ABSORB V 7.2
Programmers manual

RJ ANGEL

rossangelsoftware@gmail.com

http://www.rossangel.com

This document is intended to provide the information necessary to interface other software, such as diffractometer control or data reduction programs, with the Absorb program. It should be read in conjunction with the *Users' Manual* for ABSORB.

This version of December-2014.

CONTENTS

INTRODUCTION

ABSORB is a program to correct single-crystal X-ray intensity datasets for the effects of absorption by the crystal and by diamond-anvil pressure cells, separately or together. It can be used for data collected with either an area detector or a point detector.

Version 7 was started in January 2012. It includes the reconfiguration of the main program to run independently of any calling program, so as to allow it to be run from commercial and other software applications.

New Features in Version 7

This is a brief list of new features and changes to ABSORB, compared to the previous version 6.2:

- ABSORB is now a stand-alone program that can be run from other data reduction programs.
- There is a new GUI to set up the description of the crystal and diamond-anvil cells in the *experiment* file.
- Absorption coefficients are now in mm^{-1}.
- Sizes of DAC components are now in mm.
- New handling of negative intensities and $\sigma(I)$
- Mass absorption coefficients added for Ag radiation. And wavelength can be specified by target material.
- ABSORB ORIGIN to specify model origin.
- DAC SMALLBEAM to handle cases where the beam size is much smaller than the crystal.
- DAC CRYSTAL defined to allow ABSORB FACE cards to be used to describe a crystal in a DAC.
- DAC PHIZERO to handle DACs which are not set face-on to the incident beam.
- Improved formatting of information in print file.
- A distinction is now made between the *sample* coordinate system and the ϕ-axis axial system.
- Further improvements to the checking of the consistency of the input information about the crystal and DAC.
- Correction factors now written to a *scales* file to enable the absorption corrections to be applied by other programs.

Further details of all of these new features can be found in the relevant sections of this manual and the *Users' Manual*.

Version 7.2 was released in December 2014; it includes minor bug fixes, as detailed in the last section of the users' manual.

The program runs on Windows-2000, Windows-NT, Windows-XP Windows-7 (32 and 64 bit) and Win-98 machines.

The ABSORB program is distributed on a non-commercial basis and the author would appreciate its use being acknowledged by reference to both the original publication describing the first version of the program and the current description as follows:

> Angel RJ, Gonzalez-Platas J (2013) ABSORB-7 and ABSORB-GUI for single-crystal absorption corrections. *Journal of Applied Crystallography*, 46:252-254.

Details of the calculation methods and earlier versions of the program can be found in:

> Burnham CW (1966) Computation of absorption corrections and the significance of end effects. *American Mineralogist,* 51:159-167.
> Angel RJ (2004) Absorption corrections for diamond-anvil cells implemented in the software package Absorb 6.0. *Journal of Applied Crystallography*, 37:486-492.

Disclaimer

While every effort is made to ensure that the ABSORB software is free of bugs and errors, people use it at their own risk. No responsibility whatsoever is taken for either incorrect results or for any physical, mental or other damage arising from use of ABSORB or from errors in this manual.

ABSORB USER FILES

The program that performs the absorption corrections on X-ray intensity data is referred to as 'ABSORB'. The ABSORB program uses 6 files related to the user's experiment:

- Information about the crystal model, diamond-anvil cell, and diffractometer are provided by the user in the *experiment* file.
- Intensity data for correction is supplied in the *input data* file, either in SHELX *hkl* format or RFINE format.
- The results are report in a text *print* file.
- The corrected data are written to an *output data* file, either in SHELX *hkl* format or RFINE format.
- The scale factors for the corrections calculated by ABSORB are written to a *scales* file.
- Information about the corrections are written to a *cif* fragment.

The details concerning the content and format of these files are given below. One critical point to note – the SHELX *input data* file **must** contain direction cosines for each reflection. Other data file formats can be added to ABSORB if necessary.

INTERFACING

The method of interfacing uses text files located in the same folder as the *absorb.exe* file. This is rather primitive but is intended to allow flexibility and interaction with a variety of other programs, and without having to install ABSORB in the Windows registry.

However, note that installation of the ABSORB-GUI program does specify the environment variable ABSORB in the Windows registry, and sets it to point to the location of Absorb.exe.

