Chapter 4.1

NUMERICAL

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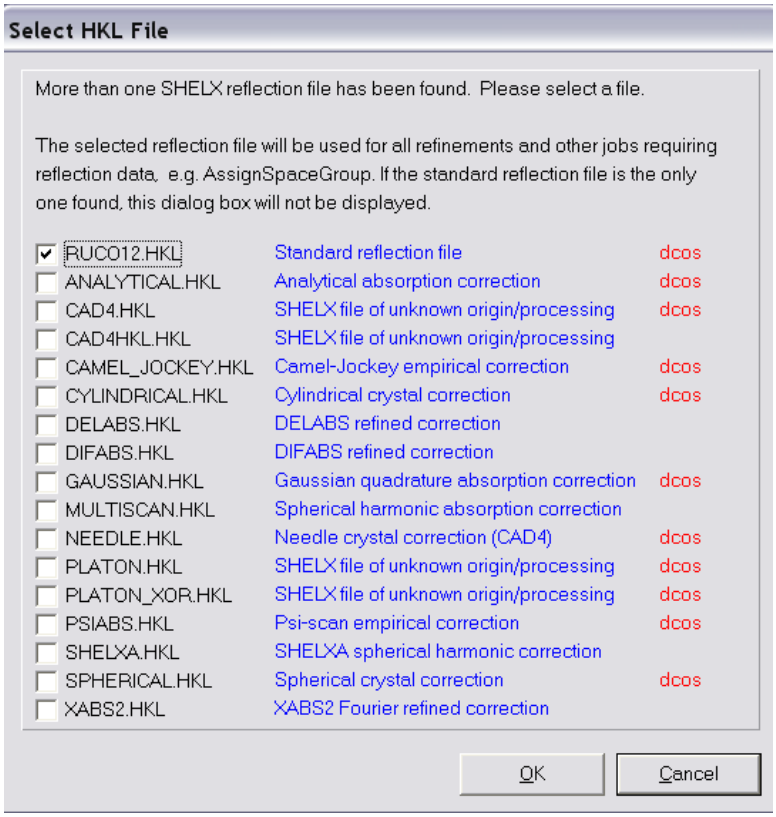
These methods provide mathematically exact absorption corrections, providing of course that the input data are correct. The first two methods require that the crystal faces have been indexed, and the distances of the crystal faces from the centre of rotation have been measured. This can be very difficult to do accurately.

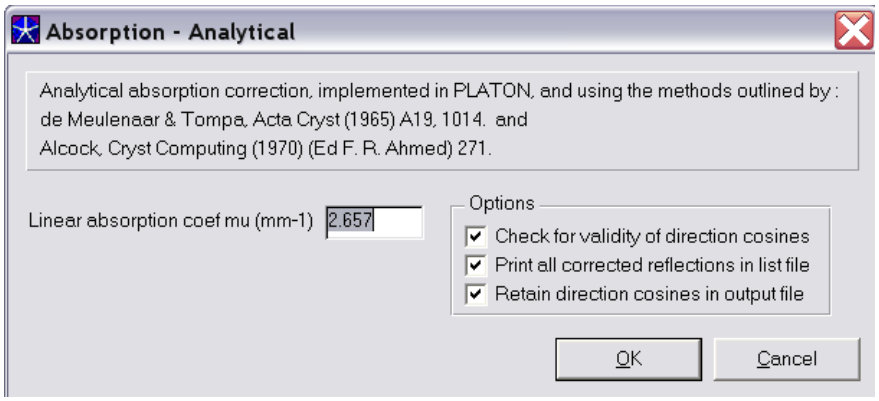
The reflection file that is actually used for input (though indicated as *name.HKL* in the following descriptions) is the file selected through the "Set HKL File" menu item If more than one SHELX style reflection file is found, the following window is displayed :



This window indicates whether the reflection file contains direction cosines. For many absoprtion corrections, these are essential. The Serial data processing programs XCAD4/PROFIT will normally include direction cosines in their output reflection files, but this will not normally be the case for Area detector processed data.

The auxilliary program XtalView is provided as a useful check that the proposed set of indices and distances accurately describe the crystal. XtalView reads the file FACES.DEF (section 4.1.6) and allows the user to edit it interactively. This file is read by the programs ANALYTICAL and GAUSSIAN.

4.1.1 - ANALYTICAL Absorption Correction



Synopsis

The procedure of de Meulenaar, Tompa and Alcock as implemented in PLATON is used. The required data are the indices of the faces (which must make up a closed polyhedron) and the distance of the centre of rotation of the polyhedron to each face (in mm). The required files are name.INS and name.HKL. The latter file MUST contain direction cosines corresponding to the cell in the name.INS file. The direction cosines are removed in the output file.

