18.37	0.00	0.61	42.41
4	0.00	3.83	0.00	0.26	3.05	0.00	1.96	0.00	9.10
5	0.00	0.17	0.00	3.05	32.56	0.00	2.73	0.00	38.51
6	0.53	0.00	18.37	0.00	0.00	5.12	0.00	23.76	47.79
7	0.00	4.15	0.00	1.96	2.73	0.00	32.77	0.00	41.62
8	1.47	0.00	0.61	0.00	0.00	23.76	0.00	4.40	30.24

Continued on next page.

 FOR POWDER MEASUREMENTS

The transition matrix elements $|\langle ij|t|k\rangle|^2$

	1	2	3	4	5	6	7	8	
1	32.01	15.65	24.46	8.00	0.01	0.48	3.14	1.25	85.00
2	15.65	53.74	1.24	2.59	8.39	0.11	3.14	0.14	85.00
3	24.46	1.24	14.68	23.81	3.24	14.73	0.50	2.33	85.00
4	8.00	2.59	23.81	29.66	5.07	4.26	8.46	3.14	85.00
5	0.01	8.39	3.24	5.07	24.83	24.75	19.74	2.97	85.00
6	0.48	0.11	14.73	4.26	24.75	24.21	2.51	17.94	85.00
7	3.14	3.14	0.50	8.46	19.74	2.51	22.33	25.19	85.00
8	1.25	0.14	2.33	3.14	2.97	17.94	25.19	32.06	85.00

The sum of each row I is : $2/3*j*(j+1)*n_i$
 n_i is the degeneration of the energy level i
 which belongs to the row I. See above : THE
 CALCULATED ENERGY LEVELS for the
 convention of labeling of the energy levels.

#

The calculated crystal electric field energy levels and transition matrix elements for a single crystal or powdered sample of Er³⁺ at a temperature of 4.5 Kelvin. The parameter settings are described in the command explanation **@focus display excitation**.

Command : **@focus display operator**

Abbreviation : **@ d o**

Action : Shows the status of the operator flag.

@focus display operator

The operator flag is OFF.

The hamiltonian is calculated by 3j-symbols!

Use @ s o to change the operator flag.

#

Output if the operator flag is off.

```
# @focus display operator
The operator flag is ON
The hamiltonian is calculated by steven-operators!
Use @ s o to change the operator flag.
#
```

Output if the operator flag is on.

Command : @focus display moment
Abbreviation : @ d mo
Action : Shows the calculated rare earth moment for a given temperature. The position of the magnetic moment within the x-, y- and z-axis depends on the values of the three Euler-angles α , β and γ . The z-axis is always the axis of quantization. The easiest wavefunctions will be achieved for a z-axis lying on the magnetic moment. If a message *ERROR: Excitation spectrum not yet determined* appears, type **go**.

```
# @focus display moment
```

```
mx = 9.00 myb
my = 0.00 myb
mz = 0.00 myb
```

The R3+ moment in units of the full measurable R3+ moment $m_r = g_j \cdot m_y b \cdot j$

```
mx/mr= 100.00%
my/mr= 0.00%
mz/mr= 0.00%
```

```
if we choose: mx = m*sin(theta)*cos(phi)
              my = m*sin(theta)*sin(phi)
              mz = m*cos(theta)
```

Continued on next page.

we find:

```

m= 9.00 myb   theta = 90.00   phi = 0.00

```

The x-, y- and z-axes are defined by the Euler-angles alpha, beta and gamma
Type @ d a to show what values they have.

#

The full magnetic moment of Er³⁺ is in x-direction for a magnetic field in x-direction and vanishing crystal field parameters. The Euler-angles α , β and γ are all zero.

Command : @focus display wavefunctions

Abbreviation : @ d w

Action : Shows the calculated wavefunctions of the rare earth ion. Remarkable is however that the easiest wavefunctions are achieved for a quantization axis (z-axis) lying parallel to the magnetic moment. Type @ d mo to find out what position the magnetic moment in the (x y z) frame has. For a non vanishing moment set the Euler-angles α , β and γ to reasonable values.

