MIBEMOL
Graphical representation, data reduction and/or treatment.

Table of content

Recall: *How to recover and install the software.*
(on the site « http://www-llb.cea.fr/Phocea/Page/index.php?id=21 »)

- After loading of "Fitmib data treatment suite.zip"

- Set the content of the .zip file, that is to say the directory "\mibemol_dat" with every file inside, directly under a root.

  > Ex : « C:\mibemol_dat »

- Inside the directory "\mibemol_dat\tdvmib\data", include all the run files you'll need later on.

  > Ex : « C:\mibemol_dat\tdvmib\data\d21758.nxs
  > \d21759.nxs
  > ..…………….. »

Note : If necessary, the intermediate files as « d21758.nxs1, d21758.nxs2, ….. » must be set in the directory « \mibemol_dat\tdvmib\dpro ». They can be visualized with '*visnex.exe*'.

Running the data treatment software

All programs are inside the directory « \mibemol_dat » as executable files (.exe). They can be run:
- either by click on their icons
- or " RUN " in the start menu :
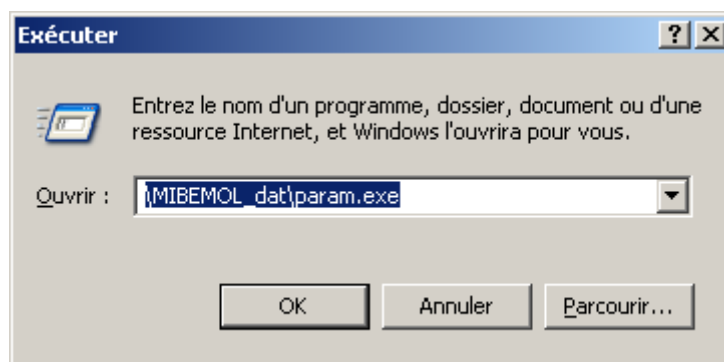
How to use the programs

List of existing programs

NAME	USE
param	Reading of the experimental parameters (user table)
grpnrj	Data reduction, grouping and save of file I (θ,ω)
evolux	Evolution with time of the data acquisition: compare intermediate runs
teknex	Graphical representation of the data (one run only)
visnex	Simultaneous representation of runs or ''intermediate runs''(dyyyyy.nxsj)
window	Integrated intensity over an energy window (ω_1,ω_2): evolution of $\mathbf{I}(\theta)$
elscat	Analysis of an « elastic scan »
densix	Getting the frequency distribution g (ω)
fitrun_theta	Fit of the θ constant scattering intensity to an analytic curve
fitrun_q	Getting $\lvert Q \rvert$ constant scattering intensity; then, fit to an analytic curve

* not available yet

These programs allow either:
- To visualize, on a chosen scale, after normalization and reduction the experimental data.
- To get, through various methods, numerical values of some physical parameters which are assumed to produce the main interactions in the scattering function $S(Q,\omega)$.

They all are 'interactive' that means they ask questions.

Program structure

***Input*:**
The asked run numbers are those of data measured by "Mibemol" and stored either in the directory « **\mibemol_dat\tdvmib\data** » (final run) or « **\mibemol_dat\tdvmib\dpro** » (intermediate run). They all are in the "**Nexus file format**".
    Ex **: \mibemol_dat\tdvmib\data\ dxxxxx.nxs** *where xxxxx is the run number (5 digits)*

***Output*:**
Graphical output uses the **PGPLOT** library.
Save of all the numerical results are in text file format (.txt)
Save of all graphical representation are in postscript file format (.ps)

All programs start by a reduction of the raw data. At first, series of question asks the run(s) number(s), the grouping of detectors that has to be made and point out different options.

Nota bene *: excepted very few case, all programs use the same numerical logic :*

*« **Run** »*
If the final data is obtained from one single run, type is number (5 digits)
*If it is obtained from an addition of several runs, type **each run number** with comma between:*

Example: 12220,12221,12225 (sum of 3 runs)

*« **Grouping** »*
In order to increase the statistic, one often whish to sum the data obtained by several detectors :
    - If they are located side by side (block of detectors) give the number of first and last column (comma between).
    - If the sum has to be made on non adjacent blocks (for instance, in order to eliminate column(s) located in a Bragg peak direction), give the number of first and last column of the first block, then first and last column of the second block, ... (comma between).
Example :
        - 25,42 (sum over all detectors from column 25 to 42, bounds included)
        - 25, 31,34,42 (sum from column 25 to 31 and from 34 to 42, bounds still included)

The program asks for :
- "sample run number": it is the main run ; it contains the parameter which are to be measured.
- "empty container" : the sample is usually enclosed in a container which scattering can be subtracted. If sample and empty container has not been measured at the same temperature, a correction based on a phonon Debye model is proposed.
- "check sample" : The scattering of some reference sample, chosen because very similar to the main sample but without the searched component (ex : phonon contribution in a dynamical magnetic measurement; solvent contribution in a two components system; ....).

Beware *: because of "self shielding" corrections, results from*
    [(sample-container) – (check sample – container)] and[(sample – container)]
     are not equivalent.

- "normalization" : All experimental data scattering are normalized to a common monitor level (10^6 counts). Inside one run, the groups of detector (one detector is in fact the column set at angle θ) can be normalized among themselves for elastic

scattering detector efficiency and surface detection, if a vanadium scattering has been measured. If not, intensity scattering are bring back to one single column.

Method : *Within the same grouping of detector than for the sample, one calculate the integrated intensity beneath the elastic peak of the vanadium run.**

$$J_{elast}(k) = \sum_{\pm\sigma} I_k(n) \; ; \; \sigma = \text{calculated résolution}$$

The group k_0 showing maximal intensity is chose as reference : $J_{max} = J(k_0)$.
The other groups (k) are normalized among this one by multiplying its intensity by a factor ($J_{max} / J(k)$.).

- Data correction

- Taking in account the characteristics of "Mibemol" detectors, final data are **always** corrected for the detection efficiency variation with energy of the scattered neutron at energy *E*

$$\sigma_{abs} \# 1/\sqrt{E}$$

- The program propose a shielding correction.

For a plane geometry (parallelepipedic container) this correction is "exact" : self-shielding of the scattering from the content and shielding from the container.
For a cylindrical geometry, shielding from the walls of the container is not considered.
If this correction is asked, you will have to answer questions on the geometry and the neutron scattering characteristic (absorption and scattering) of the sample and it's container.

Beware *: absorption and scattering length must be given as "mean free path" in cm^{-1} unit.*

$$l_{abs} = \sum_{i} \left[n_i \times (\sigma_{abs})_i \right]$$

$$l_{diff} = \sum_{i} \left[n_i \times (\sigma_{diff})_i \right]$$

n_i = number, per unit volume, of i type nucleus (cm^{-3})
($\sigma_{abs})_i$ = i type nucleus absorption cross section (cm^{-2}) (for neutron of V = 2200 m/s)
($\sigma_{scatt})_i$ = i type nucleus total scattering cross section (cm^{-2}) [($\sigma_{scatt})_i$ = ($\sigma_{cohf})_i$ + ($\sigma_{incohf})_i$]

Few final remarks

- For each question where one option is no (0), <*return*> only is OK.
- Before ending, most programs propose to redo the calculation with an other run. Assumption is then made that the data reduction is identical (for instance same vanadium run) and the question is skipped. If not true, you must end the program and restart it.

Program details

param

Reading of the experimental parameters *(user table)*
Reading of a data file content *(or result of a grouping)*

For any run, this program reads and write on the computer screen the parameter (neutron characteristics, sample environment, time and monitor counting, ….) and the raw data as stored in the data file for a single or a grouping of detectors. Indeed nexus file are not directly readable.

Direction for use

langue, language: francais (fr) ou english (en)? *en*
USER table (rep=1) or data file (rep = 2) ? *1*
run number ? *17352*
   User table for run 17352
sample name ====> blg (h/D) 0.46 D20 T =270K
user name ======> Zanotti
container ======>
monitor (1.e6 neutrons) :   0.4415
time counting (second) :   21599
Asked temperature (K) :   267.90
TOF delay (musec) :   1801
TOF channel width (musec) : 17.4
wavelength (Angstrom) :   5.20
sample angle (d°) :   135.00
frequency chopper 1 (rpm): 9999
frequency chopper 2 (rpm): 3333
frequency chopper 4 (rpm): 3333
number of used detectors : 84
Position of detectors :
 0.00 23.50 24.80 26.10 27.50 36.50 37.59 38.69 40.16 41.27
 42.38 43.87 44.99 46.11 47.62 48.76 52.20 53.36 54.53 56.09
 57.27 58.45 60.04 61.25 62.46 63.67 64.90 67.79 69.05 69.89
 71.59 72.44 73.88 75.47 76.35 77.68 79.01 79.92 84.04 85.44
 86.39 87.82 89.27 90.25 91.73 92.73 94.24 95.26 96.81 98.92
 99.99 101.62 102.72 103.84 104.96 106.11 107.85 108.44 110.24 110.85
112.69 115.24 116.54 117.87 119.22 120.60 121.30 122.73 124.19 125.69
126.45 128.01 131.26 132.11 132.97 134.73 135.64 136.57 138.48 139.46
141.48 141.51 143.67 147.16 0.00 0.00 0.00 0.00 0.00 0.00
other file (yes = run number , no =0) ? *0*

grpnrj

After a preliminary phase for data reduction and grouping of detectors, this program change into energy unit the time of flight data.

