An Example input file for Gudrun

The parameter file is divided up into 6 parts. These contain the information Gudrun requires about the instrument, the beam, the vanadium rod, the empty diffractometer, the sample and the can. The last four sections will require the most corrections.

In all instances, the run numbers will need to be altered. These numbers are always read in using two lines. The first line is gives the number of runs recorded and the period number (which is always 1). The second line then lists each run number. For example:

4 1
19000 19001 19005 19014

These values, and other lines which will always need altering are highlighted in red in the example file below. Other possible alterations which should be concidered are highlighted in blue. For alternate can sizes, see appendix B.

'INSTRUMENT'

Very little needs changing in the instrument section, provided you are consistent about the locations in which you store your files. The three lines which may require altering are highlighted in blue.

'GEM'	*Instrument abbreviation*
'C:\gem_data'	*Directory of Raw data files*
'RAW'	*Extension of data files*
'C:\Gudrun\GEM_DET_034c1.DAT'	*location of detector file*
6	*User Table column number for phi values*
'C:\Gudrun\groups_def.dat'	*location of the bank grouping file*
2 5 8 0.000	*No. of spectra and spectrum numbers for incident monitor*
0.5 3	*Wavelength range for monitor normalisation*
1 4 0.000	*No. of spectra and spectrum numbers for transmission monitor*
30 4980	*First and last channel numbers for spike analysis (0s for full range)*
1 4	*Flag to decide whether spike analysis will be done*
0.1 3.5 0.1	*Min. and max. wavelengths to be used, and wavelength step size*
100 30	*No. of smoothings on monitor and vanadium*
0.1 0.02 60	*Q_min, Q_step, Q_max,*
0 0 0 0	*signals end of individual group Q ranges,otherwise group number,*
1	*Flag to get 1 group (0) or nn groups (1)*
650	*Number of spectra to read and process at one time*
0.4 4	*Acceptance factor and merge power.*
0 1	*Single atom scattering subtraction (1,0), Statistical weights on merge*
0 0 50	*Q width of smoothing function and R-min for background subtraction on DCS data, and Lorch width in Q for window function*
0	*Spectrum number for diagnostic files (0 to give no files)*

'BEAM'

Again, this section will require very little alteration, if you are using the standard beam size of 15 x 40 mm. If an alternative beam size is used, this can be altered in the line printed in blue.

2	*No. of profile values*
1.0 1.0	*Profile values*
0.05 0.2 100	*Attenuation step (cyl), m.s. step (cyl), no. of slices (flat)*

10 *Angular step (integer degrees) to calculate corrections at*
-0.75 0.75 -2.0 2.0 *Incident beam edges relative to centre of sample*
-2.000 2.000 -2.1 2.1 *Scattered beam edges relative to centre of sample*
'spectrum000.dat'
1.0 *Background factor*

'VANADIUM'

If the 8mm vanadium rod was used, then only the run numbers will need altering in this section. The run numbers for the data measured of the vanadium rod are given first, followed by the data for the empty diffractometer. If a V rod with an alternative radius is used, the line highlighted in blue will need to be changed to give the correct inner and outer radius. For a rod

4 1 *No. of files for vanadium and period number*
30718 30729 30739 30747 *Run number(s) to be used for vanadium*
3 1 *No. of files for vanadium background and period number*
30722 30731 30746 *Run number(s) to be used for vanadium background*
1 *=1 forces calculation of corrections, else 0*
'V' 0 1.0 *Element symbol, mass no. (0=natural), relative abundance*
' ' 0 0 *Signals no more elements*
1 *V geometry: 1 = cylinder, 2 = flat plate*
0.0 0.417 *Inner and outer radius of vanadium in cm*
7.0 *"Height" (cyl) or "angle and width" (flat) of vanadium (deg and cm)*
-0.07216 *Density (gm/cm**3) (or Atoms/A**3 if negative)*
300.0 *Vanadium Temperature (K) for Placzek correction*
'TABLES' *Calculate from tables*
' ' 0 0 *Vanadium merged dcs file and smoothing parameters*

'SAMPLE BACKGROUND'

The run numbers for the empty diffractometer data is required.

3 1 *No. of files for sample background and period number*
30722 30731 30746 *Run number(s) to be used for sample background*

'SAMPLE'

Several things are required to be inputted for the correct analysis of the sample data. The run numbers are required first. And then the elements in the samples along with the isotope (0=natural, otherwise imput the correct isotope value – remember to enter each isotope present) and the fractional abundance.

*The inner and outer radius is defaulted for the contents of the 8.3 mm can. If you used an alternative can, this needs to be altered. Finally the height of the sample in the can, and the effective density (mass in can/ pi*r^2*height of sample) are needed.*

4 1 *No. of files for sample and period number*
30742 30743 30744 30745 *Run number(s) to be used for sample*
1 *=1 forces calculation of corrections, else 0*
'Mn' 0 0.0772 *Element symbol, mass no. (0=natural), relative abundance*
'P' 0 0.2416
'O' 0 0.6812
' ' 0 0 *Signals no more elements*
1 *S geometry: 1 = cylinder, 2 = flat plate*

0.0 0.541	*Inner and outer radius of sample in cm*
8.0	*"Height" (cyl) or "angle and width" (flat) of sample (deg and cm)*
1.635	*Density (gm/cm**3) (or Atoms/A**3 if negative)*
0	*Sample Temperature for Placzek correction*
'TABLES'	*Gets c/s from tables*
1.0	*Sample tweak factor*

0.0 0.0 *Min and max wavelength for each resonance. 0 0 to signal end*

'CONTAINER'

The final section needs to have the run numbers for the empty can entered. If the can size is not 8.3 mm, then the inner and outer radii, and the height of the can also need to be altered. This assumes that a vanadium can has been used. If this is not the case, the elemental makeup and density will also need altering.

2 1	No. of files for container and period number
30740 30741	Run number(s) to be used for container
'V' 0 1.0	Element symbol, mass no. (0=natural), relative abundance
' ' 0 0	Signals no more elements
1	V geometry: 1 = cylinder, 2 = flat plate
0.541 0.557	Inner and outer radius of container in cm
8.10	"Height" (cyl) or "angle and width" (flat) of container (deg and cm)
-0.07216	Density (gm/cm**3) (or Atoms/A**3 if negative)
'TABLES'	Gets c/s from tables
1.0	Sample tweak factor

'GO'
'END'