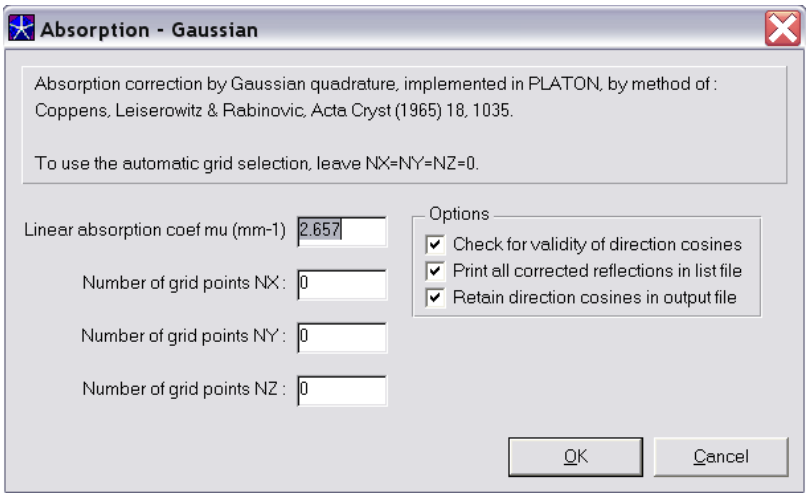
Files read

name.INS (for unit cell information only).
name.HKL - uncorrected reflection file.
FACES.DEF - face indices and distances. This file may also be created interactively by the program.

Files written

ANALYTICAL.HKL - absorption corrected reflection file
ABSORB.LST - PLATON list file giving a list of the applied corrections
ABSORB.CIF - CIF containing relevant information

4.1.2 - GAUSSIAN Absorption Correction



Synopsis

The method of Gaussian integration as implemented in PLATON is used. The required data are the indices of the faces (which must make up a closed polyhedron) and the distance from the centre of rotation of the polyhedron to each face (in mm). The required files are name.INS and name.HKL. The latter file MUST contain direction cosines corresponding to the cell in the name.INS file. The direction cosines are removed in the output file.

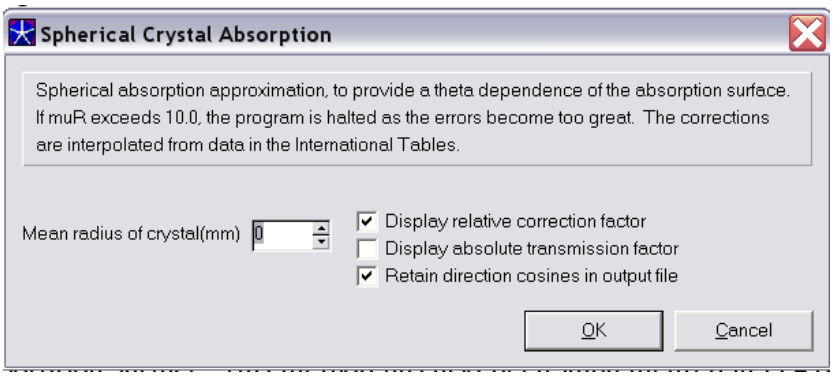
Files read

name.INS (for unit cell information only)
name.HKL - uncorrected reflection file
FACES.DEF - face indices and distances. This file may also be created interactively by the program.

Files written

GAUSSIAN.HKL - absorption corrected reflection file
ABSORB.LST - PLATON list file giving a list of the applied corrections
ABSORB.CIF - CIF containing relevant information