Whether the degenerated energy levels of the crystal field are combined or not depends on the status of the degeneration flag. Type @ d d to display the status of the degeneration flag. Use @ s d to change it. If a message *ERROR: Excitation spectrum not yet determined* appears, type go.

```
# @focus display wavefunctions
```

```
-----  
THE CALCULATED WAVEFUNCTIONS  
-----
```

```
! 1 1> = 1.000 + 0.000*i !-7.5>
```

```
! 2 1> = 1.000 + 0.000*i !-6.5>
```

Continued on next page.

```

! 3 1> = 1.000 + 0.000*i !-5.5>
! 4 1> = 1.000 + 0.000*i !-4.5>
! 5 1> = 1.000 + 0.000*i !-3.5>
! 6 1> = 1.000 + 0.000*i !-2.5>
! 7 1> = 1.000 + 0.000*i !-1.5>
! 8 1> = 1.000 + 0.000*i !-0.5>
! 9 1> = 1.000 + 0.000*i ! 0.5>
!10 1> = 1.000 + 0.000*i ! 1.5>
!11 1> = 1.000 + 0.000*i ! 2.5>
!12 1> = 1.000 + 0.000*i ! 3.5>
!13 1> = 1.000 + 0.000*i ! 4.5>
!14 1> = 1.000 + 0.000*i ! 5.5>
!15 1> = 1.000 + 0.000*i ! 6.5>
!16 1> = 1.000 + 0.000*i ! 7.5>

```

```
#
```

The wavefunctions of Er^{3+} for a magnetic field in [010]-direction and vanishing crystal field parameters. The magnetic moment has the same direction as the magnetic field. If the Euler-angles are chosen to $\alpha=0^\circ$, $\beta=-90^\circ$ and $\gamma=0^\circ$ then the quantization axis will be the b-axis and the wavefunctions are the pure Zeeman levels.

Remark: read $(a+b*i) ! n>$ for $a+b*i ! n>$.

Command : @focus display shape of lines
Abbreviation : @ d s
Action : Shows the lineshapes of the excitations. Only those excitations with positive transition energy are shown. The excitations are ordered by ascending energies. If a message *ERROR: Excitation spectrum not yet determined* appears, type *go*.

```
# @focus display shape of lines
ERROR: Excitation spectrum not yet determined
# go
Do you wish to restore the old parameters [N]?
# @focus display shape of lines

The sample temperature is : 4.50 Kelvin
Energy levels which are closer than 0.06 Kelvin are assumed to be degenerated.
Only those excitations are printed out whose intensities are greater or
equal 0.01 barn.
Excitations with negative energies are not printed out.
The lineshape of a negative excitation is determined by the positive one.
The excitations are ordered by ascending energies.

0 : elastic line          Gauss
1 : 0.00 meV  24.66 barn  Lorentz*Bosefactor
2 : 0.41 meV   7.59 barn   Gauss
3 : 2.42 meV   0.21 barn   Gauss
4 : 2.83 meV  11.87 barn   Gauss
5 : 3.51 meV   0.44 barn   Gauss
6 : 3.92 meV   3.88 barn   Gauss
7 : 7.22 meV   1.42 barn   Gauss
8 : 7.76 meV   0.02 barn   Gauss
9 : 8.17 meV   0.23 barn   Gauss
10 : 9.05 meV  0.53 barn   Gauss
11 : 9.46 meV  1.52 barn   Gauss
12 : 10.43 meV 0.02 barn   Gauss
13 : 10.83 meV 0.60 barn   Gauss

#
```

The calculated excitation spectrum of Er³⁺ at a temperature of 4.5 Kelvin. For the parameter settings look to **@focus display excitations**.

Monte-Carlo commands provided by FOCUS

The Monte-Carlo commands provided by FOCUS should help to find reasonable starting parameters if there are none existing by physical reasons or other measurements. Actually, the FOCUS command **@focus montecarlo new** (or **@ m n**) generates random values of all those parameters which have been previously limited by a lower and an upper limit. Remember that the MULTI_FRILLS command **limit [n1 n2-n3 ...]** (or **l [n1 n2-n3 ...]**) supports this task. In addition make sure that all parameters which should be varied by Monte-Carlo are not fixed. If so, use the MULTI_FRILLS command **clear parameter** (or **c p [n1 n2-n3 ...]**) to free those parameters you are interested in. After typing **@ m n** the user is asked for the number of Monte-Carlo steps and for the maximum χ^2 which should be considered. FOCUS 1.0 will store the best 100 parameter sets which are ordered by ascending χ^2 values and labeled by their position in the χ^2 - list. If you want to display the χ^2 values which have actually been found by Monte-Carlo, use the **@focus montecarlo display** (or **@ m d**) command. A quick view how those parameter sets fit to the experimental neutron data is achieved by the **@focus montecarlo plot [n1 n2-n3 ...]** (or **@ m p [n1 n2-n3 ...]**) command. If you are interested in a special Monte-Carlo parameter set for further fitting, you can load the parameter set by typing **@focus montecarlo load [n1]** (or **@ m l [n1]**).

