

# Calibration of the SLAD diffractometer

Version 2.3

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This document describes the use of a series of programs intended for fast and more-or-less automatic calibration of various instrumental parameters of SLAD. First some basic concepts about assumptions on geometry and similar is presented together with references to the second section where the various programs are described in detail and a recommended way of using the programs is given. Extracts from some sample input/output files are also given.

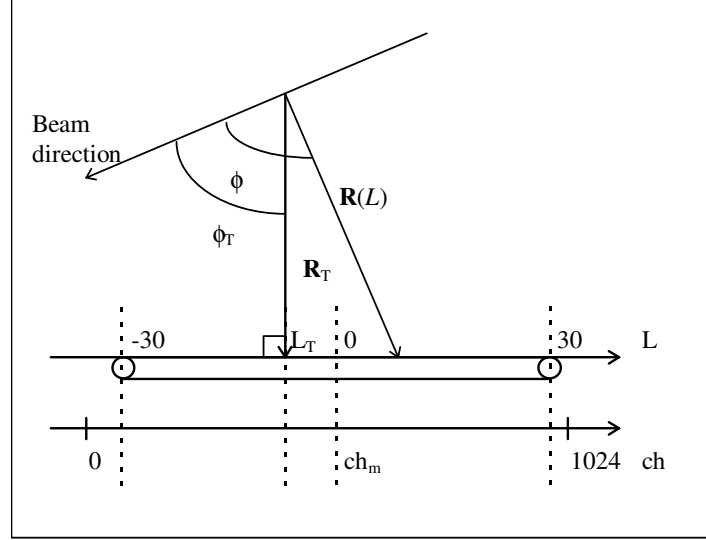
## Changes with respect to version 2.2

- A completely new format for PEAKOT input files name.inp. Now, only h,k,l indices are given and the program automatically determines which peaks are relevant for each block data, and also finds automatically initial values of parameters.
- MSK and PRM files are now updated only if the fits in MASKOT and CALSLAD were succesful, so that the previous results are not lost.
- An option to fit a second wavelength component has been introduced, which is controlled by the new parameters lamda2, wlamda2 in the PRM file.

1.	Geometry .....	2
1.1	The position sensitive detector, PSD .....	2
1.2	The PSD orientation .....	3
1.3	Peak shape and position as a function of channel number .....	4
1.4	The detector array arrangement .....	5
2.	The programs .....	6
2.1	General .....	6
2.2	Mask programs .....	7
2.3	Powder programs .....	7
2.4	Recommended use of programs .....	8
2.5	Some examples of the structure of input and output files .....	9
3.	References .....	11

# 1. Geometry

## 1.1 The position sensitive detector, PSD



**Figure 1** The PSD together with the definitions of linear position and scattering angle.

The PSD is taken to have an active length of  $L_0 = 60.0$  cm, an outer radius  $r_{PSD} = 2.54$  cm and totally  $N_{ch} = 1024$  position channels. Ideally the relation between channel and linear position should be strictly proportional, i.e.  $L = K \cdot (ch - ch_m)$ , where  $K = L_0/N_{ch} \approx 0.0586$  cm/channel and  $ch_m \approx 512$  is the detector centre channel for which  $L = 0$ . In practice the relationship is non-linear but a polynomial of degree three usually describes the situation well. To determine this relationship a measurement is performed with an isotropic scatterer (such as vanadium or Plexiglass) and Cd masks with 2 mm slits each 2 cm. By using *MASKOT* to get the slit channel positions one gets maximum  $n_m = 29$  slit positions to determine the coefficients. To get a well-conditioned problem we write the linear position as measured from the detector centre as

$$L = \sum_{i=1}^{n_l} l_i \cdot (ch - ch_m)^i \quad \{1.1\}$$

The definition of  $L$  is shown in figure 1. The channel resolution of the PSD can also be obtained from the mask measurements. Since the observed FWHM resolution  $> 5$  mm the PSD resolution standard deviation is approximately the one obtained in a Gaussian fit. (Possibly a large) part of this broadening is due to the projected trajectory of detection events in the PSD (with a width roughly given by  $d/\sqrt{1+(R/L)^2}$ ) where  $d$  is the average penetration depth of the neutrons into the detector. Since the same projection occurs e.g. with powder peaks the channel-linear position relationship above should still be valid. The slit peak width is also described by a polynomial, expressed in linear position as