Method

In channel n, we found the number [$\mathbf{I}(Q, t_n)$] of neutrons which have been detected in one detector during a time interval δt around $t_n = n\Delta$ (the neutron pulse is supposed to leave the sample at time 0; Δ is the channel width). It represents the number of neutrons whose "time of flight", that is the time take for covering the distance L between sample and detector, has change from t_{n_0} (n_0 = elastic channel number) to t_n after being scattered in the sample.

Using together the relations between energy E_n and velocity v_n for these neutrons :

$$E_n = \frac{1}{2}mv_n^2 = \frac{1}{2}m\frac{L^2}{t_n^2} \quad \blacktriangleright \quad \delta E_n = \left(\frac{dE}{dt}\right)_{t_n} \delta t = -mL^2 \frac{\delta t}{t_n^3}$$

and between intensity and scattering cross section :

$$\mathbf{I}(Q, t_n) = \frac{k_n}{k_0}\left(\frac{d^2\sigma}{d\Omega\, dt}\right) = \left(\frac{t_0}{t_n}\right)\left(\frac{t_0}{t_n}\right)^3 \left(\frac{d^2\sigma}{d\Omega\, d\omega}\right)_n$$

we get for a sample at temperature T (classical statistic) :

$$\widetilde{S}(Q, \omega_n) = \left(\frac{t_n}{t_0}\right)^4 \mathbf{I}(Q, t)$$

$$S(Q, \omega_n, T) = \exp\left[-\frac{1}{2}\left(\frac{\hbar\omega_n}{kT}\right)\right]\widetilde{S}(Q, \omega_n)$$

Result

For each grouping, the final result is saved in a text format file. Its pathname is **\mibemol_dat\tdvmib\grpnrj\dxxxxx\kyyy** where xxxxx is the sample run number and yyy a file serial number.

Each file is a 6 columns and 512 lines table:

channel number	Energy transfer	$\widetilde{S}(Q,\omega)$	$\Delta\widetilde{S}(Q,\omega)$	$S(Q,\omega,T)$	$\Delta S(Q,\omega,T)$
…..					
j	ω_j	$\widetilde{S}(Q,\omega_j)$	$\Delta\widetilde{S}(Q,\omega_j)$	$S(Q,\omega_j,T)$	$\Delta S(Q,\omega_j,T)$
…..					

Direction for use

langue, language: francais (fr) ou english (en)? en
grouping and/or subtraction of spectra
to treat: standard(0), personal(1) ' or single detector grouping(1)? 0
Sample
run(s) number(s)? 17352
an empty box to subtract
(yes=run(s) number, interpolation=-1, no=0)? 17347
do you wish to correct for self shielding (yes=1, no=0)? 0
do you want to subtract a spectrum (yes=run(s) number, no=0)? 0
do you wish normalization to vanadium(yes=1,no=0)? 1
run(s) number(s)? 17343
same empty box to subtract (yes=1, no=0)? 1
saved on \mibemol_dat\tdvmib\grpnrj\d17352\k001
saved on \mibemol_dat\tdvmib\grpnrj\d17352\k002
saved on \mibemol_dat\tdvmib\grpnrj\d17352\k003
saved on \mibemol_dat\tdvmib\grpnrj\d17352\k004
saved on \mibemol_dat\tdvmib\grpnrj\d17352\k005
saved on \mibemol_dat\tdvmib\grpnrj\d17352\k006
saved on \mibemol_dat\tdvmib\grpnrj\d17352\k007
saved on \mibemol_dat\tdvmib\grpnrj\d17352\k008
saved on \mibemol_dat\tdvmib\grpnrj\d17352\k009
saved on \mibemol_dat\tdvmib\grpnrj\d17352\k010
saved on \mibemol_dat\tdvmib\grpnrj\d17352\k011
saved on \mibemol_dat\tdvmib\grpnrj\d17352\k012
an other case (yes=1,no=0)?

evolux
Time evolution of data acquisition
"part runs" : graphical representation of their integrated intensity

With this program, one can detect a counting rate variation during one total run time acquisition and thus, the possible appearance of a non wanted effect. Indeed, the use of the spectrometer allows to cut up the total counting time in "slices" (generally of 1 hour). At the end of each its counting result is, on one hand, saved and on the other hand add to the total counting already stored. By following the evolution of the integrated (over time of flight) intensity of these "part runs" one can see if a change has come out during the run time.

Direction for use

The pathname file of the "part runs" is made with the five digits number (xxxxx) of the run plus an extension 1, 2, 3, ….,j , ….. (that is file ….\dxxxxx.nxsj) according to their rank in the total time measuring interval.

- One can compare among themselves all the "part run" (then answer: [0,0])or only some of them (answer: [j,j'] being the numbers of the first and last "part run" to compare.
- Evidently, this comparison makes sense only if each "part run" is normalised to a common monitor count (reactor power change, cold source efficiency, possible "interrupt", …..); nevertheless if the actual monitor count is to low (now less than 100) the statistical error on this number becomes higher than the other relevant terms. In such case, in order to avoid appearance of a false anomaly, there is no normalisation to monitor.

langue, language: francais (fr) ou english (en)? en
evolution with time, run number ? 21721
which is your detector grouping
(for details, make <return>)? 2,84
\MIBEMOL_dat\tdvmib\dpro\d21721.nxs1
\MIBEMOL_dat\tdvmib\dpro\d21721.nxs2
...
\MIBEMOL_dat\tdvmib\dpro\d21721.nxs16
there is 16 partial runs, 'which do you want ?
give first and last (0,0 = all of them) 0
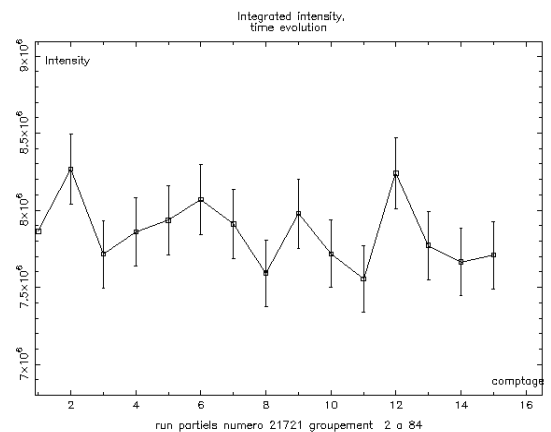*Run partiel N° 1 Monit= 0.00048*
Run partiel N° 2 Monit= 0.00046
………………………………………
Run partiel N° 15 Monit= 0.00047
partial N° 16 CAUTION : monitor to low, no normalization
other scale (yes=1, no=0)? 0

N.B. As explained above this application compute the total intensity (Σ over all channels) counted in a detector (or a group of). If necessary, it can be easily transform in order to compute the time evolution over a given energy interval of the scattering function $S(Q,\omega)$ (dynamical experiment).

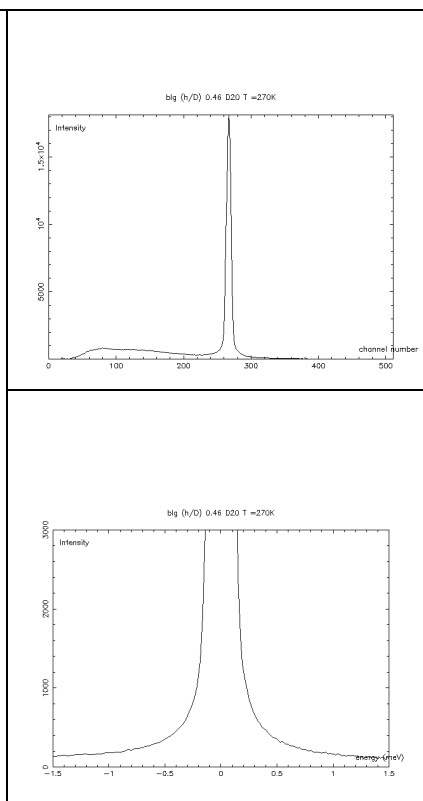**back to**: *List of existing programs*

teknex

Graphical representation of the data for one or a grouping of detectors.