The sequence of operations for running ABSORB is as follows:

1. The intensity data are integrated and stored with direction cosines in the *input data* file (usually a SHELX *hkl* file).
2. The *experiment* file containing information about the experiment, and instructions for the corrections to be performed is created.
3. The names of the *output data* file and the *print* file are decided.
4. The information about file names and formats is written to the *absorb_config.dat* file that is located in the same folder as *absorb.exe.*
5. The *absorb.exe* is run. The actions of the program are:
   a. It creates an *absorb.lck* file in the same folder as *absorb.exe.*
   b. It deletes the *absorb_error.log* from the same folder as *absorb.exe.*
   c. It reads the filenames and some configuration flags from the *absorb_config.dat.*
   d. It reads the *experiment* file and performs the absorption corrections on the data, and writes the results to the *print* file, and the *output data* file.
   e. If there are warnings or errors, they are recorded in both the *print* file and the *absorb_error.log*. The existence of the *absorb_error.log* indicates an error or warning has occurred.
   f. On completion (with or without error), the *absorb.lck* file is deleted.
6. The program calling ABSORB should test for the existence of the *absorb.lck* file. When it no longer exists, ABSORB has finished.
7. On completion of ABSORB, the calling program should check for the existence of the *absorb_error.log* file. If it does not exist, no error occurred.

THE LOCK FILE

The existence of the *absorb.lck* file in the same folder as *absorb.exe* indicates that either ABSORB is running, or that the program crashed (very unusual for release versions). ABSORB checks for the existence of the *absorb.lck* file, so ABSORB cannot be run if the lock file exists. Therefore it is the responsibility of the calling program to determine whether the *absorb.lck* file exists and, if it does, what action to take. Our own ABSORB-GUI presents the user with the opportunity to delete the *absorb.lck* file and to run ABSORB, or to exit.

THE CONFIGURATION FILE

Starting with Absorb version 7, the names of files to be used by *absorb.exe* to perform the absorption corrections are provided with other run-time instructions to the program via a *configuration file*. This file must be named *absorb_config.dat* and it must reside in the same directory or folder as the executable. This is a text file and can be created by a suitable editor such as *Windows Notepad* or *Wordpad*, or written by another program. This allows ABSORB to be called from other software.

For example, the program Absorb7browser allows the user to select files, writes the *absorb_config.dat*, and runs the ABSORB program.

The general *format* of the configuration file is that the first six characters of each line are read as a label. The label defines the content of the rest of the line. If the first six characters of a line are blank, then the remainder of the line is ignored; blank labels can therefore be used to space out the information or to add comments (see the example below). The lines can appear in any order within the file. The information is read by Fortran free-format read statements, so floating-point values should include a decimal point, and integer values must not contain a decimal point. Otherwise the format is free. Individual numerical values on the same line can be separated by commas or spaces.

Here is an example of *absorb_config.dat*:

```
    This is the configuration file for Absorb
    Created on: 02-FEB-12   at 20:49:30

RUN   1
EXP   C:\Users\rangel\Documents\RJA_Software\Reduce_Refine\Absorb\Absorb7\test\example3.exp
PRINT  C:\Users\rangel\Documents\RJA_Software\Reduce_Refine\Absorb\Absorb7\test\new.prt
INPUT
C:\Users\rangel\Documents\RJA_Software\Reduce_Refine\Absorb\Absorb7\test\example234.hkl
OUTPUT C:\Users\rangel\Documents\RJA_Software\Reduce_Refine\Absorb\Absorb7\test\test3.hkl
INFORM 2
OFORM  2
INCOMM 0
```

The first three lines have blanks in the first six characters and are therefore treated as comments. It is recommended to document the creation of the file in some way, as illustrated here. The remainder of the key words are:

RUN sets the run configuration. Values:
- 0 suppresses all interactive communication (e.g. warning and error boxes) from ABSORB, so that these messages only appear in the print and error log files.
- 1 allows all interactive communication (e.g. warning and error boxes) from ABSORB, so that these messages appear both in pop-up dialog boxes and in the print and error log files.

EXP specifies the location and name of the *exp* (experiment) file.

PRINT specifies the location and name of the *print* file.

INPUT specifies the location and name of the *input data* file.

OUTPUT specifies the location and name of the *output data* file.