How does the Monte-Carlo simulation work in detail? All limited parameters are transformed to angles with values between $[0, \pi]$. These angles are then varied randomly. For more details see *Appendix: Monte-Carlo on n parameters with finite boundaries*.

If you have no idea what the limits of the magnetic field or crystal field parameters might be, it is recommended by the author to alter to the (x,R)-parameter scheme (see *Appendix: The n-dimensional spherical parameters*) first. Use the **@focus alter parameter xR** (or **@ a p x**) command. As this transformation will affect the magnetic

field and crystal electric field parameters only, make sure that at least one of those parameters are not fixed. If the transformation to the (x,R)-parameter scheme is successful, the n unlimited parameters will be transformed to n-1 x_i parameters with finite boundaries of -1 and 1, and one unlimited R parameter which represents the over-all-splitting of the excitation spectrum. After some Monte-Carlo runs it is not difficult to get a feeling what the upper and the lower limit of the R parameter is.

Command : **@focus montecarlo**
Abbreviation : **@ m**
Action : An entry to all **montecarlo** commands.

```
# @focus montecarlo
Which Monte-Carlo command do you want to use? Implemented are:
New, Display chi**2, Load parameters, Plot parameters : 1
Enter below the number of the Monte-carlo-set you want to load.
REMARK: The number of the Monte-Carlo-sets are displayed by @ m d.
Which set do you want to load [1=default]? 1
#
```

After calling the entry command **@focus montecarlo** (or **@ m**), the user is asked for a further specification what Monte-Carlo command he wants to use. In the example above the command **@focus montecarlo load** (or **@ m 1**) command was called by choosing *1* for *load*.

Command : **@focus montecarlo new**
Abbreviation : **@ m n**
Action : Starts a Monte-Carlo on all free and limited parameters. FOCUS 1.0 will store the 100 best parameter sets.

```
# @focus montecarlo new
Enter the number of Monte-Carlo steps [100=default]: 10
Enter the maximum value of Chi**2 [100=default]: 50
The following parameters will be varied by Monte-Carlo:
Re V20 : R (meV) [ 5.0000 , 15.0000 ]
Re V40 :x2 [ -1.0000 , 1.0000 ]
Re V44 :x3 [ -1.0000 , 1.0000 ]
Re V60 :x4 [ -1.0000 , 1.0000 ]
Re V64 :x5 [ -1.0000 , 1.0000 ]
Monte-Carlo starts on 19 :25 :34

2. Monte-Carlo Step Chi**2 = 14.2
3. Monte-Carlo Step Chi**2 = 15.0
4. Monte-Carlo Step Chi**2 = 39.0
5. Monte-Carlo Step Chi**2 = 13.9
6. Monte-Carlo Step Chi**2 = 18.4

Monte-Carlo starts on 19 :25 :34
Monte-Carlo ends on 19 :25 :40
Do you wish to store the best Monte-Carlo parameters [Y]?
#
```

After calling the Monte-Carlo command **@focus montecarlo new** (or **@ m n**), the user is asked for the number of Monte-Carlo steps and for the maximum of χ^2 which should be considered.

Command : **@focus montecarlo display chi**2**
Abbreviation : **@ m d**
Action : Displays the χ^2 - values which have been found by **@focus montecarlo new**.

```
# @focus montecarlo display chi**2
Enter the maximum value of Chi**2 [100=default]: 16
  1. stored Monte-Carlo Chi**2 is      13.9
  2. stored Monte-Carlo Chi**2 is      14.2
  3. stored Monte-Carlo Chi**2 is      15.0
#
```

The Monte-Carlo command **@focus montecarlo display chi**2** or (**@ m d**) is used for displaying all parameter set numbers up to a χ^2 - value of 16.0. In this example there are only three parameter sets which fulfill this restriction. The parameter set number are 1-3, respectively.

Command : **@focus montecarlo load [n1]**
Abbreviation : **@ m l [n1]**
Action : Loads the n1-th parameter set in the actual parameter table. Use the MULTI_FRILLS command **display parameters** (or **d p**) to check that the parameter set has been loaded. To find an appropriate parameter set number n1 use the FOCUS command **@focus montecarlo display chi**2** (or **@ m d**).

```
# @focus montecarlo load 5
#
```

The Monte-Carlo command **@focus montecarlo load 5** loads the fifth parameter set to the actual parameter table.