This program visualize the content of **a single file** (one curve). It allows to see the effect of various reduction (grouping, subtraction, normalization, …) and correction on data of a run. It offers also the possibility to detect small details which might be more difficult to see with other graphical representation. We hardly recommend to use it before any fitting program (choice of the grouping, optimisation of the fitting interval, choice of the most significant analytic representation, ……).

At last, it is a fast and easy way to visualize the state of the run in progress

Direction for use

langue, language: francais (fr) ou english (en)? en
VISUALISATION of data
sub-run = data from a (series of) detector; run = sigma(s/run)
*   Sample*
run(s) number(s)? 17352
an empty box to subtract
(yes=run(s) number, interpolation=-1, no=0)? 17347
do you wish to correct for self shielding (yes=1, no=0)? 0
do you want to subtract a spectrum (yes=run(s) number, no=0)? 0
which is your detector grouping (for details, make <return>)? 60,84
do you want to subtract a constant number (value or no=0)?
Lambda= 5.2 A; Theta=128.7deg; Q0=2.178A-1; T= 267.9 K
channel (0) or energy (1) scale? 0
automatic scale (rep=0),or chosen(rep=1)?
other scale (yes=1,no=0)?1
channel (0) or energy (1) scale? 1
Bose factor (yes=1,no=0)? 0
automatic scale (rep=0),or chosen(rep=1)? 1
minimum de x= -20.00 maximum de x=   2.19
minimum de y= 0.21556E-08 maximum de y= 0.18155E+05
xmin, xmax ? -1.5,1.5
ymin, ymax ? 0,3000
other scale (yes=1,no=0)?
paper output (yes = 1 ; no = 0) ? 1
saved in file \MIBEMOL_dat\tdvmib\teknex\d17352\graph.ps/PS
an other case (yes=1,no=0)?

.

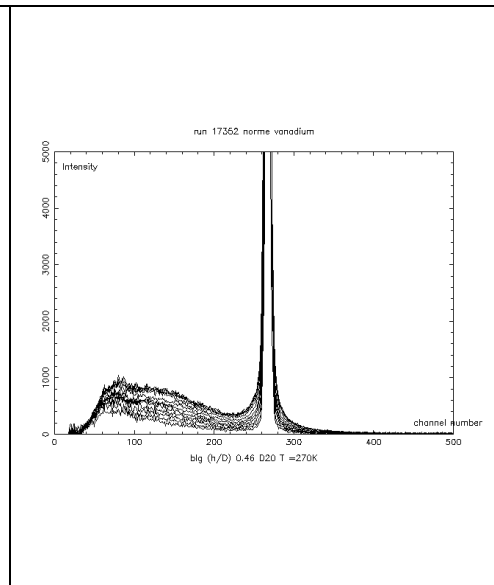
back to: *List of existing programs*

visnex
Graphical comparison of different run or grouping
Time evolution (from part run xxxxx.nexk)

By superposition of many curves on a same graphic, this program allows to compare among themselves several data file. It can be the result in various groups of detectors for one run or in one specific group for several runs. Also, using the "part run" saved at fixed time interval during the data acquisition, it detect any evolution with time for a particular run. When time evolution is not concerned, several data reduction (grouping, subtraction, normalization) and correction are proposed. Evidently, the data processing asked for the first run will be automatically used for the others. For instance, if you chose a self-shielding correction and compare different runs, it will be apply to all with the same parameter (geometry, scattering and absorption lengths).

- Normalisation must always occurs when comparing different grouping for one run: either from a "vanadium" run if exists, or if not, only by reducing the data to one single column (the coefficient is 1 for the smallest number of column).
- The 'automatic grouping' option gives 12 groups which are then visualised:
  2,5 ; 6,10 ; 11,15 ; 16,20 ; 21,25 ; 26,35 ; 36,45 ; 46,55 ; 56,64 ; 65,72 ; 73,78 ; 79,84

Direction for use

langue, language: francais (fr) ou english (en)? en
VISUALISATION of several runs
compare different grouping (0) or different runs (1) ? 0
        Sample
run(s) number(s)? 17352
an empty box to subtract
(yes=run(s) number, interpolation=-1, no=0)? 17347
 do you wish to correct for self shielding (yes=1, no=0)? 0
do you want to subtract a spectrum (yes=run(s) number, no=0)? 0
standard(0), perso(1) grouping? 0
Vanadium for normalization ; run(s) number(s)? 17343
vanadium box to subtract (yes=run number, no=0)?
 channel (0) or energy (1) scale? 0
automatic scale (rep=0),or chosen(rep=1)? 1
minimum de x=   0.00maximum de x= 511.00
minimum de y=-0.16865E+03maximum de y= 0.21675E+05
xmin, xmax ? 0,500
ymin, ymax ? 0,5000
other scale (yes=1,no=0)?

back to: *List of existing programs*

window

Integrated intensity over the [ω₁, ω₂] energy change interval

$I(\vartheta_j,[\omega_1, \omega_2]) \Leftrightarrow I(\vartheta_j,[n_1, n_2])$

(ω = neutron energy change; n = connected channel number

For any neutron energy change interval [ω₁, ω₂] (± according to neutron energy gain (-) or loss (+)) , this program compute the total number of neutron scattered in one (or a group of) detectors set in the ϑ_j direction. The energy change interval can be prescribe either in energy unit (meV) or by the channel numbers which collect the neutrons with final energy $E_0 + \omega$. In both cases it calculates :

$$I(\vartheta_j,[n_1,n_2]) = \sum_{i=n_1}^{n_2} I(\vartheta_j, n_i)$$

n₁, n₂, channel numbers corresponding to energy transfer [ω₁, ω₂]
ϑ_j = scattering angle (one or grouped detector)

This calculation is made after subtraction (if wanted) of a container and/or a reference sample, vanadium normalisation and shielding corrections. The result is shown in a graphical form and numerical values can be printed.

Notes
- Reduction and correction are made on the raw data. The integration over the energy interval comes only after.
- The vanadium normalisation is not mandatory (answer **0** to *spectrum number*); then results shall be normalise to constant detectors number (coefficient 1 for the group with the largest number of detectors)
- In order to get the angular variation of the elastic scattering choose option "*energy window*" (answer **1**) and **0** when asked "*energy transfer, min, max*" (caution: here this **0** is not equivalent to a "return"). The program computes $\Sigma_{E_0-\delta, E_0+\delta}$ where E_0 is the neutron incident energy and $\delta = 3\ \sigma$ (σ^2 calculated quadratic error of the elastic resolution).
- In order to get the angular variation of the integrated intensity, choose option "*channel window*" (answer **0**) and then ask for the total channel interval (**1, 512**).

Direction for use

langue, language: francais (fr) ou english (en)? en
  I=f(theta) pour omega=+- delta (omega)
to treat : ' standard grouping(0) or personal grouping(1)? 0
        Sample
run(s) number(s)? 17352
an empty box to subtract
(yes=run(s) number, interpolation=-1, no=0)? 17347
 do you wish to correct for self shielding (yes=1, no=0)? 0
do you want to subtract a spectrum (yes=run(s) number, no=0)? 0
Vanadium for normalization ; 17343
vanadium box to subtract (yes=run number, no=0)? 0
window in channel(rep=0) or energy(rep=1) unit? 1
 min, max of energy transfer (neutron energy: +=lost; -=gain) ?-
2.5,2.5
caution (omega+hwhm) out of the table
---
spectre17352 (norme moniteur)
monit data= 0.44147E+06 monit "tampon"= 0.00000E+00
somme sur energie de -2.50, 2.50 mev ; canaux 203 a 511 ;
*omega -2.50, 2.*

2	3	4	5	6	7	8
146789	90990	154277	167407	188459	194152	197874

9	10	11	12	13
203042	209608	226466	220367	215603

*abscise: column(rep=0), angle(rep=1) Q(rep=2), Q**2(rep=3)? 3*
other graph (yes=1, no=0) ? 0
change the window (yes=1, no=0)? 1
window from channel(rep=0) or energy(rep=1)? 1
 min, max of energy transfer (neutron energy: +=lost; -=gain) ?-
1,1
---
spectre17352 (norme moniteur)
monit data= 0.44147E+06 monit "tampon"= 0.00000E+00
somme sur energie de -1.00, 1.00 mev ; canaux 237 a 333 ;
omega -1.00, 1.