All four of these filenames must be present. They must all include the full absolute path name of the file, and the extension.

INFORM specifies the input file format with a single integer.

OFORM specifies the output file format with a single integer.

The allowed values for INFORM are:

- 1 RFINE format files (*int* for input)
- 2 SHELX format files with direction cosines
- 3 Raw format files

The allowed values for OFORM are:

- 1 RFINE format files (*abs* for output)
- 2 SHELX format files with direction cosines

INCOMM specifies whether the data files include incommensurate data. Values:

- 0 normal data
- 1 incommensurate data. Only valid for SHELX and Raw files. The incommensurate indices must always be given as 6 integers (3 for the Bragg indices plus 3 for the satellite, whatever the dimensionality of the incommensurate structure). The indices are not used by ABSORB, but just copied to the output file.

Other instructions and controls could be added to this file, if required.

THE ERROR LOG FILE

The *absorb_error.log* is deleted when ABSORB is run. It is only created in the same folder as *absorb.exe* if a warning or error occurs. There are two levels of errors:

- *Warnings* alert you to *potential* problems with the model described in the *experiment* file that may or may not be fatal to the calculation depending on other details in that file. Program execution continues after a warning.

- *Errors* are fatal and prevent further execution of the program. An example would be a dataset supplied as a SHELX file, but without the orientation matrix being given in the *experiment* file. Program execution is halted after an error.

In the log file the warning or error message is prefaced by the string *****WARNING or *****ERROR as appropriate. These messages are duplicated in the *print* file.

AXES AND COORDINATE SYSTEMS

Cartesian Axial Systems

In order for the program to calculate the correct path lengths for the incident and diffracted X-ray beams in both the crystal and the DAC (if present), the reflection data, the crystal shape, and the DAC must all be described on a self-consistent set of coordinate axes, diffractometer circle parities and zero positions. This section expands upon the information provided in the *User's Manual.*

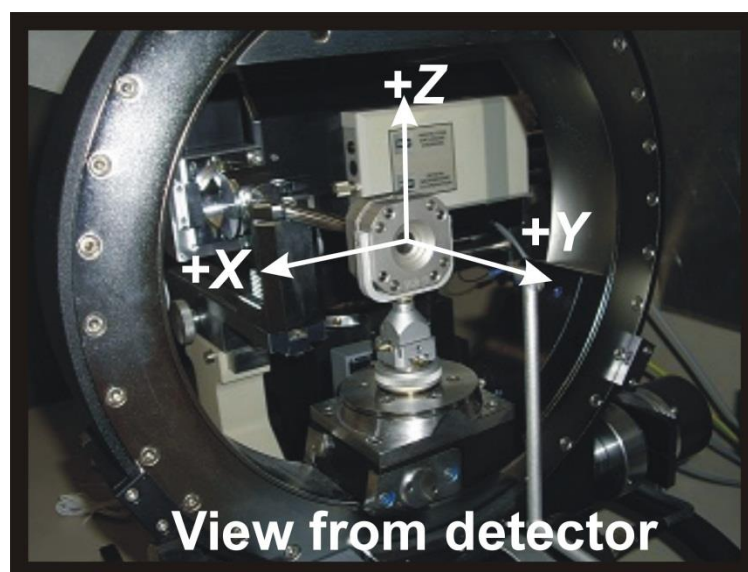The origin of all coordinate systems is at the centre of the diffractometer. Note the following:

- ABSORB does not require that the origin lies within the crystal.

- If a crystal is described in terms of the distances and indices of faces (by ABSORB MODEL HKL) from a point that is not at the goniometer centre the coordinates of that reference point can be specified by ABSORB ORIGIN.

- With DACs the origin is at the middle of the culet face of the anvil on the incident-beam side of the cell when the diffractometer is at zero. This means we assume that the middle of the DAC gasket hole is at the centre of the goniometer.

Internally the ABSORB program uses the axial conventions defined by Busing and Levy (1967), with the addition of the DAC coordinate axes.

The Cartesian basis of the "ϕ-axis" coordinate system (Busing and Levy 1967) has its axes defined as follows:

- the positive Y-axis extends from the crystal towards the beamstop (i.e. along the un-diffracted direct beam),

- the positive Z-axis is parallel to the ϕ axis, and away from the ϕ-axis carrier,

- the positive X-axis makes a right-handed set, and corresponds to an imaginary diffraction vector at $2\theta = 0$.

