

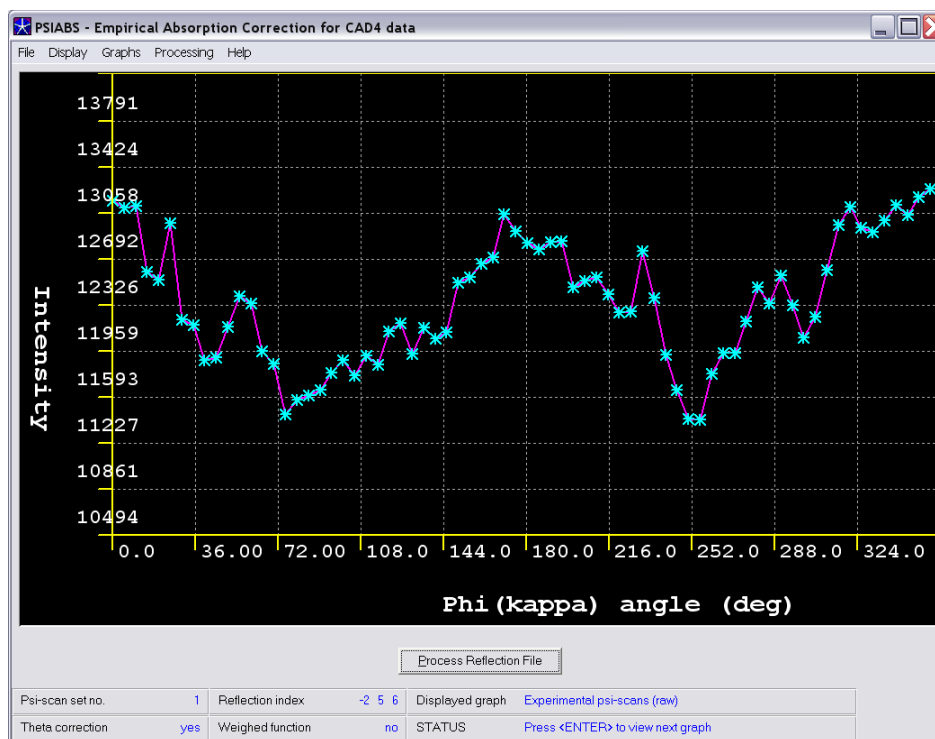
Chapter 4.2.1

SEMI-EMPIRICAL METHODS

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These methods provide an approximate correction, based on an experimentally determined absorption surface. They require extra intensity measurements to be performed. The least demanding of extra information is the PSI-SCAN method, the most demanding is Blessing's MULTISCAN method. CAMEL_JOCKEY has effectively been superseded by MULTISCAN.

4.2.1.1 - PSIABS absorption correction



Synopsis

This routine uses the method described by North, Phillips and Mathews, and is specific for CAD4 data. Up to 10 psi-scan sets may be processed and the present implementation has an important restriction in that ALL sets must contain the SAME number of measurements for the SAME incremental psi-angles. This is because this data is averaged in the calculation of the transmission surface. The psi-scan curve may be Fourier smoothed and specified curves may be omitted from the averaged transmission surface. A theta (spherical crystal) correction may also be applied. Graphical output is provided to display the original psi-data, the averaged psi-curve and Fourier smoothed psi-curves, and a final comparison between the corrected and uncorrected data. Once the transmission surface has been adopted, a corrected reflection file may be written using the Process menu item. If direction cosines are present in the uncorrected file name.HKL, these will be echoed to the corrected output file.

NOTE The approximations inherent in the psi-scan method make it unsuitable for

highly absorbing crystals. For these samples a GAUSSIAN or ANALYTICAL or refined absorption correction should be used.

Files read

name.INS (for unit cell information only).

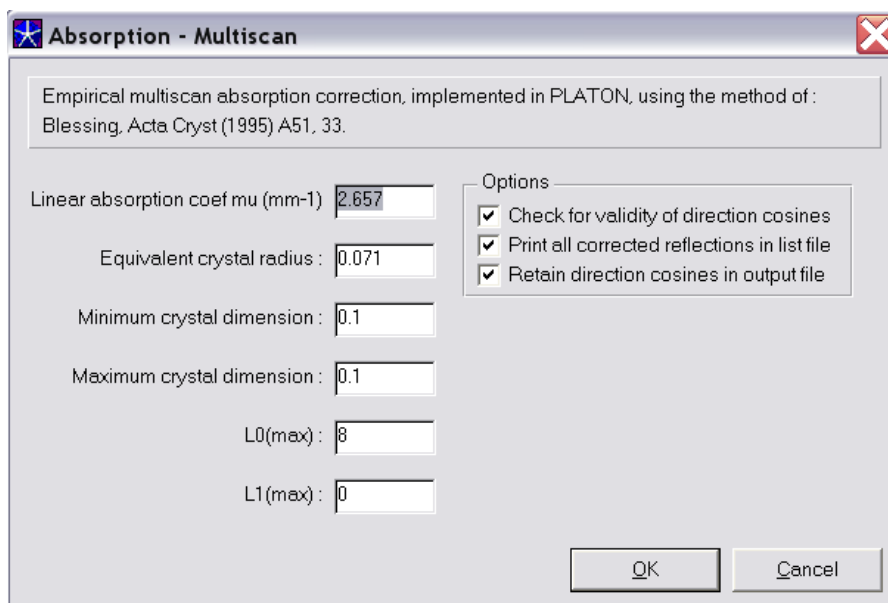
name.HKL - uncorrected reflection file.

name.PSI (or PSI.DAT) - CAD4 diffractometer file containing psi-scans.

Files written

1. PSIABS.HKL - absorption corrected reflection file
2. PSIABS.LST - List file giving summary of the applied corrections
3. PSIABS.CIF - CIF containing relevant information

4.2.1.2 - MULTISCAN absorption correction



Synopsis

This program requires the data set to contain an extensive set of equivalents, and is primarily of interest for data collected using area-detectors, which routinely have a large degree of over-determination. It models the absorption surface using a spherical harmonic series based on differences between equivalent reflections and will probably not be very effective for triclinic and monoclinic crystal systems (since these have fewer equivalences).

It is based on the code of **Blessing** in SORTAV and is implemented in PLATON. It requires a .INS and .HKL file. The latter must have direction cosines consistent with the cell in the .INS file.

Files read

name.INS (for unit cell information only).

name.HKL - uncorrected reflection file containing as many equivalents as possible.

Files written

MULTISCAN.HKL - absorption corrected reflection file

ABSORB.CIF - CIF containing relevant information

ABSORB.LST - PLATON list file giving summary of the applied corrections