2	3	4	5	6	7	8
138761	87622	148579	160187	179661	183809	186217

9	10	11	12	13
189448	194286	210011	203788	198897

*abscise: column(rep=0), angle(rep=1) Q(rep=2), Q**2(rep=3)? 3*
other representation (yes=1,no=0)?
change the window (yes=1, no=0)??
Treat an other run (iyes=1,no=0)?
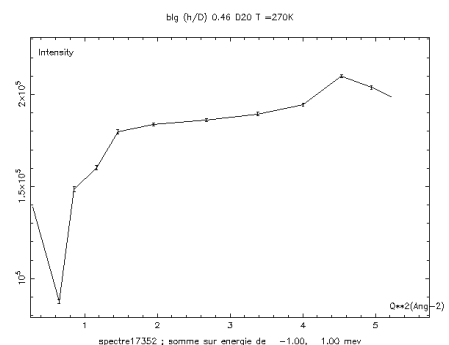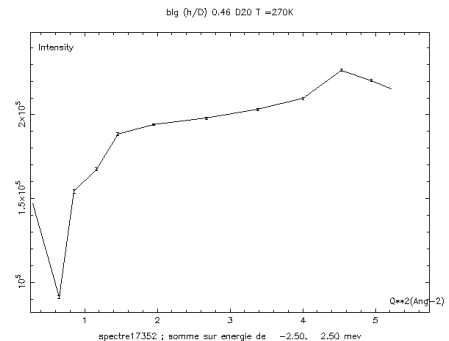
back to: *List of existing programs*

elscat
"Elastic scan"
Evolution with an external parameter of the elastic scattering

This program process the N runs provide by a step by step variation (scan) of an external parameter T (in general temperature). The wanted experimental result is the variation, with the parameter T and/or with the scattering angle ϑ, of the *total elastic scattered intensity*.

Notes
Input :
Mandatory :
- First and last run number of the scan
- Number of the vanadium run (for normalization to the detection surface and efficiency)

Optional :
- Subtraction of an other scan (reference sample) : if asked, the second scan must have the same number of runs.
- Subtraction of a container (for sample and reference if exists). Either this measurement is a scan which must also consist of N runs ; or it has just been made for one T value and then the program offer a temperature correction using a Debye model;
- Correction for self-shielding and/or shielding by the container.

The integration range (in order to take all the elastic scattering) is taken by the program to be $\pm 3\ \sigma_{el}$ (σ_{el}^2 calculated quadratic error of the elastic resolution)

- Total elastic scattering is calculated for each scattering angle (individual column or from a grouping) and for each T value.
- For each T parameter value, the result $Y = \text{Log}\ [\ I_{el}(Q)\ ]$ is fitted, with a least square criterion, to the line

$$Y = <u^2>\ Q^2 + C \text{ (adjusted parameter } <u^2> \text{ and C)}$$

Output
- For each T value, graphical representation of the elastic intensity variation with Q.
- Graphical representation of $<u^2>$ in function of T

Direction for use (without container or reference; non grouped run, standard detector grouping) :

langue, language: francais (fr) ou english (en)? en
*   sample:*
give first and last run number for each series => 14218,14317
*   check sample(s) to subtract, no(0), yes (1): 0*
Vanadium (angular normalization) : 14436
vanadium box to subtract (yes=run number, no=0)? 0
automatic scale (rep=0),or chosen(rep=1)?
other scale (yes=1,no=0)? 0
empty container no = return or run number ?
to treat : ' standard (0) or personal (1) grouping? 0
Do you want to group "n" runs together: no (0), yes ("n") ?0
* 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19,*
* 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37,*
38, 39, 40, 41, 42, 43, 44, 45, 46,14264 ce spectre n"existe pas
* 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65,*
66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84,
85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99,100,
* graph ? <u2>=f(T) => rep=1 ; (Ielast)=f(T,Q) => rep=2 :1*
do you want error bars (yes=1, no=0) 1
paper output (yes = 1 ; no = 0) ? 1
saved in file \MIBEMOL_dat\tdvmib\elscat\d14218\result.ps/PS
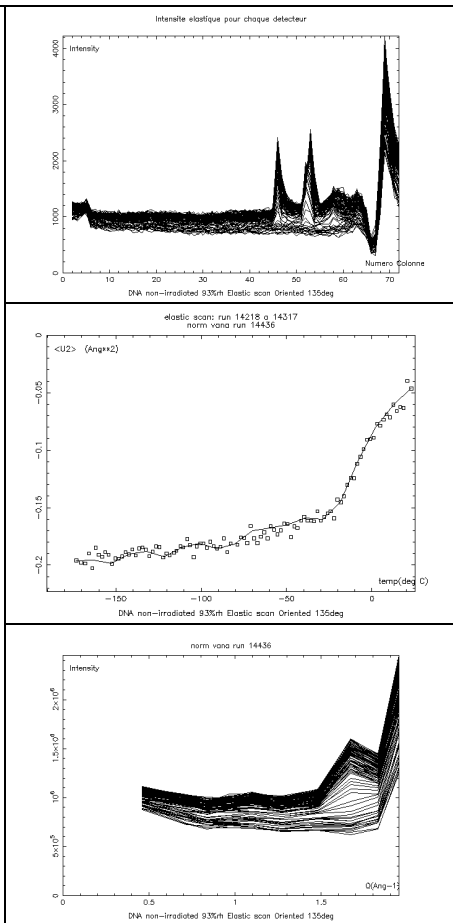* graph (Ielast)=f(T,Q) yes=2, no=0 ? 2*
*abscise: angle(rep=1), Q(rep=2), Q**2(rep=3) 2*
automatic scale (rep=0),or chosen(rep=1)? 0
other scale (yes=1,no=0)? 0
Change the grouping (yes=1, no=0)? 0
An other scan (yes=1,no=0)? 0

back to: *List of existing programs*

densix
Extraction of a phonon density of state

From the angular variation of the inelastic component of the scattering, one can extrapolate the phonon density of state **G(ω)** of the solid which scatter.

Method
The incoherent inelastic term in the scattering cross-section of thermal neutrons by a mono-atomic harmonic solid is :

$$\mathbf{S}_{inc}(\mathbf{Q},\omega) = \alpha Q^2 \left[\exp - \left(Q^2 \left\langle u^2(T)\right\rangle\right)\right]\left[1 + n(\omega)\right]\left[\frac{\mathbf{G}(\omega)}{\omega}\right]$$

α = constant factor which include the incoherent cross section of the nucleus, its atomic weigh, ….. .

|Q| = modulus of the momentum transfer for a scattering angle θ and an energy transfer ω :

$$\left(Q^2(E_0, E_f) = \left(\frac{2\pi}{\lambda}\right)^2 \left\{1 + \frac{E_f}{E_0} - 2\cos(\vartheta)\sqrt{\frac{E_f}{E_0}}\right\}\right) \quad (1)$$

$\omega = (E_f - E_0)$ => neutron energy change due to the scattering process.
Conventionally, $\omega > 0$ when the neutron increase its energy (energy gain)
(caution : it is inverse to the convention in « Marshall – Lovesey » book).

$<u^2(T)>$ = mean quadratic displacement of the nucleus (at temperature T) ;
n(ω) = occupation number of the energy level ω (above the normal state, Bose statistic)

$$1 + n(\omega) = \frac{1}{\exp\left(\omega/kT\right) - 1}$$

Now, if N is the number of the channel which receive the neutrons having the final energy E_N (energy change $\omega_N = (E_N - E_0)$), the quantity of neutrons collected by this channel is the result of a convolution between the scattering function $\mathbf{S}(Q,\omega_N)$ and the resolution function $R[(\omega_N - \omega), N)]$:

$$\mathbf{I}(Q, N) = \int \mathbf{S}(Q,\omega) R(\omega_N - \omega, N) d\omega \cong \alpha E_N^2 \, \mathbf{S}(Q,\omega_N)$$

Combining the expressions above it comes:

$$\left[\exp - \left(Q^2\left\langle u^2(T)\right\rangle\right)\right]\mathbf{G}(\omega) = \left\{\left[\frac{\omega}{1 + n(\omega)}\right]\left[\frac{\mathbf{S}_{inc}(Q,\omega)}{Q^2}\right]\right\} \quad (2)$$

and thus:

$$\mathbf{G}(\omega_N) = \mathrm{Lim}_{Q \to 0}\left\{\left[\frac{\omega_N \left(\exp\left(\frac{\omega_N}{kT}\right) - 1\right)}{E_N^2}\right] \times \left[\frac{\mathbf{I}_{inc}(Q, N)}{Q^2}\right]\right\} \quad (3)$$

Note
- The energy unity is the milli-eV (meV)

As a consequence of the low energy (compare to the one of a characteristic phonon) of the incident neutrons (cold neutrons), only the neutron energy gain part of the spectrum is used.