$$\sigma_{PSD}(L) = \sum_{i=0}^{n_\sigma} \sigma_i \cdot L^i \quad \{1.2\}$$

$n_\sigma = 2$ ,  $\sigma_0 = 0.12$  cm,  $\sigma_1 = -0.001$  cm<sup>-1</sup>,  $\sigma_2 = 0.0002$  cm<sup>-2</sup> are typical values, i.e. the broadening is worst at the endpoints. If the mask measurement is normalised by vanadium the  $n_m$  peak areas are all approximately equal and the complete mask profile can be fitted by

$$I(L(ch)) = A \sum_{j=1}^{n_m} \frac{1}{\sigma_{PSD}(L_j)} \exp \left[ -\frac{1}{2} \left( \frac{L - L_j}{\sigma_{PSD}(L_j)} \right)^2 \right] + \sum_{i=0}^{n_B} B_i ch^i \quad \{1.3\}$$

Here the linear position of slit  $j$  is  $L_j = 2(j-1)$  and the  $B_i$  are coefficients for a polynomial background. This is the expression which is fitted in *MASKOT*. For reference we also write down the parameter derivatives used in the program. Using the definitions

$$Y = \frac{L - L_j}{\sigma_{PSD}(L_j)} \quad \varepsilon_j = \frac{1}{\sigma_{PSD}(L_j)} \exp\left[-\frac{1}{2}Y^2\right] \quad \{1.4\}$$

the derivatives needed are

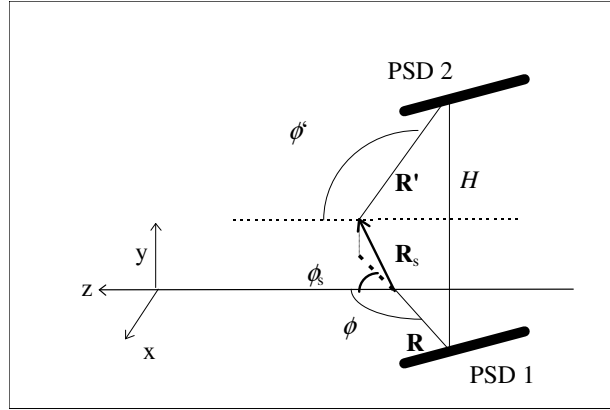
$$\begin{aligned} \frac{dI}{dch_m} &= A \left( \sum_{j=1}^{n_m} \frac{Y \varepsilon_j}{\sigma_{PSD}(L_j)} \right) \sum_{i=1}^{n_l} i \cdot l_i (ch - ch_m)^{i-1}, \quad \frac{dI}{d\sigma_i} = A \sum_{j=1}^{n_m} \frac{(Y^2 - 1)}{\sigma_{PSD}(L_j)} \varepsilon_j L_j^i \\ \frac{dI}{dl_i} &= -A \sum_{j=1}^{n_m} \frac{Y \varepsilon_j}{\sigma_{PSD}(L_j)} (ch - ch_m)^i, \quad \frac{dI}{dA} = \sum_{j=1}^{n_m} \varepsilon_j, \quad \frac{dI}{dB_i} = ch^i \end{aligned} \quad \{1.5\}$$

## 1.2 The PSD orientation

The orientation of the PSD relative to the sample is shown in figure 1 and can be described as the detector perpendicular to a sample radius vector  $\mathbf{R}_T$ . This implies that a linear position  $L$  corresponds to a scattering angle according to

$$\phi = \phi_T + \arctan((L - L_T)/R_T) \quad \{1.6\}$$

where  $\phi_T$  is the scattering angle at  $L_T$  and  $R_T$  is the (obviously) shortest distance between the sample and the detector. Note that this expression covers all cases where the detector is oriented so that its extrapolation cuts the direction of the incoming beam and also adjusts for any misalignment in the positioning of the Cd mask.