These definitions are illustrated for an Eulerian cradle in the picture below, with all of the circles at zero. These definitions do not, however, depend on the geometry of the goniometer.

For the crystals inside DACs, there are some important additional points:

The crystal must be described on the DAC axial system. The origin of this coordinate system is the center of the gasket hole, on the surface of the culet of the anvil on the incident beam side of the DAC (when the diffractometer is at zero). If the DAC is face on to the beam when the diffractometer circles are zero, then this DAC axial system coincides with the Busing-Levy φ-axis system, as shown here:
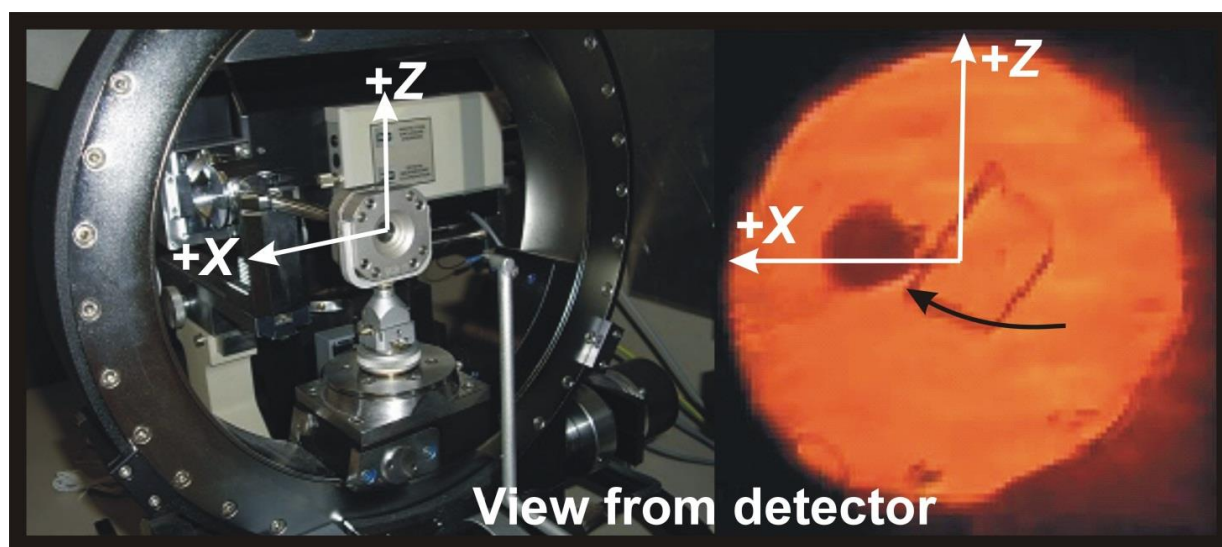
If the DAC is rotated when the diffractometer circles are all at zero, the DAC axial system *does not* coincide with the Busing-Levy φ-axis system. The DAC system rotates with the DAC, and the crystal corners must still be described in terms of the X- and Z-axes shown in the picture on the right above. The Y-axis of this coordinate system always remains parallel to the load-axis of the DAC. Rotations of the DAC from the face-on position can be specified with DAC PHIZERO, as described below. *However, it is strongly recommended that users are very very strongly discouraged from conducting experiments with rotated cells unless*

absolutely necessary, as the rotations will lead to all sorts of problems in data collection and ambiguities in later data reduction.

Thus, whether the DAC is rotated or not, the coordinates of the crystal corner indicated by the black arrow in the picture above are $x = 37$um, $z = -16$um (the gasket has a radius of 150um).

The y-coordinates depend on which anvil the crystal is lying. Suppose the crystal is on the 'incident beam anvil' – this is the anvil on the side of the DAC that is towards the X-ray source when the diffractometer is at zero. We also call this 'Anvil 1'. When the crystal is on this anvil, the y-coordinates of its corners will be either 0 or the thickness of the crystal.

If the crystal is on the other anvil (the diffracted-beam anvil or anvil 2), the y-coordinates of one face of the crystal will be equal to the thickness of the gasket, and the other face will have coordinates equal to the thickness of the gasket minus that of the crystal.