- The density of state value is found as the limit, when Q➔ 0 of the quantity **I**(Q,N). This procedure make sense only if the data are normalized to equal detector efficiency: this means that a vanadium run must exist.
- We recall that the treatments of "subtraction of a container" and "subtraction of an other spectrum" are different.
- The geometry of the sample, or the failure of a detector may result in a abnormally low intensity in one (or a grouping of) detector. In such case, the normalisation coefficient would be very high leading to an enormous statistical uncertainty. We then prefer to eliminate those points. The criterion is: keep if **[normalisation coefficient] < 10**
- Starting from equation (2), two ways are proposed for obtaining **G**(ω):

1) **Take the Q➔0 limit** of the right hand part of the equality **for each ω_N value.** Indeed, for each detector (or grouping of) we have a measured intensity I(Q,N) and a Q value calculated from equation (1). Then, for each ω_N one can calculate a series of *y*:

$$y = \log\left\{\left[\frac{\omega_N\left(\exp\left(\frac{\omega_N}{kT}\right)-1\right)}{E_N^2}\right] \times \left[\frac{\mathbf{I}_{inc}(Q,N)}{Q^2}\right]\right\} = f\left(Q^2\right)$$

G(ω_N) is the Q = 0 ordinate of the best fitted line through the *y* value (a least square criterion is used).

For each energy, a quality fit factor K(χ^2) is calculated. When it is too low (less than 5. 10^{-3}, as recommended by "Numerical Recipies") a warning appears. If, by graphical observation, one be in no doubt that the bad fit comes primarily from particular angles, they can be "eliminated" and a succession of fit can be done again.

2) **Bredov approximation** [*M.M Bredov et al, Sov.Phys.Solid State, **9**, 214,(1967)*]

Instead of looking for a limit, a angular summation is made for each ω_N :

$$\mathbf{G}\left(\omega_N\right) = \sum_Q\left\{\left[\frac{\omega_N\left(\exp\left(\frac{\omega_N}{kT}\right)-1\right)}{E_N^2}\right] \times \left[\frac{\mathbf{I}_{inc}(Q,N)}{Q^2}\right]\right\}$$

This second method should be prefer :

- When the number of neutron collected is low, thus with a high statistical error, the limit extrapolation in the first method might produce non-reliable result.
- When the sum of scattering length of the atoms of the elementary cell is such that $\sigma_{coh} \approx \sigma_{inc}$ add to some long range order leads to a non negligible "distinct correlation" term, compare to the "auto-correlation term, in the scattering function. Indeed, the $\left(\sum_Q\right)$ operation reduce, by an averaging effect, the impact of the coherent intensity.

After giving a graphical representation of **G(ω),** the program propose a fitting procedure of all, or part, of the energy interval to an **G(ω_N) = $\delta \times (\omega_N)^{\alpha}$** analytic function (one fits the experimental result to the line Log[G(ω_N)] = α Log(ω) + C^{te}).

At last, the graphical representation of the results is saved in the file :

\mibemol_dat\tdvmib\densix\dxxxxx\graph.ps

Direction for use (subtraction of a container; standard grouping, Bredov extrapolation)

langue, language: francais (fr) ou english (en)? en
Density of state as (q==>0) limit from sub/spectrum at
different angles
run(s) number(s)? 17361
a spectrum to subtract yes=run(s) number, no or empty
container=0)? 0
to treat : ' standard (0) or personal (1) grouping0
an empty box to subtract (yes=run(s) number, no=0)? 17347
vanadium for detector calibration: run(s) number(s)? 17343
do you wish to correct for self shielding (yes=1, no=0)? 0
g(omega), energy interval and step
(in meV): min, max, delta ? 0.5,25,.2
recorded temperature = 268.0 K
do you wish to modify this value, (yes=value, no=0)? 0
using Q=>0 limit(rep=1) or BREDOV method(rep=2)? 2
* RESULTS ; graph and fit of G(omega)*
X axe lin (rep=1) or log (rep=2)? 1
Y axe lin (rep=1) ou log (rep=2)? 1
automatic scale (rep=0),or chosen(rep=1)? 0
do you want error bars (yes=1, no=0)1
do you want a fit (yes=1,no=0)? 0
other coordinates : no (0), yes (1) ? 1
X axe lin (rep=1) or log (rep=2)? 2
Y axe lin (rep=1) ou log (rep=2)? 2
automatic scale (rep=0),or chosen(rep=1)? 0
do you want error bars (yes=1, no=0)
do you want a fit (yes=1,no=0)? 1
Omega mini et maxi or <return> if total interval ? 0.5,5
do you want error bars (yes=1, no=0)1
other coordinates : no (0), yes (1) ? 0
paper output (yes = 1 ; no = 0) ? 1
saved in file
\MIBEMOL_dat\tdvmib\densix\d17361\graph.ps/PS
lattice heat capacity (yes=1,no=0)? 1
how many atoms in the molecule ? 5
molecular weight (grams) ? 79
PHONON HEAT CAPACITY =   0.50 J/(g.K)
results are in files :\MIBEMOL_dat\tdvmib\densix
other run (yes=1,no=0)? 0
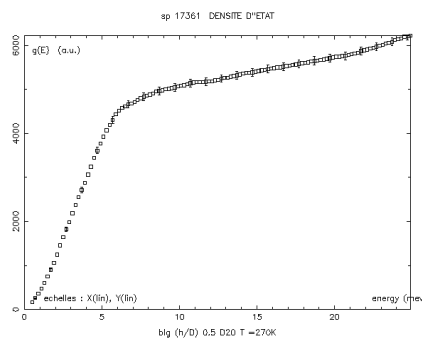
échelle linéaire-lineaire
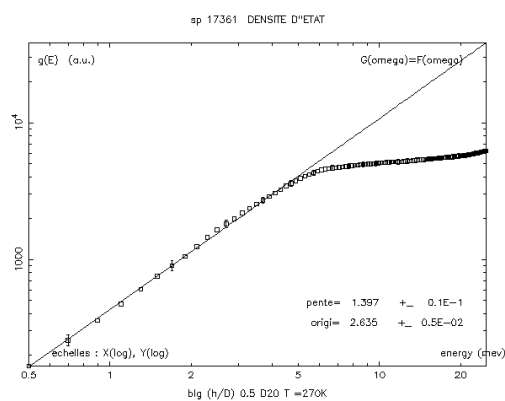
échelle log-log

back to: *List of existing programs*

fitrun_theta

This program fits experimental data to various analytical functions. The selected function made by the experimentalist will be an image of the theoretical expression $S(Q,\omega)$ of the thermal neutron scattering by the sample. The fitting procedure is done on non transformed data, that is in time of flight unit.

$$\mathbf{I}_{calc}(\mathbf{Q},\mathbf{n}) = \mathbf{Fd}(\mathbf{n}) + \int_{-e_0}^{\infty} \mathbf{S}(\mathbf{Q},\omega)\mathbf{R}(\mathbf{n},\omega)\,d\,\omega + \mathbf{Bf}(\mathbf{n})$$

Fd = elastic peak ; R = résolution function ; Bf = background noise

Fitting means : found the set of parameters $\{(a_j)\ ;\ j \in [1,k]\}$ which minimize the function :

$$\chi^2(a_1, a_2, ..., a_k) = \sum_{\mathbf{n}} \left\langle \left\{ \frac{[\mathbf{I}_{calc}(\mathbf{Q},\mathbf{n},a_1,a_2,...,a_k) - \mathbf{I}_{mes}(\mathbf{Q},\mathbf{n})]}{\sigma_{\mathbf{I}}} \right\}^2 \right\rangle$$

The quality factor of the fit over the "npoints" of the zone to match is

$$P = \left[\frac{\chi^2}{(\text{npoints - nvar})} \right]$$

nvar = number of parameters in the analytical function.

The program progresses in successive phases :

Building of the data to be fit
- Reading of the sample run
- Eventually subtraction of a container
- Eventually self shielding correction
- Eventually subtraction of a reference sample (with or without a container)
- Eventually accounting for detectors efficiency
- Grouping of several detectors columns (for better statistic)

Fitting procedure preparation
- Find the elastic full width half maximum (σ_{el}) by fitting a nearly purely elastic scattering run with a gaussian profile: indeed, as the elastic component of the scattering by the sample is often the dominant part of its spectrum, it is absolutely necessary to found this parameter from a reference run, measured in the same geometrical and neutron conditions with a sample in which the scattering function has no quasi-elastic component (usually vanadium).
- Choose of the analytical form to fit to the experimental data. This choice is made in a number form. Connection between this number and the various possible analytical functions are found in a table ***List_fitrun_options*** attached to this document.
- Choice of the part of the spectrum which has to be fit. This choice is fixed by giving the first and last channel number of the zone. One can wish to exclude some part inside the total zone: then gives the first and last channel number of each partial zone.

*Example: **150,210,230,340,350,450***
fitting will concerned the part of the spectrum between channel 150 and 450 but will exclude channel 211 to 229 and 341 to 349

- Choice of the starting set parameter value. For each function the ***List_fitrun_options*** gives the number of required adjustable parameter and their meaning.

Remark If some other fit has already been complete with the same option (for instance for an other scattering angle) one can take its final set parameter as starting values. The nearest angle value already handled will be selected automatically

- Plot on a same graphic of the experimental data, the calculated intensity of each component[*] and of the total intensity allows to revise the initial choice for some starting values. Actually it is important to ensure that the discrepancy between experimental and calculated values is not too important (without being able to specify what "too important" means) at the beginning of the fitting procedure; from this gap depend the probability to get the real, and not a local, χ^2 minima.