**Figure 2** Geometry for the case of a non-centred sample and a PSD position out of the horizontal  $y = 0$  plane.  $\phi$  is the scattering angle for PSD 1 in the horizontal  $y = 0$  plane and  $\phi'$  the scattering angle for PSD 2 in the  $y = H$  plane.

If the detector is displaced a distance  $\Delta H$  perpendicular to the horizontal plane and the sample is centred at  $\mathbf{R}_s$  this could be described, with reference to figure 2 by

$$\begin{aligned} \mathbf{R} &= (R \sin \phi, 0, R \cos \phi) & \mathbf{R}_s &= (R_s \sin \phi_s, Y_s, R_s \cos \phi_s) \\ \mathbf{R}' &= \mathbf{R} + \Delta H \hat{\mathbf{y}} - \mathbf{R}_s = (R \sin \phi - R_s \sin \phi_s, \Delta H - Y_s, R \cos \phi - R_s \cos \phi_s) \\ \cos \phi' &= \frac{\mathbf{R}' \cdot \hat{\mathbf{z}}}{R'} = \frac{(R \cos \phi - R_s \cos \phi_s)}{\left( R^2 + R_s^2 - 2RR_s \cos(\phi_s - \phi) + (\Delta H - Y_s)^2 \right)^{1/2}} \end{aligned} \quad \{1.7\}$$

Here  $\phi' = 2\theta$ , the true scattering angle. Now, letting

$$\begin{aligned}
H &= \Delta H - Y_s & \Lambda &= L - L_T & R &= \sqrt{R_T^2 + \Lambda^2} = R_T / \cos(\phi - \phi_T) \\
R'^2 &= R_T^2 + \Lambda^2 + R_s^2 - 2R_s[R_T \cos(\phi_s - \phi_T) + \Lambda \sin(\phi_s - \phi_T)] + H^2
\end{aligned} \tag{1.8}$$

we finally have

$$\phi' = \arccos \left[ \frac{R_T \cos \phi_T - R_s \cos \phi_s - \Lambda \sin \phi_T}{R'(\Lambda)} \right] \tag{1.9}$$

This is the fundamental equation for the process of converting channel positions into scattering angles. For calibration purposes we instead solve {1.8} for  $\Lambda$  as a function of  $\phi'$  obtaining

$$\begin{aligned}
\Lambda &= \left\{ R_T \sin \phi_T \cos \phi_T - R_s \left[ \cos^2 \phi' \sin(\phi_s - \phi_T) + \cos \phi_s \sin \phi_T \right] \right. \\
&\quad \left. - \cos \phi' \sqrt{(R_T - R_s \cos(\phi_s - \phi_T))^2 \sin^2 \phi' + H^2 (\sin^2 \phi' - \cos^2 \phi_T)} \right\} \\
&\quad / (\sin^2 \phi' - \cos^2 \phi_T)
\end{aligned} \tag{1.10}$$

### 1.3 Peak shape and position as a function of channel number

If the powder peak, as a function of scattering angle, is a Gaussian with amplitude  $A$ , centre at  $\phi_0 \leftrightarrow ch_0$  and width  $\sigma_0$ , we have for the (vanadium normalised) intensity

$$I(\phi') = A \exp \left( -\frac{1}{2} \left[ \frac{\phi' - \phi_0}{\sigma_0} \right]^2 \right) \tag{1.11}$$

where  $\phi' = \phi'(\Lambda(ch))$  and  $\phi_0' = \phi'(\Lambda(ch_0))$  are evaluated using {1.9}. Defining

$$\Phi = \frac{\phi' - \phi_0'}{\sigma_0}, \quad R_0' = R'(\phi_0'), \quad \phi_0' \triangleq \arccos \left\{ \frac{R_b}{R_0'} \right\} \tag{1.12}$$

we have

$$\begin{aligned}
\frac{\partial R_0'}{\partial \Lambda_0} &= \frac{\Lambda_0 - R_s \sin(\phi_s - \phi_T)}{R_0'} \\
\frac{\partial \phi_0'}{\partial \Lambda_0} &= \frac{1}{\sqrt{R_0'^2 - R_b^2}} \left\{ \sin \phi_T + \frac{R_b}{R_0'} \frac{\partial R_0'}{\partial \Lambda_0} \right\} \\
\frac{\partial \Lambda_0}{\partial ch_0} &= \sum_{i=1}^{n_i} i \cdot l_i (ch_0 - ch_m)^{i-1}
\end{aligned} \tag{1.13}$$