Command : @focus montecarlo plot [n1 n2-n3 n4 ...]
Abbreviation : @ m p [n1 n2-n3 n4 ...]
Action : Choose the n1-th, n2-th to n3-th, n4-th, ... parameter sets found by Monte-Carlo and plot the calculated excitation spectra over the experimental neutron data. This command is designed for having a quick view on the Monte-Carlo sets. Actually, the command will not change the actual parameter table. If you want to load a special parameter set in, use the FOCUS command @focus montecarlo load [n1] (or @ m l [n1]).

```
# @focus montecarlo plot 1-4
Enter min energy [ 0.0]:
Enter max energy [ 67.0]: 20
Enter min intensity [ 0.0]:
Enter max intensity [ 300.0]: 600
...
...
#
```

Plot the calculated excitation spectra of the first four Monte-Carlo parameter sets over the experimental neutron data.

MULTI_FRILLS Commands

This section gives only a short survey over the possible MULTI_FRILLS commands because a MULTI_FRILLS manual will be available soon. The word MULTI_FRILLS stands for MULTIPLE Fitting of Results Interactively by Least Squares and allows therefore a simultaneously fitting of multiple spectra. FOCUS Version 1.0 does not support multiple spectra fitting. Type **help** (or just **h**) at the # prompt to show all the implemented MULTI_FRILLS commands.

help

Possible commands are:

- Help - Help provided on each command
- Display - Display Data, Parameters, Calculation, Fit or Matrix
- Input - Input parameters from file
- Output - Output Parameters, Calculation or Fit to a disk file
- Use - Use specified dataset in subsequent commands
- Plot - Plot Data, Calculation, Fit, Residuals or Over
- Keep - Store previous plot in a disk file
- Modify - Modify data points
- Remove - Remove data points
- Set - Set parameters
- Fix - Fix parameters
- Bind - Bind two parameters together in fits
- Clear - Clear fixed Parameters or modified Data
- Limit - Limit parameters
- Alter - Alter fitting constants and output characteristics
- Title - Set plot points
- Go - Fit function to data
- Jump - Issue DCL command or spawn DCL sub-process
- Exit - exit from routine
- @focus - FOCUS defined commands

Each command may be abbreviated by the first letter

Type **Help** followed by the command for further information

#

You will find no description of the command **@focus** in the MULTI_FRILLS manual, because it has been defined by FOCUS itself to have an entry to FOCUS defined commands.

References

R Osborn, *FRILLS: an interactive Least-Square Fitting Package*, Rutherford Appleton Laboratory report RAL-91-011, January 1991

R Osborn and T G Perring, *MULTI_FRILLS :an interactive Least-Square Fitting Package*, Rutherford Appleton Laboratory preprint, March 1995

Appendix

The hamiltonians used in FOCUS

FOCUS calculates the crystal electric field in two different ways. The first method uses Stevens' operator-equivalents while the second method applies 3j-symbols. However, both methods should give exact the same result. Implementation of both provides therefore an easy check of the CEF calculation. The total hamiltonian \hat{H} is a sum of three terms

$$\hat{H} = \hat{H}_{CEF} + \hat{H}_{EXT} + \hat{H}_{MOL}$$

$$\hat{H}_{EXT} = \mu_B \cdot g_J \cdot \mathbf{B}_{EXT} \cdot \hat{\mathbf{J}}$$

$$\hat{H}_{MOL} = 2 \cdot \mu_B \cdot (g_J - 1) \cdot \mathbf{B}_{MOL} \cdot \hat{\mathbf{J}} .$$

\hat{H}_{EXT} and \hat{H}_{MOL} are magnetic field contributions due to an external and a molecular magnetic field coupling to the total angular momentum \mathbf{J} of a rare earth 3+ ion. The following crystal electric field hamiltonian \hat{H}_{CEF} is used in Stevens' operator-equivalent notation

$$\langle JM | \hat{H}_{CEF} | JM' \rangle = \sum_{k=2,4,6} B_{k0} \cdot \langle JM | \hat{O}_{k0}(\mathbf{J}) | JM' \rangle + \frac{1}{2} \sum_{k=2,4,6} \sum_{\substack{q=-k \\ q \neq 0}}^k B_{kq}^* \cdot \langle JM | \hat{O}_{kq}(\mathbf{J}) | JM' \rangle$$

where the B_{kq} are complex crystal field parameters and the $\hat{O}_{kq}(\mathbf{J})$ are the full Stevens' operator-equivalents. The sum over q only takes those values which are not forbidden by the point symmetry of the rare earth ion. In the notation of 3j-symbols the crystal electric field hamiltonian \hat{H}_{CEF} has a different form

$$\langle JM | \hat{H}_{CEF} | JM' \rangle = \sum_{k=2,4,6} \sum_q D_{kq}^* \cdot (-1)^{J-M} \cdot \begin{pmatrix} J & k & J \\ -M & q & M' \end{pmatrix} \cdot \langle J || \hat{C}_k(\mathbf{J}) || J \rangle.$$