Thus, the crystal in a DAC can always be described in terms of the coordinates of its corners. It is also possible to describe a crystal in a DAC by the indices and distances of its faces. But, in order to avoid ambiguities this is not allowed when the DAC is rotated (DAC PHIZERO). With DAC PHIZERO the crystal must be described in terms of the coordinates of the corners. *From the point of view of interfacing, it is therefore easier to always specify the crystal shape and position in terms of the micron coordinates of its corners.*

Units

The units used to input various physical quantities into the ABSORB are chosen for ease of use:

* Radiation wavelengths are written in Ångstrom.

* Dimensions of the crystal (as in distances to a face, or coordinates of corners) are in microns (10^{-6}m).

* Dimensions of the DAC components are in mm.

* Absorption coefficients of the crystal and diamond-cell components are in mm^{-1}.

Point detector data

If reflection intensities are collected with a point detector, then the reflection data can be supplied to the ABSORB program with the setting angles of the goniometer. In this case the axial conventions must follow those defined by Busing and Levy (1967). When all circles are at their zero positions:

* the 2θ arm lies in the position of the undiffracted direct beam (i.e. at $2\theta = 0$)

* the plane of the χ circle is perpendicular to the direct beam ($\omega = 0$)

* the ϕ-axis is perpendicular to the diffraction plane ($\chi = 0$)

* the choice of $\phi = 0$ is arbitrary.

These conventions also define the "normal-beam equatorial geometry" of Arndt and Willis (1966) subsequently generalised by Dera and Katrusiak (1998).

The sense of positive rotations of the four diffractometer circles under the Busing and Levy (1967) convention are left-handed for all axes except for the χ-axis. To be explicit, when viewed *from the +z direction* (looking down on the diffractometer from above), positive movement of the 2θ, ω and φ axes away from their zero positions is clockwise. When viewed *from the +y direction* (looking towards the crystal from the detector arm) positive movement of the χ-axis is anti-clockwise. These senses of rotations are hereinafter defined as having *positive parities*. Circles on diffractometers that rotate in the opposite sense will be said to possess *negative parities*. If the data file contains angles with a different set of parities, this can be specified on the PARITIES card in the *experiment* file.

SHELX hkl datafiles

These contain direction cosines for the incident and diffracted beams defined with respect to the crystal reciprocal axes. To convert this information to direction cosines on the φ-axis system, the *experiment* file must contain the orientation matrix. In addition the orientation of the axial system used to describe the orientation matrix must be given by the BLAXES card.

EXPERIMENT FILE EXAMPLES

Before another program calls ABSORB it must create an experiment file. The experiment file contains three types of information:

- Information about the diffractometer (wavelength etc.)
- Information about the diffraction experiment (orientation matrix, DAC)
- Information about the sample crystal (size, composition)

The entries for two common ways of giving this information, one for a crystal in air, and one for a DAC are given below. Full information about the *experiment* file is given in the user's manual.

The *experiment* file is a text file. The general *format* of the instrument parameter file is that the first six characters of each line are read as a label. The label defines the content of the rest of the line. If the first six characters of a line are blank, then the remainder of the line is ignored; blank labels can therefore be used to space out the information or to add comments (see the example files). Comment lines can also be marked with a #. The lines can appear in any order within the file.

The information is read by Fortran read statements, so floating-point values should include a decimal point, and integer values must not contain a decimal point. Otherwise the format is free. Individual values can be separated by commas or spaces.

Describing the diffractometer

It is almost always necessary to provide basic information about the diffractometer, the wavelength, and the conventions used in the diffractometer software for describing the orientation matrix of the crystal. Here is a simple example that describes an Oxford Diffraction/Agilent Technologies diffractometer with a Mo radiation source:
WAVEL 1,0.7093
BLAXES -2,1,3

The wavelength is given as the α_1 wavelength (the '1' specifies one wavelength is given). The entry BLAXES specifies the orientation of the axes for the orientation matrix from the Crysalis software package. Use the same for Bruker instruments. For data collected with Stoe diffractometers, use 1,3,-2.

An alternative way to specify the wavelength is by target material:
WAVE Mo

Experiment information

If the input data is in a SHELX *hkl* file, you must provide the orientation matrix that indexes the dataset, and the *hkl* file must contain the direction cosines of the incident (i.e. primary) and diffracted beams.