Varying  $A$ ,  $\sigma_0$  and  $ch_0$  we need the derivatives

$$\begin{aligned}
\frac{\partial I}{\partial A} &= \frac{I}{A}, \quad \frac{\partial I}{\partial \sigma_0} = \frac{I \cdot \Phi^2}{\sigma_0} \\
\frac{\partial I}{\partial ch_0} &= \frac{\partial I}{\partial \Phi} \frac{\partial \Phi}{\partial \phi_0'} \frac{\partial \phi_0'}{\partial \Lambda_0} \frac{\partial \Lambda_0}{\partial ch_0} = \\
&= \frac{I \cdot \Phi}{\sigma_0} \left\{ \sum_{i=1}^{n_i} i l_i (ch_0 - ch_m)^{i-1} \right\} \frac{1}{\sqrt{R_0'^2 - R_b^2}} \times \\
&\quad \left\{ \sin \phi_T + \frac{R_b}{R_0'^2} (\Lambda_0 - R_s \sin[\phi_s - \phi_T]) \right\}
\end{aligned} \tag{1.14}$$

*PEAKOT* uses this to fit mean channel positions of powder peaks. In *MASKOT*, however, a simple channel Gaussian lineshape is used.

## 1.4 The detector array arrangement

The present arrangement of PSD:s on SLAD is an array of three banks, each with 4 detectors, above each other making a total of 12 detectors. The up and down banks are displaced  $\pm \Delta H \approx \pm 3.65$  cm from the middle bank. In addition there might also be a common y displacement,  $H_0$ , for a detector *column* (e.g. detectors 1,5 and 9).

To cover a continuous set of scattering angles the whole detector array is possible to rotate about the sample position in the horizontal plane. Measurements are usually done at two such orientations, called the A and B position, and thus introduces another parameter,  $\Delta\phi$ , the rotation angle between the A and B position. Presently,  $\Delta\phi \approx 11.89^\circ$ .

The origin of the xyz co-ordinate system in figure 2 is defined by the intersection of the rotation axis of the detector array and the horizontal plane which is at the vertical centre of the full height of the incoming beam. This full height is about 4 cm at the sample position and the lower (fixed) limit of the beam is thus 2 cm below the  $y = 0$  plane. Reducing the beam height is done by lowering the upper limit and so displaces the sample centre from the origin as defined above. If the sample height *in the beam*,  $H_s$ , is less than the actual beam height,  $H_b$ , (e.g. in case of a half-full container) then the sample centre is even more offset from the origin. In principle the sample y offset could be obtained by fitting but a good estimate can be calculated as  $Y_s = -2 + (H_s/2)$ .  $H_s$  is the minor of  $H_b$ , and the sample height *in the container* less the part of the container below the lower beam limit. The latter is usually 1 cm in the furnace set-up and 1.4 cm in the CCR for the standard 8mm containers. For a 'full' container obviously  $H_s = H_b$ .

This means that in the general formulation of {1.10} for detector  $j$  we substitute

$$\phi_{T,j} \rightarrow \phi_{Tot,j} = \phi_{T,j} + \Delta\phi_j, \quad \Delta\phi_j = \begin{cases} 0, & \text{A position} \\ \Delta\phi, & \text{B position} \end{cases} \quad \{1.15\}$$

and

$$H = \begin{cases} H_0 + \Delta H - Y_s, & \text{Up bank} \\ H_0 - Y_s, & \text{Middle bank} \\ H_0 - \Delta H - Y_s, & \text{Down bank} \end{cases} \quad \{1.16\}$$