4.1.3 - SPHERICAL Absorption Correction

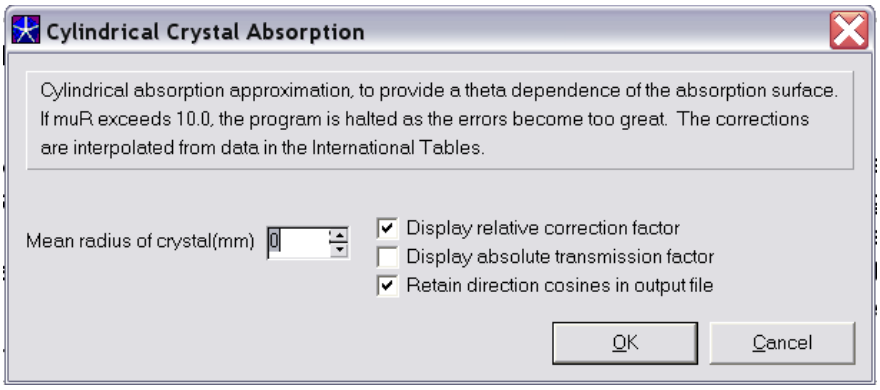


Synopsis
This provides a correction for spherical crystals, effectively the theta dependence of the absorption surface. If muR exceeds 10.0 the program is aborted, as the errors will be too large. The only required input is the mean spherical radius of the crystal in mm. The correction is calculated by interpolation of data from International Tables. If direction cosines are present in the input reflection file, these will be echoed to the output file.

Files read
name.INS (for unit cell information only)
name.HKL - uncorrected reflection file

Files written
SPHERICAL.HKL - absorption corrected reflection file
ABSORB.CIF - CIF containing relevant information

4.1.4 - CYLINDRICAL Absorption Correction



Synopsis

This provides a correction suitable for cylindrical or needle crystals, where the crystal is mounted along the cylinder axis. If muR exceeds 10.0 the program is aborted, as the errors will be too large. The only required input is the mean cylindrical radius of the crystal in mm. The correction is calculated by interpolation of data from International Tables. If direction cosines are present in the input reflection file, these will be echoed to the output file.

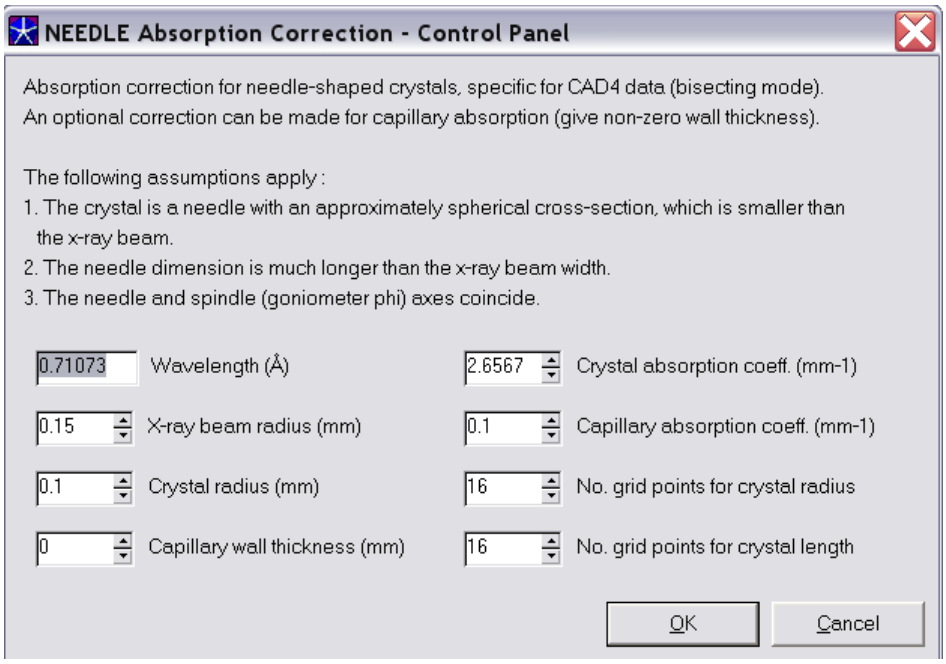
Files read

name.INS (for unit cell information only)
name.HKL - uncorrected reflection file

Files written

CYLINDRICAL.HKL - absorption corrected reflection file
ABSORB.CIF - CIF containing relevant information

4.1.5 - NEEDLE Absorption Correction



Synopsis
This provides a CAD4 specific correction suitable for cylindrical or needle crystals, where the crystal is mounted along the spindle axis. It will be useful for crystals where the needle axis is very much longer than the X-ray beam width. A GUI is presented for further information and user input. If direction cosines are present in the input reflection file, these will be echoed to the output file.