There are two formats for the input of the orientation matrix. If you are using a system run by the Crysalis software, put the orientation matrix in to the *experiment* file like this:
UBL   0.019490 -0.021849 -0.125444
UBL   0.129750 0.123922 -0.001238
UBL   0.125763 -0.124432 0.020638

If you are using other software systems, for which the orientation matrix does not contain the wavelength in the entries (e.g. Stoe, Bruker or Single software) use:
UB   0.149868 0.099295 0.004852
UB   -0.004849 -0.005076 0.126745
UB   0.102091 -0.146011 -0.001063

You can also specify a title for your experiment:
TITLE   My first absorb run

If you want to make corrections for absorption by the crystal, you can specify the absorption coefficient by one of two methods.

If you have data from a laboratory diffractometer with an X-ray tube or rotating anode, you can ask ABSORB to calculate the absorption coefficient for you, by specifying the unit-cell volume (with the UB or UBL entries or CELL), the X-ray wavelength, and the unit-cell contents thus:
CONTENTS Ca1 Al2 Si2 O8 Z=8

Note that values can only be calculated for Mo, Cu, Fe, Cr and Co $K\alpha$ radiations. The number of formula units within the unit cell is specified by the "Z=" entry: this example specifies a unit-cell content of $Ca_8Al_{16}Si_{16}O_{64}$.

An alternative is to give the program the absorption coefficient of the crystal directly in mm^{-1}:

ABSORB MU 12.27

If you have synchrotron data, you must use this method. If no absorption coefficient is given or the absorption coefficient is zero and no CONTENTS card is present, no crystal absorption will be calculated.

Crystals in air – examples

For crystals in air, there are four possible types of crystal absorption model. One example of each of three of them is given here (the fourth ABSORB MODEL XYZFACE, is not often used). These examples also illustrate the different ways of defining the absorption coefficient. Full details of all input options can be found in the section 'The Experiment File' in the *Users' Manual*.

A spherical crystal in air would be specified like this:

```
WAVEL    2  0.709260  0.713543  0.500000
UB     0.149868  0.099295  0.004852
UB    -0.102091  0.146011  0.001063
UB    -0.004849 -0.005076  0.126745
ABSORB MU 10.3
ABSORB MODEL SPHERE 100.0 4 0
```

This specifies a spherical crystal of radius 100um and an absorption coefficient of 10.3 mm^{-1}. The second number (4) on the 'sphere' card tells the program to use $2^4 = 16$ points in the Gaussian grid, and the '0' suppresses printing of grid information. Because there is no BLAXES card, the coordinate axes for the orientation matrix are assumed to be the same as Busing-Levy (1967).

With video capture systems on diffractometers, the most common will be the specification of the crystal shape by the indices of its bounding planes. To use this method, the following entries are required in the *experiment* file:

```
TITLE  Demonstration test crystal in air.
UB     0.149868  0.099295  0.004852
UB    -0.004849 -0.005076  0.126745
UB     0.102091 -0.146011 -0.001063
BLAXES 1,3,-2
   #         (Stoe UB matrix)
ABSORB MU 12.2
ABSORB MODEL HKL 4,4,4,0
ABSORB FACE 1,1,0,51.
ABSORB FACE 1,-1,0,51.
ABSORB FACE -1,-1,0,51.
ABSORB FACE -1,1,0,51.
ABSORB FACE 0,0,1,60.
ABSORB FACE 0,0,-1,60.
```

The ABSORB MODEL HKL means that the crystal will be described in terms of the *hkl* indices of its faces, and their distance from the centre of the diffractometer in microns. This crystal is a rectangular box bounded by {110} and {001} forms.

The first three numbers on the ABSORB MODEL line specify the number of grid points to be used for Gaussian integration.