These generalisations are used in *CALSLAD* to get the final calibration of the SLAD instrument. The program can fit three general parameters, the wavelength  $\lambda$ , the rotation angle  $\Delta\phi$  and the detector spacing  $\Delta H$ . Then for each detector  $j$  there are two further adjustable parameters,  $R_{T,j}$  and  $\phi_{T,j}$  and one fix,  $H_{0,j}$ . The current versions of the programs uses the fundamental assumptions that  $R_s = 0$ , all  $L_{T,j} = 0$  and that bank planes are parallel to each other. Totally there are thus 27 calibration parameters. Defining

$$q \triangleq \sin \theta = \frac{Q\lambda}{4\pi}, \quad \cos(\phi') = \cos(2\theta) = 1 - 2q^2 \quad \{1.17\}$$

$$R_A \triangleq \sqrt{(R_T - R_s \cos(\phi_s - \phi_T))^2 \sin^2 \phi' + H^2 (\sin^2 \phi' - \cos^2 \phi_T)}$$

the parameter derivatives needed are

Since *PEAKOT* gives mean *channel* position and errors we also need to convert the experimental errors according to  $\sigma_{\Lambda} = \frac{d\Lambda}{dch} \sigma_{ch} = \sigma_{ch} \sum_{i=1}^{n_l} i \cdot l_{i,j} (ch - ch_{m,j})^{i-1}$ . Without any sample offset and full beam height the current set-up corresponds to the following schematic diagram.

**Figure 3** The present set-up of the detector array on SLAD. The scattering angles are those at the geometrical endpoints and centres of the Middle bank detectors calculated for a full beam height,  $H_b = 4.0$  cm. Q values (in Å) are calculated using  $\lambda = 1,116$  Å.

## 2.1 General

6

solution condition. Instead the user is requested to repeat the iterations until a satisfactory result is obtained. The smoothing procedure is based on the Savitsky-Golay method [2,3]. In all input/output descriptions "sample" stands for the sample run name, "van" for the vanadium etc.

### ***PREPI***

This program reads all raw data files of a particular runname and sums the data channelwise. There is an option to perform counting statistics on individual runs/detectors and to skip them in the output file. The output is a GENIE format file, either as a function of channel or angle. For calibration purposes the channel option should be selected.

Input files:     calib.PRM       Calibration parameters for detector start,stop channels  
                   samplexx.RAW xx are the run numbers, specified in the program

Output files:    sample.SUM ( or .PRE)

## **2.2 Mask programs**

### ***MASKNORM***

Given three .SUM files measured with each bank succesively masked this program normalises the mask data with the corresponding unmasked data from the same set of files. The normalising data can optionally be smoothed. Also the A and B positions are summed for each detector. The latter is done with respect to the screening of low angles in detectors 1, 5 and 9 in the A position, below a given channel number. There is also a check that there are no zero counts or zero errors, which is essential in order for the fitting programs to work. The output file is a three-block (U, M and D bank) GENIE file with x-values = channels = [1,4000].

Input files:     calib.PRM       Calibration parameters for detector start,stop channels  
                   mask.SUM, for UP, MIDDLE and down banks

Output files:    mask.DAT       Normalised experimental mask profiles

### ***MASKOT***

Fits the mask slit peaks profile of the Cd mask using {1.3} for each detector.

Input files:     mask.DAT       The output file from *MASKNORM*  
                   mask.MSK       Initial values for peak widths

Output files:    mask.FIT       Fitted curves in a GENIE file  
                   mask.MSK       Updated list of  $b_i$ ,  $\sigma_i$  and errors for all fitted detectors

## **2.3 Powder programs**

### ***SUMSMO***

Smooths background, vanadium and empty container. If the background is specified it is subtracted before smoothing vanadium and container and then *added on again*. The smoothing interval width can be individually chosen and if it is zero no smoothing is performed. Vanadium peaks are however always removed by fitting quadratic functions to the surrounding regions and extrapolating. The output file is in the .SUM format.

Input files:     calib.PRM       Calibration parameters for van Bragg removal etc.  
                   [back.SUM, ] van.SUM [ ,can.SUM]

Output files: [back.SUMS, ] van.SUMS [ ,can.SUMS]

### ***SUMNORM***

Subtracts container data from the powder data and normalises with vanadium, corrected for background, if desired. The data sets can also be scaled, e.g. if they have different beam heights. In order to get an estimate of the absolute cross-section one can also supply the radii and atomic densities of the sample and vanadium. There is also here a check that there are no zero counts or errors. The output file is in the .SUM format.