Search of the best set of parameters by minimization of χ^2

- Before starting the minimization process, one can freeze one or several parameters to their starting values. For doing this give, when asked, the order number(s) of the parameter(s) which must not vary.

This can be useful when several components are mixed in some part of the spectrum (successive approximations should then give an adequate answer) or if, for some reasons, the elastic peak zone has been discarded from the fitting interval. In that case, obviously one must give the elastic channel number.

- Throughout the minimization: its progression is represented by drawing the function $\chi^2 = $ f(number of cycles). The process ends when $\delta(\chi^2) < 10^{-5}$ between two successive cycles.
- Final values of the parameters are displayed on the terminal screen and written in a specific file :

<div align="center">

C:mibemol_dat\tdvmib\fitrun_theta\par_ini\dxxxxx\kwww.yyyy

</div>

xxxxx ➔ sample run number ;
www ➔ mean angle for the actual detector grouping (in degrees).
yyyy ➔ option number

This file will be used for getting some starting value of the parameters in a subsequent running with the same option.

Looking and saving the results

- A graphical comparison between experimental and calculated data is proposed. The diverse components[*] of the analytic function are drawn. One can select either time of flight or energy scale.
- The "error curve" $\Delta(\mathbf{I}) = [\mathbf{I}_{mes} - \mathbf{I}_{calc}]$ allows to call attention to interval(s) where, even if the global quality parameter is good, systematic discrepancy between calculation and measure is obvious.
- The final result of the minimization (fit parameter, final value and statistical error on the fitted parameters) is automatically saved in a text file :

<div align="center">

C:MIBEMOL_dat\tdvmib\fitrun_theta\resultat\dxxxxx\kzz_yy.txt

</div>

xxxxx ➔ sample run number
yy_zz ➔ first and last column numbers of the detector grouping
On demand, the previous graphical comparison is saved in a postscript file.

<div align="center">

C:MIBEMOL_dat\tdvmib\fitrun_theta\resultat\dxxxxx\kzz_yy_aa.ps

</div>

aa ➔ **tv** or **en** according as time of flight (tv) or energy (en) scale has been chosen.

---

[*] For clearness of the graphic, we are forced to limit at 3 the number of drawn components (+ the global intensity as the sum of the calculated components).

In all options we have used the same rule :

Points (●) ➔ experimental data (($\mathbf{I}_{mes}$)

Continuous black line (——) ➔ total computed intensity ($\mathbf{I}_{calc}$)

Hatched green line (- - - -) ➔ elastic + background + phonon component

Hatched red line (- - - -) ➔ first component (quasi elastic or inelastic)

Hatched blue line (- - - -) ➔ second component (quasi elastic or inelastic)

Direction for use (here: option 102 ➔ elastic + Lorentz + BdF + Debye phonon)

langue, language: francais (fr) ou english (en)? *en*
fitting program;
    answer question and then make <return>
    CAUTION : separator between two values is ALWAYS ","
       Sample
run(s) number(s)? *17352*
an empty box to subtract
(yes=run(s) number, interpolation=-1, no=0)? *17347*
 do you wish to correct for self shielding (yes=1, no=0)? *0*
do you want to subtract a spectrum (yes=run(s) number, no=0)? *0*
do you wish normalization to vanadium(yes=1,no=0)? *1*
run(s) number(s)? *17343*
same empty box to subtract (yes=1, no=0)? *1*
which is your detector grouping (for details, make <return>)? *65,78*
Reference run for elastic peak shape
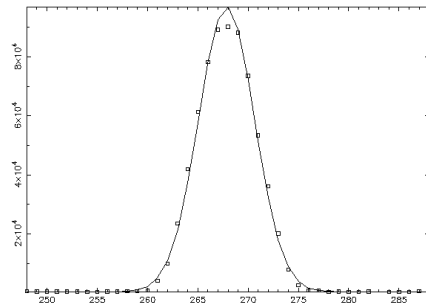*Run(s) number(s)?* **17343**
Same empty box to subtract (yes=1, no=return) ? **1**
    54 cycles, Gauss parameters
 0.96738E+05 0.26786E+03 0.27874E+01
0.26407E+03 0.12018E+03
 see elastic peak and fit (yes=1) ? **1**

which option do you want? *102*
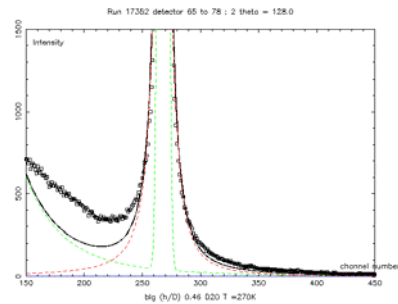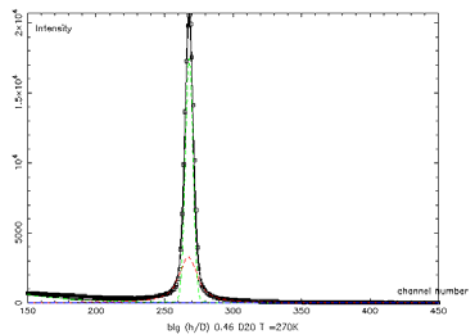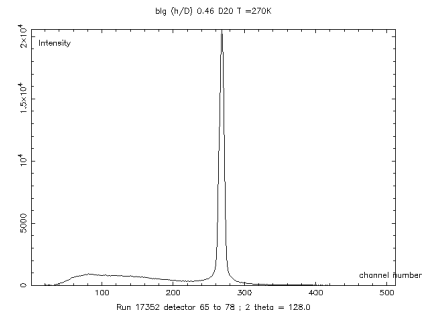*you shall give a channel interval to fit*
do you want a graph (yes=1,no=0)? *1*
automatic scale (rep=0),or chosen(rep=1)? *0*
another graphic (yes=1, no=0)? *0*
first channel, last channel,.. (several zones allowed)?
150,450

*Debye-factor <U2> (angstr**-2)=* *0*
starting parameter-values already in a file (yes=1,no=0)? *0*
give the 8 starting values of the parameters;
all numbers on same line
7000,268,3500,0.15,1,1,80,0.01
computed resolution = 0.07326meV
measured resolution = 0.07328meV
automatic scale (0) or your choice (1)? *0*
do you want error bars (yes=1, no=0) *0*

other graph (yes=1, no=0) *1*
automatic scale (0) or your choice (1)? *1*
x minimum= 150   x maximum= 450
y minimum=   0.0   y maximum= 20728.1
xmin, xmax ? *150,450*
ymin, ymax ? *0,1500*
do you want error bars (yes=1, no=0)
other graph (yes=1, no=0) *0*

do you want to modify a parameter (yes=1, no=0)? *1*
present values:

zc(1)= 0.70000E+04
zc(2)= 0.26800E+03
zc(3)= 0.35000E+04
zc(4)= 0.15000E+00
zc(5)= 0.10000E+01
zc(6)= 0.10000E+01
zc(7)= 0.80000E+02
zc(8)= 0.10000E-01

for changing a parameter give its number and its new value,
then <return>
 n , zc(n)? 7,150
 n , zc(n)? 8,0.03
 n , zc(n)?
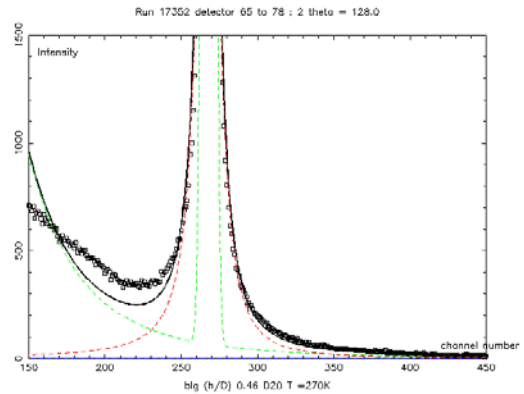*automatic scale (0) or your choice (1)? 1*
 same limits as previous case (yes=1, no=0)? 1
do you want error bars (yes=1, no=0) 0
other graph (yes=1, no=0) 0
do you want to modify a parameter (yes=1, no=0)? 0
do you keep the last values (yes=1, no=0)? 1

initial values of parameters:
     c(1) =   7000.0
     c(2) =   268.00
     c(3) =   3500.0
     c(4) =   0.15000
     c(5) =   1.0000
     c(6) =   1.0000
     c(7) =   150.00
     c(8) =   0.30000E-01
   freeze some ?
list number, separator comma. <return>=all free
     Starting of the fit khi2 = 0.34819E+03
                RESULT
           blg (h/D) 0.46 D20 T =270K
   Run N° 17352Run 17352 detector 65 to 78 ; 2 theta = 128.0
   Option 102 Elast => gauss ; T= 267.9 K
   fit between chnl 150 and 450 on 301 channel
   lambda = 5.2 A; angle = 128.0 deg; q0 = 2.17 A-1
   resolution mesuree = 73. ; calculee = 73. micro-eV
        fit parameter=   0.21

