**Fitting 3D Single Crystal X-ray Diffuse Scattering in RMCProfile.**

The input file with diffuse-scattering intensities must have the following format:

* The 1st line contains two digits: the total number of pixels and the number of symmetrically equivalent points, *nsym*. If no symmetrization is used, nsym=1.
* The first 3 columns are digits enumerating pixels in a 3D data grid;
* The following 3 columns specify *k*x, *k*y, and *k*z coordinates (in Å-1) of each pixel, which represent components of the corresponding reciprocal-lattice vector (i.e. **k**=2π/**a**);
* The last column specifies the intensity on either linear or logarithmic scale.

Symmetry can be used to improve signal-to-noise ratio. Space group symmetry applies to Bragg reflections but not necessarily to diffuse scattering. If certain symmetry is assumed, it can be accounted for by inserting sets of additional 3(*nsym*-1) columns between the 1st set of three *k*-coordinates and the intensity column. Each of these sets specifies the coordinates *k*x, *k*y, and *k*z of symmetrically equivalent reciprocal-lattice points that are expected to have the same intensity. The program will calculate the average intensity over the equivalent *nsym* points and compare it with the corresponding experimental value. Since I(**k**)≡I(-**k**), there is no benefit in using this symmetry.

If certain pixels/*k*-points need to be excluded from the fit, their intensity should be set to zero. The program will still calculate and printout the diffuse-scattering intensities at these points but ignore their values while evaluating the residual.

If noise in the calculated signal as caused by limited statistics presents a problem, it can be smoothed using a Gaussian filter. The size of the kernel is specified in the control .**dat** file as described below.

The 3D diffuse-scattering capability is activated using the following block of keywords in the .**dat** file:

DIFFUSE\_SCATTERING3D ::

> FILENAME :: ! specify name of the input file with diffuse-scattering intensities

> FITTED\_SCALE :: ! use this card for fitting the scale factor for diffuse-scattering or

> CONSTANT\_SCALE :: ! use this card to keep the scale fixed. The scale-factor value must be specified here.

> FITTED\_OFFSET :: ! use this card to fit the signal offset

> CONSTANT\_OFFSET :: ! use this card to set a constant offset; the offset value must be specified

> WEIGHT :: ! weight assigned to the diffuse-scattering dataset in the total residual; if using the WEIGHT\_OPTIMIZATION option (recommended) set to 1.0

> KERNEL3D :: 3 3 3 ! size of the kernel (in pixels) for the Gaussian filter; in this example it’s a cube with a side of 3 pixels

The intensity scale, linear or logarithmic, is specified using keywords LINEAR ::

or LOGARITHMIC :: as in

NUMBER\_DENSITY ::

MINIMUM\_DISTANCES ::

MAXIMUM\_MOVES ::

R\_SPACING ::

PRINT\_PERIOD ::

TIME\_LIMIT ::

SAVE\_PERIOD ::

ATOMS ::

BOX\_SIZE ::

VALENCE ::

LINEAR ::

NO\_BACKGROUND ::

INPUT\_CONFIGURATION\_FORMAT ::

SAVE\_CONFIGURATION\_FORMAT ::