Again the D_{kq} are complex crystal field parameters and the sum over q is taken over all values between $-k$ and k which are not forbidden by the point symmetry of the rare earth ion. Both the D_{kq} and the B_{kq} are connected via the equations

$$\begin{aligned} B_{k0} &= D_{k0} \cdot \epsilon_{k0} \cdot \omega_{k0} & \text{for } q = 0 \\ B_{kq} &= 2 \cdot D_{kq} \cdot \epsilon_{kq} \cdot \omega_{kq} & \text{for } q \neq 0 \end{aligned}$$

and the reduced matrix elements is

$$\langle J || \hat{C}_k(\mathbf{J}) || J \rangle = \frac{1}{2^k} \cdot \sqrt{\frac{(2J+k+1)!}{(2J-k)!}}.$$

References

For the definition of the full Stevens' operator-equivalents $\hat{O}_{kq}(\mathbf{J})$ and the constants ϵ_{kq} and ω_{kq} look to (and references therein) :

P Hoffmann, *Generalization of Stevens' operator-equivalent method*, J. Phys. A: Math. Gen. **24** (1991) 35-44

The calculation of 3j-symbols is described in:

A Lindner, *Drehimpulse in der Quantenmechanik*, Teubner Studienbuecher Physik, Stuttgart 1984, ISBN 3-519-03061-6, page 39 ff

M Rotenberg, *The 3j and 6j Symbols*, Cambridge, MA: MIT Press 1959

The rotation of the crystal electric field hamiltonian

The crystal electric field hamiltonian in the fixed crystallographic (single crystal) system with the axis a b c may be written to

$$\hat{H} = \sum_{k,q} F_{kq}^* \cdot \hat{C}_{kq}$$

where both the F_{kq} , the multiple moments of the crystal electric field (i.e. crystal field parameters) and the \hat{C}_{kq} which are tensor operators of order k, are defined in the fixed crystallographic system of the single crystal. A Rotation

$$\hat{R}(\alpha\beta\gamma) = \exp(-i \cdot \alpha \cdot \hat{\mathbf{J}}_c) \cdot \exp(-i \cdot \beta \cdot \hat{\mathbf{J}}_b) \cdot \exp(-i \cdot \gamma \cdot \hat{\mathbf{J}}_a)$$

of the crystal electric field hamiltonian by the three Euler-angles α , β and γ yields new crystal field parameters F'_{kq} and new tensor operators \hat{C}'_{kq}

$$\hat{R}(\alpha\beta\gamma) \cdot \hat{H} \cdot \hat{R}(\alpha\beta\gamma)^{-1} = \hat{H}' = \sum_{k,q'} F'_{kq'}^* \cdot \hat{C}'_{kq'}$$

The $F'_{kq'}$ are now the multiple moments of the crystal electric field in the rotated system with the axis x y z. They are connected to the F_{kq} by the equation

$$F'_{kq'}^* = \sum_{q=-k}^k F_{kq}^* \cdot D_{q'q}^{(k)}(\alpha\beta\gamma)$$

For the rotation matrix $D_{q'q}^{(k)}(\alpha\beta\gamma)$ the following equation holds

$$D_{q'q}^{(k)}(\alpha\beta\gamma) = \exp(-i \cdot \alpha \cdot q') \cdot d_{q'q}^{(k)}(\beta) \cdot \exp(-i \cdot \gamma \cdot q)$$

where the reduced functions $d_{q'q}^{(k)}(\beta)$ can be calculated by

$$d_{q'q}^{(k)}(\beta) = \sqrt{\frac{(k+q')!(k-q')!}{(k+q)!(k-q)!}} \\ \times \sum_n (-1)^{k-q-n} \binom{k-q}{n} \binom{k+q}{k-q'-n} \cos^{2n+q'+q} \frac{\beta}{2} \sin^{2k-2n-q-q'} \frac{\beta}{2}$$

with n fulfilling $\max\{0, -(q+q')\} \leq n \leq \min\{k-q, k-q'\}$. Pay attention to the fact that $d_{q'q}^{(k)}(0)$ is the Kronecker delta function $\delta_{q'q}$.