Input files:     calib.PRM     Calibration parameters for detector start,stop etc.  
                 sample.SUM [ can.SUM, van.SUM, back.SUM or .SUMS]

Output files:    sample.DAT

### ***PEAKOT***

Finds the positions of the Bragg peaks in channel units by fitting an angular Gaussian, corrected for channel lineshape according to {1.11}, and a linear background. This is done individually for each specified peak, one at the time. There is an option to check each peak interactively or just run 30 iterations on each of them.

Input files:     calib.PRM     Calibration parameter file for calculating channel peakshapes  
                 sample.DAT    The output file from *SUMNORM*  
                 sample.INP    Initial values for lattice parameters, peak positions etc.

Output files:    sample.OUP    General output file with fitting statistics  
                 sample.FIT    Fitted curves in a GENIE file  
                 sample.PKS    Peak list with Q values and positions etc.

### ***CALSLAD***

The final calibration parameter fit program. Parameters, in the .PRM file, or peaks, in the .PKS file, can be omitted by clearing the corresponding flags.

Input files:     mask.MSK     The result of *MASKOT*  
                 calib.PRM     The parameter file with initial values and fix/free flags  
                 sample1.PKS   The list from *PEAKOT* for the first calibration sample  
                 [sample2.PKS] Next sample  
                 ...            etc.

Output files:    sample.OUS    General output file  
                 calib.PRM     Updated calibration parameter file

## **2.4 Recommended use of programs**

First of all the relevant .DAT files has to be created by running *PREPI* and *MASKNORM* / *SUMNORM*. This probably only has to be done only once unless there is some problem with certain detectors, backgrounds, vanadium or similar. Using an old .MSK file as starting point *MASKOT* is then run at least twice, first adjusting the channel midpoint, background and amplitude, second time allowing all parameters to vary. Occasionally one needs to consider the order of the different polynomials. Next thing is to run *PEAKOT* and *CALSLAD* iteratively until satisfactorily small changes are observed in the resulting .PRM file. To do this you initially need a trial .PRM file for input to *PEAKOT*. Usually you can copy an old file. If you have powder data from (structurally) different samples you can run *PEAKOT* individually for the samples and then edit together the .PKS files. You can also fit peaks by



other means (e.g. if they are multiple) and then edit the result into a file suitable for input to *CALSLAD*. Note that the program suite is very sensitive to the number of digits; lattice parameters etc. should be given with at least 3 decimal digits in order to get overall consistency (which is one of the major intentions with these programs).

## 2.5 Some examples of the structure of input and output files

MASK.MSK:

```

12 3 2 2 4                                ! ndet, nl, nσ, nB, ninrow
1 10 1024.123169 0.04848 525.92023        ! idet, iter,  $\chi^2$ , A, chm + errors
0.64139E-03 0.43152E-01
0.63104E-01 0.39272E-05 -0.78183E-11      ! linear position coefficients + errors
0.25602E-04 0.74763E-07 0.42048E-09
0.11988E+00 -0.11281E-02 0.18677E-03      ! PSD width coefficients + errors
0.21539E-02 0.17198E-03 0.14946E-04
0.11015E-01 -0.23916E-04 0.67051E-07      ! background coefficients + errors
0.38768E-02 0.15985E-04 0.15170E-07
...                                         ! repeated for each detector
1 1                                         ! flags for varying A, chm
1 1 1                                       ! flags for varying linear coefficients
1 1 1                                       ! flags for varying width coefficients
1 1 1                                       ! flags for varying background coeff.
...                                         ! repeated for each detector
201 860                                    ! start and stop channels
...                                         ! repeated for each detector

```

SAMPLE.INP:

```

1          ! Symmetry code
2.866000   ! lattice parameter
.0 .0 3.6   ! Rs,  $\phi$ s, and Hs
1 1 1 0 1 1 ! fit flags for p0, A0,  $\sigma_1$ ,  $\sigma_2$ , A, B
2 3 11 6    ! npos, nrows, npks, nsig
h k l
1 1 0
2 0 0
2 1 1
2 2 0
3 1 0
2 2 2
3 2 1
4 0 0
3 3 0
4 2 0
3 3 2