                              stat 90%   gradient
   -c(1)= 0.74309E+04 plus ou moins 0.290E+03   0.107E-09
   -c(2)= 0.26810E+03 plus ou moins 0.255E-01   -0.824E-07
   -c(3)= 0.29313E+04 plus ou moins 0.259E+02   -0.207E-09
   -c(4)= 0.12403E+00 plus ou moins 0.322E-02   -0.420E-05
   -c(5)=-0.18370E+02 plus ou moins 0.139E+00   -0.594E-08
   -c(6)=-0.39646E+02 plus ou moins 0.300E+00   -0.180E-08
   -c(7)= 0.16739E+04 plus ou moins 0.177E+02   -0.123E-09
   -c(8)= 0.31880E+00 plus ou moins 0.171E-02   -0.582E-06
Graph in ToF (1) or 'energy scale (2) ? 1
automatic scale (0) or your choice (1)? 0
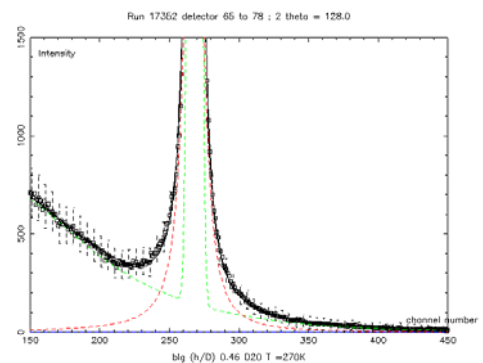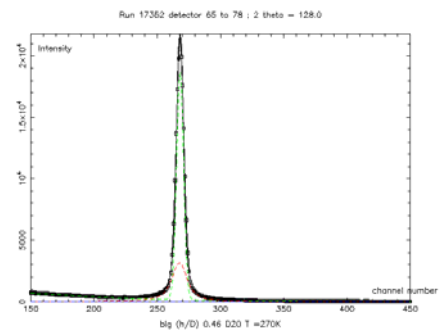*do you want error bars (yes=1, no=0) 0*
other graph (yes=1, no=0) 1
*automatic scale (0) or your choice (1)? 1*
 same limits as previous case (yes=1, no=0)? 1
do you want error bars (yes=1, no=0) 1
other graph (yes=1, no=0) 0

change ToF <=> energy (no(0), ToF(1), energy(2)) 2
automatic scale (0) or your choice (1)? 1
x minimum= -6.48   x maximum= 1.95
y minimum=   -14.5   y maximum=   21801.5
xmin, xmax ? -3,1.9
ymin, ymax ? 0,1000
do you want error bars (yes=1, no=0) 1
other graph (yes=1, no=0) 0
change ToF <=> energy (no(0), ToF(1), energy(2)) 0
error-curve (ToF)(no=0, yes=1) 0
Change a parameter, then new fit (yes=1,no=0)? 0
save graph file(no(0), ToF(1), energy(2))? 2
saved in file
\MIBEMOL_dat\tdvmib\fitrun_theta\resultat\d17352\k65_78_en.ps
end (0), other grouping and same run(1),
other run and same grouping (2) ? 0
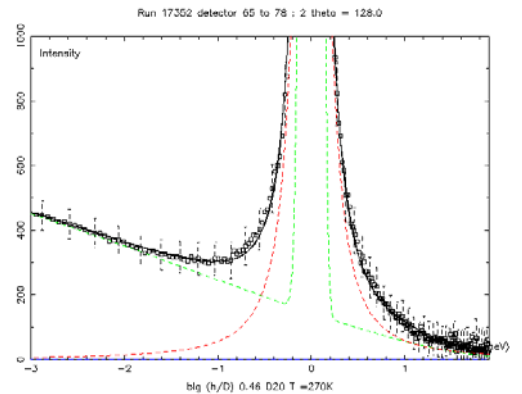
back to: *List of existing programs*

fitrun_q

Constant Q scattering function
Data interpolation and fitting

List_fitrun_options

N.B. *In the table behind, when the option number is followed by an asterisk (*), it signify that the option with terminal digit 1, 2 and 3 also exist and have the same meaning than options 100, 101, 102, 103.*

OPTION			CONTENT	Nbe Coeff
C	D	U		
1	**0**	**0**	$Ep + L_{3D}(\Delta) + (BG_{incl})$	2+2+(2)
		1	$Ep + L_{3D}(\Delta) + (BG_{incl} + P_h\ approx)$	2+2+(2+1)
		2	$Ep + L_{3D}(\Delta) + (BG_{incl} + P_h\ Debye)$	2+2+(2+2)
		3	$Ep + L_{3D}(\Delta) + (BG_{incl} + Damped\_Osc)$	2+2+(2+3)
	1	**0**	$Ep + L_{3D}(\Delta) + (BG_{incl}) + Gauss(inel)$	2+2+(2)+3
	2	**0***	$Ep + F_{MAG}(Q)*L_{3D}(\Delta) + (BG_{incl})$	2+3+(2+x)
	8	**0**	$Ep + a/\omega^b + (BG_{incl})$	2+2+(2)
2	**0**	**0***	$Ep + L_{3D}(\Delta_1) + (BG_{incl}) + L_{3D}(\Delta_2)$	2+2+(2)+2+(x)
	1	**0**	$Ep + L_{3D}(\Delta_1) + (BG_{incl}) + L_{3D}(\Delta_2) + Gauss(inel)$	2+2+(2)+2+3
	2	**0***	$Ep + F_{1MAG}(Q)*L_{3D}(\Delta_1) + (BG_{incl}) + F_{2MAG}(Q)*L_{3D}(\Delta_2)$	2+2+(2)+2+(x)
3	**0**	**0***	$Ep + L_{3D}(DQ^2) + (BG_{incl})$	2+2+(2+x)
	1	**0**	$Ep + L_{1D}(DQ^2)$ *(with powder averaging)* $ + (BF_{incl})$	2+2+(2)
4	**0**	**0***	$Db + L_{3D}(D_1Q^2) + (BG_{incl}) + L_{3D}(D_2Q^2)$	2+2+(2)+2+(x)
5	**0**	**0***	$Ep + L_{3D}(DQ^2) + (BG_{incl}) + L_{3D}(\Delta)$	2+2+(2)+2+(x)
	1	**0***	$Ep + L_{1D}(DQ^2) + (BG_{incl}) + L_{3D}(\Delta)$	2+2+(2)+2+(x)
6	**0**	**0***	$Ep + L_{3D}(A_1, DQ^2) + (BG_{incl}) + L_{3D}[A_2, (DQ^2 + \Delta)]$	2+2+(2)+2+(x)
7	**0**	**0***	$Ep + L_{3D}(kA_1, DQ^2) + (BG_{incl}) + L_{3D}[k(1-A_1), (DQ^2 + \Delta)]$	2+2+(2)+2+(x)
8	**0**	**0***	$Ep + TF(stretch\_exp) + (BG_{incl})$	2+3+(2+x)
	1	**0**	$Ep + TF(stretch\_exp) + (BG_{incl}) + L_{3D}(\Delta)$	2+3+(2)+2
9	**0**	**0**	$Ep + L_{3D}(\Delta_1) + (BG_{incl}) + L_{3D}(\Delta_2) + L_{3D}(\Delta_3)$	2+2+(2)+2+2
	1	**0**	$Ep + Distrib(lorentz) + (BG_{incl})$	2 + 3 + (2)

0PTION			CONTENT	Nbe Coeff
C	**D**	**U**		
0	**1**	**0**	**Ep + Gauss**(inel +et -**) + (BG**incl**)**	2+3+**(2)**
		1	**Ep + Gauss**(inel +**) + (BG**incl**)**	2+3+**(2)**
	2	**0**	**Ep + Gauss**$_1$**(+/ -) + (BG**incl**) + Gauss**$_2$**(+/ -)**	2+3+**(2)**+3
	3	**0**	**Ep + Gauss**$_1$ **+ (BG**incl**) + Gauss**$_2$ **+ Gauss**$_3$	2+3+**(2)**+3+3
	5	**0**	**Ep + Damped_Osc + (BF**incl**)**	2+3+**(2)**
	6	**0**	**Ep + Damped_Osc** $_1$ **+ (BF**incl**) + Damped_Osc** $_2$	2+3+**(2)**+3

Caution: *The coefficient succession and their number is indicated in the last column.*
*For "asterisked" options, the coefficients numbers in parentheses are for **BG**$_{incl}$ (2 coeff) and*
*the various "**Approx ph**" (x = 1, 2 or 3 coefficients) at their respective position.*

Symbol meaning :