For a crystal field spitting within one J -multiplet the tensor operator \hat{C}_{kq} of rank k is equal to $\theta_k \cdot \hat{C}_{kq}(\mathbf{J})$. Where $\hat{C}_{kq}(\mathbf{J})$ is an operator-equivalent and the θ_k are the operator-equivalent factors θ_2, θ_4 and θ_6 well known as the Stevens' factors α_J, β_J and γ_J . Stevens' operator-equivalent $\hat{O}_{kq}(\mathbf{J})$ and the $\hat{C}_{kq}(\mathbf{J})$ are connected by $\hat{C}_{kq}(\mathbf{J}) = \varepsilon_{kq} \cdot \omega_{kq} \cdot \hat{O}_{kq}(\mathbf{J})$.

References

A Lindner, *Drehimpulse in der Quantenmechanik*, Teubner Studienbuecher Physik, Stuttgart 1984, ISBN 3-519-03061-6, page 39 ff

H A Buckmaster, R Chatterjee, and Y H Shing, *phys. stat. sol. (a)* **13**, (1972) page 9 ff

The rotation of the external magnetic field hamiltonian

FOCUS rotates simultaneously the external magnetic field and the crystal electric field hamiltonian. The molecular magnetic field is assumed to be parallel to the spin moment and therefore is not influenced by any rotation. The hamiltonian for the external magnetic field can be written to the form

$$\hat{H}_{EXT} = \mu_B \cdot g_J \cdot \left[B_{EXT}^Z \cdot \hat{J}^Z + \frac{1}{2} \left(B_{EXT}^+ \cdot \hat{J}^- + B_{EXT}^- \cdot \hat{J}^+ \right) \right].$$

The components of the external magnetic field and the total angular momentum operator are based in the fixed crystallographic (single crystal) system with axis a b c. Now the following identity holds between the total angular momentum operator \hat{J} and a tensor operator \hat{V}_{1q} of rank one

$$\begin{aligned} \hat{V}_{10} &= \alpha \cdot \hat{J}^Z \\ \hat{V}_{1,\pm 1} &= \mp \frac{\alpha}{\sqrt{2}} \cdot \hat{J}^{\pm} \end{aligned}$$

and the constant α is equal to

$$\alpha = \sqrt{\frac{3}{J(J+1)(2J+1)}}.$$

The reduced matrix element $\langle J || \hat{V}_1 || J \rangle$ is by definition $\sqrt{3}$. Rewriting of the hamiltonian in the tensor operator scheme gives

$$\begin{aligned} \hat{H}_{EXT} &= \mu_B \cdot g_J \cdot \sum_q M_{1q} \cdot \hat{V}_{1q} \\ M_{1,\pm 1} &= \mp \frac{1}{\alpha \sqrt{2}} B_{EXT}^{\mp} \\ M_{10} &= \frac{1}{\alpha} B_{EXT}^Z \end{aligned}$$

A rotation of the hamiltonian leads to new tensor operators of rank one with different magnet field components M'_{1q}

$$\hat{R}(\alpha\beta\gamma) \cdot \hat{H}_{EXT} \cdot \hat{R}(\alpha\beta\gamma)^{-1} = \hat{H}'_{EXT} = \mu_B \cdot g_J \cdot \sum_q M'_{1q} \cdot \hat{V}'_{1q}.$$

They are calculated by

$$M'_{1q} = \sum_{q'=-1}^1 M_{1q'} \cdot D_{q'q}^{(1)}(\alpha\beta\gamma).$$

The external magnetic field has in the rotated system the values

$$B'_{EXT} = \pm \alpha \cdot \sqrt{2} \cdot M'_{1,\mp 1}$$

$$B^z_{EXT} = \alpha \cdot M'_{10}$$

The transformation to a normalised parameter scheme

The idea of a normalised parameter scheme is that FOCUS varies a parameter set where all parameter are comparable in size. This is achieved if the hamiltonian has the form

$$\hat{H} = \hat{H}_{CEF} + \hat{H}_{EXT} + \hat{H}_{MOL}$$

$$\hat{H}_{CEF} = \sum_{k=2,4,6} V_{k0} \cdot \frac{\hat{O}_{k0}(\mathbf{J})}{\|\text{Re}(\hat{O}_{k0}(\mathbf{J}))\|} + \frac{1}{2} \sum_{k=2,4,6} \sum_{\substack{q=-k \\ q \neq 0}}^k V_{kq}^* \cdot \frac{\hat{O}_{kq}(\mathbf{J})}{\|\text{Re}(\hat{O}_{kq}(\mathbf{J}))\|}$$