```

where

Symmetry code 1 = cubic , 2 = tetragonal, 3 = orthorhombic, 4 = hexagonal  
Lattice parameter: a (cubic) a,c (tetragonal) a,b,c (orthorhombic) a,c (hexagonal)  
R<sub>s</sub>,  $\phi$ <sub>s</sub>, and H<sub>s</sub>, sample offset parameters  
p<sub>0</sub> = peak position  
A<sub>0</sub> = peak amplitude  
 $\sigma_1$  = Peak width for lamda1 component  
 $\sigma_2$  = Peak width for lamda2 component  
A = constant background term  
B = linear background term

npos = Nr of detector array positions  
 nrows = Nr of detector banks  
 npks = No. of peaks to fit  
 nsig = Width of peak region to fit in units of peak width  
 h, k, l = Miller indices of the peaks

SAMPLE.PKS:

```

    .000    .000    3.600 ! Rs,  $\phi_s$ , and Hs, sample offset parameters
      Q      chm    echm    gsig    egsig    gsig2    egsig2    lsig ip id if
    3.100407 306.5928 .0119 .34662 .00035 .00000 .00000 .12569 1 2 1
    4.384637 671.8882 .0200 .32712 .00069 .00000 .00000 .11811 1 2 1
    6.200814 256.7963 .0178 .26533 .00052 .00000 .00000 .10698 1 3 1
    6.932721 516.9666 .0163 .32926 .00047 .00000 .00000 .07079 1 3 1
  
```

where

R<sub>s</sub>,  $\phi_s$ , and H<sub>s</sub> sample offset parameters  
 Q = Module of the scattering vector (calculated from lattice parameters)  
 chm = Peak channel position (<1000)  
 echm = Peak position error  
 gsig = Peak width  
 egsig = Peak width error  
 gsig = Peak width for lamda2 component  
 egsig = Peak width error for lamda2 component  
 ip = position code, 1 = A position, 2 = B position  
 id = detector nr  
 if = flag (set by default) to indicate if peak is used in fit

SAMPLE.PRM:

CALIBRATION PARAMETERS

```

      2      12
    1.116102 .000000 11.889000 3.650000 1 0 0 0
    2.666519 -2.466908 .870916 1 1 1
    1.115845 .000000
    .000000 .000000 .000000 0 0 0
    19.00 4096. .00
    2.5957 102.95180 .00000 1 1
    ...
    541 940 201 920
    ...
      3      2
    518.0769 .633640E-01 .188430E-05 .204460E-09
    .1145 -.658220E-03 .239680E-03
    ...
  
```

! npos,ndet  
 ! lamda,dPhi,dH and flags  
 ! U1, V1 and W1 and flags  
 ! lamda2,wlamda2  
 ! U2, V2 and W2 and flags  
 ! taumon,monmult,taudet  
 !  $\phi$ , R<sub>T</sub>, H<sub>0</sub> and flags  
 ! repeated for each detector  
 ! ista,isto  
 ! repeated for each detector  
 ! nlp,nsp  
 ! lco  
 ! sco  
 ! repeated for each detector

where

n<sub>pos</sub> = No. of detector array positions  
 n<sub>det</sub> = No. of detectors  
 U1, V1 and W1 = Gaussian peakwidth parameters for lamda1  
 lamda2,wlamda2 = second wavelength and fractional weight  
 U2, V2 and W2 = Gaussian peakwidth parameters for lamda2  
 taumon = Monitor count deadtime  
 monmult = Monitor count multiplier  
 taudet = Detector count deadtime  
 ista,isto detector start and stop channels for each position

nlp,nsp order of the linear position and width polynomials  
lco detector centre channel and linear position coefficients  
sco linear width coefficients

### 3. References

- [1] Numerical Recipes, 2nd ed., eds. William H. Press, Saul A. Teukolsky, William T. Vetterling, Brian P. Flannery, Press Syndicate of the University of Cambridge, Cambridge, 1992.
- [2] A.Savitsky and M.J.E.Golay, *Anal.Chem.*, **36** (1964) 1627
- [3] A.Proctor and P.M.A Sherwood, *Anal.Chem.*, **52** (1980) 2315