And below is the same crystal described on an instrument run by the Crysalis software, with the crystal described in terms of the coordinates of its corners (in microns, on the Busing-Levy phi-axis system), and the absorption coefficient calculated from the unit-cell contents:

```
TITLE   Crystal described by Corners
UBL    0.072413    -0.10357    -0.00075
```

```
UBL    0.106301    0.07043    0.003442
UBL    -0.00344    -0.0036    0.08990
WAVE MO
BLAXES -2,1,3
        (Crysalis UB matrix)
CONTENTS Ca1 Sn1 O3 Z=4


ABSORB MODEL XYZCORNER 4,4,4,3
ABSORB CORNER 61,-39.5, 58.0
ABSORB CORNER 56.5,-40.5,-62.0
ABSORB CORNER 43,61,58.
ABSORB CORNER 39, 60.,-62
ABSORB CORNER -39,-60., 62.
ABSORB CORNER -43.4,-60.9,-58.
ABSORB CORNER -56., 40.5, 62
ABSORB CORNER  -61, 39.5,-58.
```

Diamond Anvil cells

There are a number of entries starting with "DAC" that specify the corrections to be made for absorption and shadowing of the reflections by the components of a DAC. Note that there are several valid combinations of these cards, and many invalid combinations! The following is the easiest set of options to use. See the *Users' Manual* for other options!

If you are using a Boehler-Almax or similar type of DAC, only absorption by the anvils and shadowing by the gasket needs to be corrected, for example:

```
DAC TYPE 1
DAC ANVIL 1.4
DAC OPEN 40.
DAC GASKET 60., 150., 200., 0.2
```

The lines above describe a Boehler-Almax cell with two identical anvils, 1.4mm thick and an opening angle for X-rays of 40deg. The absorption coefficient of the anvils will be determined by the ABSORB program from the wavelength that is given on the WAVE card. The gasket is 60um thick between the anvils, and it has been drilled with a hole of radius 150um. The gasket material has an absorption coefficient of 200mm^{-1}; a value appropriate for tungsten with Mo radiation.

If the cell has beryllium backing plates, but is otherwise the same, the absorption by the backing plates can be added:
```
DAC TYPE 1
DAC ANVIL 1.4
DAC PLATE 4.0
DAC OPEN 40.
DAC GASKET 60., 150., 200., 0.2
```
Note that the absorption coefficient for the backing plates defaults to the value for beryllium at the wavelength specified. If you have backing plates made of other materials, you must specify the absorption coefficient on the DAC PLATE card.

It is normal to set up the DAC so that when the diffractometer angles are zero, the DAC is face on to the beam. You should always attempt to perform experiments in this orientation as it is easy to align the cell this way, and it avoids all sorts of complications and potential sources of errors and confusion. However, this is not always possible. If the DAC is rotated

around the phi axis from the face-on position when the diffractometer angles are zero you must use the DAC PHIZERO card to specify the rotation angle:

DAC PHIZERO 20.0

This specifies a rotation of the cell in a clockwise direction when viewed from above the phi axis (i.e. *from* the +Z Busing-Levy direction looking towards the middle of the diffractometer):
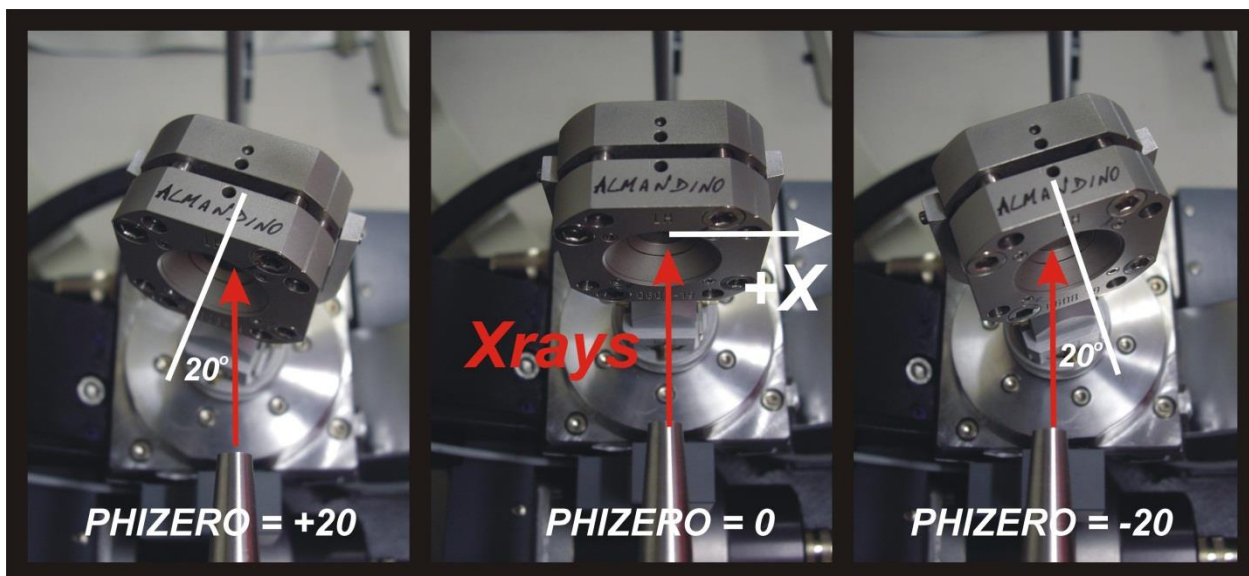
Even when the DAC is rotated in this way, you still use the same *x, y* and *z* coordinates to describe the corners of the crystal inside the cell. If you use DAC PHIZERO you cannot describe the crystal in terms of the indices of the faces.