$$\hat{H}_{EXT} = V_{EXT}^Z \cdot \frac{J^Z}{\|J^Z\|} + V_{EXT}^+ \cdot \frac{J^-}{\|J^-\|} + V_{EXT}^- \cdot \frac{J^+}{\|J^+\|}$$

$$\hat{H}_{MOL} = V_{MOL}^Z \cdot \frac{J^Z}{\|J^Z\|} + V_{MOL}^+ \cdot \frac{J^-}{\|J^-\|} + V_{MOL}^- \cdot \frac{J^+}{\|J^+\|}$$

It is not difficult to find out how these new parameters are related to the old ones and is left as an exercise for the reader. However, the normalisation of the full Stevens' operator-equivalents are consistent in the following sense. The crystal electric field hamiltonian may be written to

$$\hat{H}_{CEF} = \sum_{k=2,4,6} V_{k0} \cdot \frac{\hat{O}_{k0}(\mathbf{J})}{\|\text{Re}(\hat{O}_{k0}(\mathbf{J}))\|} + \sum_{k=2,4,6} \sum_{q>0} \text{Re}(V_{kq}) \frac{\text{Re}(\hat{O}_{kq}(\mathbf{J}))}{\|\text{Re}(\hat{O}_{kq}(\mathbf{J}))\|} + \text{Im}(V_{kq}) \frac{\text{Im}(\hat{O}_{kq}(\mathbf{J}))}{\|\text{Re}(\hat{O}_{kq}(\mathbf{J}))\|}$$

and in fact the equation

$$\|\text{Re}(\hat{O}_{kq}(\mathbf{J}))\| = \|\text{Im}(\hat{O}_{kq}(\mathbf{J}))\|$$

holds. The normalisation by the real part of the full Stevens' operator- equivalents ensures a consistent way of normalisation

for all possible point symmetries. The norm used by FOCUS is defined by

$$\|\hat{A}\|^2 = \sum_{M=-J}^J \sum_{M'=-J}^J \frac{|\langle JM|\hat{A}|JM'\rangle|^2}{2J+1}$$

for an arbitrary operator \hat{A} .

The n-dimensional spherical parameters

The components V_1, \dots, V_n ($n \geq 1$) are assumed to be free and real fitting parameters. FOCUS identifies the V_1, \dots, V_n with the normalised parameter mentioned in the last section. The transformation to spherical parameters is done by the equations

$$\begin{aligned}
 V_1 &= R \sin \varphi_n \sin \varphi_{n-1} \sin \varphi_{n-2} \cdots \sin \varphi_3 \sin \varphi_2 \\
 V_2 &= R \sin \varphi_n \sin \varphi_{n-1} \sin \varphi_{n-2} \cdots \sin \varphi_3 \cos \varphi_2 \\
 V_3 &= R \sin \varphi_n \sin \varphi_{n-1} \sin \varphi_{n-2} \cdots \cos \varphi_3 \\
 &\vdots \\
 V_{n-2} &= R \sin \varphi_n \sin \varphi_{n-1} \cos \varphi_{n-2} \\
 V_{n-1} &= R \sin \varphi_n \cos \varphi_{n-1} \\
 V_n &= R \cos \varphi_n
 \end{aligned}$$

If the radius R is chosen in the way that it can either be positive or negative, then the $n-1$ angles $\varphi_2, \dots, \varphi_n$ have values between 0° and 180° , only. It follows that $\sin \varphi_i$ is always positive and $\cos \varphi_i$ covers all values between -1 and 1 . The sign of R is equal to the sign of V_1 while R itself is equal to $\|V\|_n$. Here the i -th norm is defined by

$$V := (V_1, \dots, V_n)$$

$$\forall_{i=1 \dots n} \|V\|_i := \sqrt{\sum_{k=1}^i V_k^2}$$

The radius R is therefore

$$R = \text{sign}(V_1) \cdot \|V\|_n$$

and the $n-1$ angles $\varphi_2, \dots, \varphi_n$ are determined by

$$\forall_{i=2 \dots n} \cos \varphi_i = \frac{V_i}{\|V\|_i} \cdot \text{sign}(R) \quad \wedge \quad \sin \varphi_i = \frac{\|V\|_{i-1}}{\|V\|_i}$$