Ep ➔ **Elastic peak**

BGincl ➔ **Background with a slope**

L3D( ) ➔ **3D Lorentz-shape with constant width**

L3D(DQ2) ➔**3D Lorentz-shape with DQ2 width**

L3D(DQ2 + Δ) ➔ **convolution of the two previous Lorentz-profil**

L1D(DQ2) ➔ **1D Lorentz-profil with DQ2 width and powder averaging**

Gauss(inel) ➔ **Inelastic Gaussian peak ; frequency plus or minus** ω1**, variance** σ1

Damped_Osc_ ➔ **damped oscillator ; frequency** ω1**, damping coefficient** Γ1

Distrib(lorentz) ➔ **Uniform and continuous lorentz-profil distribution**

TF(stretch_exp) ➔ **slow relaxation**

Ph approx ➔ **Approximate scattering from low energy phonons (<< Debye energy)**

Ph Debye ➔ **Phonon scattering by a Debye solid**

Meaning of abbreviations
Number of adjustable parameters

*In the two next functions, there is no definite energy exchange between the neutron and the sample. Either because it is purely elastic or weakly inelastic (and not resolved by the spectrometer) scattering from the sample (**Ep** ➜ lastic peak) or because it is the addition of a phenomenological approach of numerous very inelastic scattering process (out of the measuring window of the spectrometer) and a non correlated background (**BG$_{incl}$** ➜ inclined background). In both cases the only variable of the fitted function is the neutron time of flight i.e. the channel number **n***

Ep ➜ **Elastic peak**
2 adjustable parameters **A, n$_0$**

$$\mathbf{Db} = \left(A \big/ \Delta\sqrt{2\pi}\right)\exp\left[-\left(\frac{\mathbf{n}-\mathbf{n}_0}{\Delta\sqrt{2}}\right)^2\right]$$

Typically the Δ parameter value has been determined previously from a reference measurement (usually a vanadium scattering).

BG$_{incl}$ ➜ Background with a slope
The baseline is the straight line which connect the two end points of the total fitting interval.
2 adjustable parameters γ and α

$$\mathbf{BG_{incl}} = \left(\frac{1}{N_{sup} - N_{inf}}\right)\left[\gamma\left(N_{sup} - \mathbf{n}\right) + \alpha\right]$$

α = number of neutrons in the upper channel number N_{sup}
γ = difference between the content in the lower N_{inf} and upper channel number (reverse slope)

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*When there is neutron energy change, the intensity collected in the time of flight channel **n** is the convolution between the scattering function of the sample S(**Q**, ω) and its energy resolution function **R**(**n**, ω).*

$$\mathbf{I(Q,n)} = \int_{-e_0}^{\infty} \mathbf{S(Q,\omega)R(n,\omega)}\, d\,\omega$$

The scattering function for thermal neutrons

$$\mathbf{S(Q,\omega)} = \mathbf{P}(T,\omega) \times \mathbf{J(Q,\omega)}$$

is the product of :
- *a term which depends only on temperature and statistic*

$$\mathbf{P}(T,\omega) = k T \frac{\beta\hbar\omega}{\exp(\beta\hbar\omega) - 1} \quad ; \quad \beta = \frac{1}{kT}$$

- *a scattering intensity*

$$\mathbf{J(Q,\omega)}$$

which depends only on the interactions between the neutron and the scattering sample. The following formula are the diverse analytical forms of this term, depending on the physic involved.

L₃D(Δ) ➔ 3D Lorentz-shape with constant width

2 adjustable parameters **A**, **Δ**

$$\mathbf{L}_{3D}(\Delta) = \left(\frac{\mathbf{A}}{\pi}\right)\left[\frac{\Delta}{(\Delta^2 + \omega^2)}\right]$$

L₃D(DQ^2) ➔ 3D Lorentz-shape with DQ^2 width

2 adjustable parameters **A**, **D**

$$\mathbf{L}_{3D}(\mathbf{D}Q^2) = \left(\frac{\mathbf{A}}{\pi}\right)\left[\frac{\mathbf{D}Q^2}{((\mathbf{D}Q^2)^2 + \omega^2)}\right]$$

L₃D(DQ^2 + Δ) ➔ convolution of the two previous Lorentz-profil

3 adjustable parameters **A**, **D**, **Δ**

$$\mathbf{L}_{3D}(\mathbf{D}Q^2 + \Delta) = \left(\frac{\mathbf{A}}{\pi}\right)\left[\frac{\mathbf{D}Q^2 + \Delta}{((\mathbf{D}Q^2 + \Delta)^2 + \omega^2)}\right]$$

L₁D(DQ^2) ➔ 1D Lorentz-profil with DQ^2 width and powder averaging

2 adjustable parameters **A**, **D**

$$\mathbf{L}_{1D}(\mathbf{D}Q^2) = \left(\frac{\mathbf{A}}{\pi}\right)\int_0^\pi \sin(\theta)\left[\frac{\mathbf{D}Q^2\cos^2(\theta)}{((\mathbf{D}Q^2\cos^2(\theta))^2 + \omega^2)}\right]d\theta$$

Gauss(inel) ➔ Inelastic Gaussian peak ; frequency plus or minus ω_1, variance σ_1

3 adjustable parameters **A**, **ω_1**, **σ_1**

$$\mathbf{Gauss}(\pm) = \mathbf{A}\left\{\exp\left[-\frac{(\omega - \omega_1)^2}{2\sigma_1^2}\right] + \exp\left[-\frac{(\omega + \omega_1)^2}{2\sigma_1^2}\right]\right\}$$

Damped_Osc_ ➔ damped oscillator ; frequency ω_1, damping coefficient Γ_1

3 adjustable parameters **A**, **ω_1**, **Γ_1**

$$\mathbf{Damped\_OSC} = \mathbf{A}\left\{\frac{\Gamma_1\omega_1^2}{[(\omega^2 - \omega_1^2)^2 + (\Gamma_1\omega_1)^2]}\right\}$$

Distrib(lorentz) ➔ Uniform and continuous lorentz-profil distribution

Width (HWHM) of the Lorentz goes from Δ_1 to Δ_2

3 adjustable parameters **A**, **Δ_1**, **Δ_2**

$$\mathbf{Distrib}(\mathbf{lorentz}) = \frac{\mathbf{A}}{(\Delta_2 - \Delta_1)}\int_{\Delta_1}^{\Delta_2}\left(\frac{\delta}{\delta^2 + \omega^2}\right)d(\delta)$$

TF(stretch_exp) ➔ slow relaxation

3 adjustable parameters **A**, **Λ**, **1/τ**

$$\mathbf{J}(\omega) = \mathbf{A}\int_0^\infty e^{-i\omega t} \exp\left[-\left(\frac{t}{\tau}\right)^{\mathbf{B}}\right] dt \approx \frac{1}{\omega}\mathbf{Im}\left[\frac{\mathbf{A}}{1+\mathrm{i}(\omega/\Lambda)}\right]^{\mathbf{B}} = \frac{\mathbf{A}}{\omega}\frac{\sin\left[\mathbf{B}\times\mathrm{arc\ tg}(\omega/\Lambda)\right]}{\left[1+(\omega/\Lambda)^2\right]^{\mathbf{B}/2}}$$

Ph approx ➔ Approximate scattering from low energy phonons (<< Debye energy)

1 adjustable parameter **A**

$$\mathbf{Ph\_approx} = \mathbf{A}(kT)$$

Ph Debye ➔ Phonon scattering by a Debye solid

2 adjustable parameters **A**, **U²**

$$\mathbf{Ph\_debye} = \left(\frac{\mathbf{A}}{\beta}\right)\left(\frac{Q}{Q_0}\right)^2 \left[\exp\left(-Q^2\,\mathbf{U}^2\right)\right]\left[\frac{\beta\hbar\omega}{\exp(\beta\hbar\omega)-1}\right] \; ; \; \beta = \frac{1}{kT}$$

Integrated Intensities

The minimization program gives the best set of coefficients for fitting the experimental data as a sum of definite analytic form. The founded values allows to compute independently the area I_p under each component. Taking into account the detail of the calculation, we have:

- *Area under the elastic peak:*

$$I_{el} = \mathbf{A}_{el}\times\left(\text{channel width in } \mu s\right) \quad (1)$$

- *Area under a quasi-elastic Lorentzian:*

$$I_{QE} = \mathbf{A}_{QE}\times\left(kT\right)_{\mathbf{meV}} \quad (2)$$

Moreover the integrated intensity over the total fitted zone

$$J = \sum_{n\,\mathbf{min}}^{n\,\mathbf{max}} j(n)$$

is computed for each component and displayed.

Usually $J_{el} \approx I_{el}$ because the fitting interval include and is larger than the elastic peak

$$J_{QE} < I_{QE} \text{ for the reason that Lorentz-shape extend up to infinity}$$