Files read
name.INS (for unit cell information only)
name.HKL - uncorrected reflection file

Files written
NEEDLE.HKL - absorption corrected reflection file
ABSORB.CIF - CIF containing relevant information

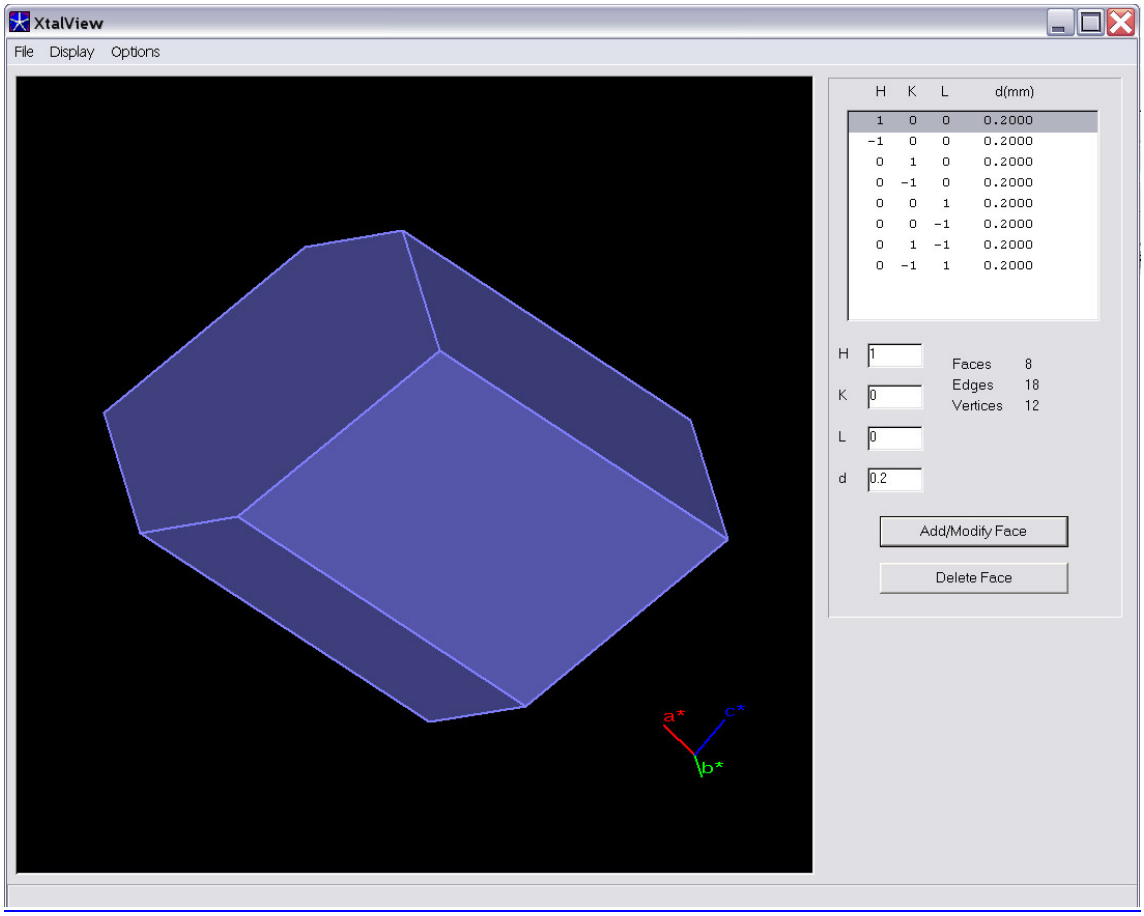
4.1.6 The FACES.DEF File

This file contains the face index and distance information about the crystal. It is a SHELX style free format text file with four-character data identifiers. It may either be created manually with a text-editor, created by the ANALYTICAL or GAUSSIAN absorption correction programs, or by the visualisation program XtalView. The format is as follows

```
TITL    test crystal shape for NaWO4.2H2O
CELL    8.4797  10.5930  13.8527   90.0   90.0   90.0
FACE    0   0   1   0.0387
FACE    0   0  -1   0.0387
FACE    1   0   0   0.1225
FACE   -1   0   0   0.1225
FACE    0   1   0   0.1375
FACE    0  -1   0   0.1375
FACE    0   1   2   0.0825
FACE    0  -1  -2   0.0825
FACE    0   1  -2   0.0825
FACE    0  -1   2   0.0825
FACE    1   0   1   0.1050
FACE   -1   0  -1   0.1050
FACE   -1   0   1   0.1050
FACE    1   0  -1   0.1050
ABSC   18.669
GRID    5
```

The TITL card is optional if you want to put a title in the picture
The GRID entry allows the user to modify the default setting of the %age accuracy required (5%). It is only used for the GAUSSIAN correction in the Area Detector programs

4.1.7 The XTALVIEW program



This program allows the user to visualise the crystal faces in the file FACES.DEF and also to edit the dimensions of add new faces. The viewpoint may be changed interactively by mouse dragging and the reciprocal space axial directions are also rotateds