$\|V\|_i \neq 0$

By the last equations we can define x_i variables by

$$\forall_{\substack{i=2 \dots n \\ \|\mathbf{V}\|_i \neq 0}} x_i := \cos \varphi_i = \frac{V_i}{\|\mathbf{V}\|_i} \cdot \text{sign}(R) \in [-1,1].$$

The transformation has now the form

$$\begin{aligned} V_1 &= R \sqrt{1-x_n^2} \sqrt{1-x_{n-1}^2} \sqrt{1-x_{n-2}^2} \cdots \sqrt{1-x_3^2} \sqrt{1-x_2^2} \\ V_2 &= R \sqrt{1-x_n^2} \sqrt{1-x_{n-1}^2} \sqrt{1-x_{n-2}^2} \cdots \sqrt{1-x_3^2} x_2 \\ V_3 &= R \sqrt{1-x_n^2} \sqrt{1-x_{n-1}^2} \sqrt{1-x_{n-2}^2} \cdots x_3 \\ &\vdots \\ V_{n-2} &= R \sqrt{1-x_n^2} \sqrt{1-x_{n-1}^2} x_{n-2} \\ V_{n-1} &= R \sqrt{1-x_n^2} x_{n-1} \\ V_n &= R x_n \end{aligned}$$

But, what happens if there exists an i_0 with $\|\mathbf{V}\|_{i_0} = 0$? Let i_0 be the first value with vanishing norm and let i_1 be the first value with non vanishing norm $\|\mathbf{V}\|_{i_1} \neq 0$. By the last equation on the left page we get

$$x_{i_1} = \frac{V_{i_1}}{\|\mathbf{V}\|_{i_1}} \cdot \text{sign}(R) \quad \wedge \quad \sqrt{1-x_{i_1}^2} = \frac{\|\mathbf{V}\|_{i_1-1}}{\|\mathbf{V}\|_{i_1}} = 0 \quad \Rightarrow \quad x_{i_1} = \text{sign}(V_{i_1}) \cdot \text{sign}(R).$$

For all $i_0 \leq i < i_1$ the x_i can be set to an arbitrary value. FOCUS set those x_i to zero

$$\forall_{i_0 \leq i < i_1} x_i = 0.$$

Monte-Carlo on n parameters with finite boundaries

First of all FOCUS brings all limited parameters to the same scale. Suppose the case of $n \geq 1$ limited parameters $p_i^{\min} \leq p_i \leq p_i^{\max}$ with $i=1 \dots n$ and given finite boundaries p_i^{\min} and p_i^{\max} . The following linear transformation f_i which acts on each limited parameter p_i separately

$$f_i: [p_i^{\min}, p_i^{\max}] \rightarrow [-1, 1]$$

$$p_i \rightarrow f_i(p_i) = \frac{2}{p_i^{\max} - p_i^{\min}} \cdot p_i - \frac{p_i^{\min} + p_i^{\max}}{p_i^{\max} - p_i^{\min}}$$

defines new parameters $f_i(p_i)$ with the finite boundaries -1 and 1. It is therefore possible to define angles $\varphi_i \in [0, \pi]$ by

$$\cos \varphi_i := f_i(p_i).$$

Here, the cosine function ensures that the x_i - parameters of the last chapter and the limited parameters p_i mentioned above have all the same functional dependence to the angles φ_i . In fact, for a x_i - parameter we find

$$\cos \varphi_i = f_i(x_i) = \frac{2}{1 - (-1)} \cdot x_i - \frac{1 + (-1)}{1 - (-1)} = x_i.$$

What is nothing else than the definition of the angles φ_i of the last chapter. We end up with having $n \geq 1$ angles φ_i with $\varphi_i \in [0, \pi]$ which have to be varied randomly between 0 and π .

FOCUS uses a random number generator which generates numbers between 0 and 1. Next, one has to decide whether a component should be varied or not and which value it should be given. FOCUS does both in a single step by choosing two random numbers r_1 and r_2 for each angle φ_i . If r_1 and r_2 are both lower than or equal to 0.5 then the angle φ_i is varied and the value is $\varphi_i = 0.5 \cdot \pi \cdot (r_1 + r_2 + 1)$. If r_1 and r_2 are both greater than 0.5,

again the angle φ_i will be varied and the value is $\varphi_i = 0.5 \cdot \pi \cdot (r_1 + r_2 - 1)$. In the two other cases where r_1 and r_2 do not share the same region, the angle φ_i stays on the old value and is not changed at all. The possibility of changing the angle φ_i is therefore 50%.