There are other ways to specify the absorption of the DAC, and to describe cells with different absorption (e.g. different sized anvils) on the two sides of the cells. For these and other details, see the full description in the section 'The Experiment File - Details' in the *Users' Manual*.

Therefore, a typical *experiment* file for a crystal in a Boehler-Almax DAC will look like the following:

```
TITLE  Demonstration test crystal in DAC.
UB     0.149868  0.099295  0.004852
UB    -0.004849 -0.005076  0.126745
UB     0.102091 -0.146011  -0.001063
WAVEL    1  0.709260
BLAXES 1,3,-2
         (Stoe UB matrix)
ABSORB MU 12.2
ABSORB MODEL HKL 4,4,4,0
        Model with 16grid pts/axis, print indicator 0
        Model is a rectangular box bounded by {110} and {001} forms with {001} lying on the anvil
face
ABSORB FACE 1,1,0,51.
ABSORB FACE 1,-1,0,51.
ABSORB FACE -1,-1,0,51.
ABSORB FACE -1,1,0,51.
        The following two lines new entries for Absorb7
```

The first specifies the origin used for the face information, the second the anvil on which the crystal is sitting, and the crystal thickness

```
ABSORB ORIGIN 20.,0, -10.
DAC CRYSTAL 1,30.0

DAC TYPE 1
DAC ANVIL 1.4
DAC OPEN 40.
DAC GASKET 60., 150., 200., 0.2
```

A typical *experiment* file for a crystal in a Be-backed DAC will look like the following:

```
TITLE  Demonstration test crystal in DAC.
UB      0.149868  0.099295  0.004852
UB     -0.004849 -0.005076  0.126745
UB      0.102091 -0.146011  -0.001063
WAVEL    1  0.709260
BLAXES 1,3,-2
          (Stoe UB matrix)
ABSORB MU 122.0
ABSORB MODEL HKL 4,4,4,0
```
        Model with 16grid pts/axis, print indicator 0
        Model is a rectangular box bounded by {110} and {001} forms with {001} lying on the anvil face
```
ABSORB FACE 1,1,0,51.
ABSORB FACE 1,-1,0,51.
ABSORB FACE -1,-1,0,51.
ABSORB FACE -1,1,0,51.
```
        The following two lines new entries for Absorb7
        The first specifies the origin used for the face information, the second the anvil on which the crystal is sitting, and the crystal thickness
```
ABSORB FACE ORIGIN 20.,0, -10.
DAC CRYSTAL 1,30.0

DAC TYPE 1
DAC ANVIL 1.4
DAC PLATE 4.0
DAC OPEN 40.
DAC GASKET 60., 150., 200., 0.2
```

And this is an example for a crystal in a Boehler-Almax DAC with data from Crysalis:

```
TITLE  Demonstration test crystal in DAC.
```
        The orientation matrix direct from Crysalis
```
UBL -0.0402096   0.0266883   0.0235661
UBL  0.0290053   0.0616744  -0.0288270
UBL -0.0596043  -0.0381398  -0.0298778
```
        To convert the Crysalis matrix to the conventions in Absorb you need the next two cards
```
WAVEL    1  0.709260
BLAXES -2,1,3
```
        The next card specifies the type of crystal description as being in terms of corner coordinates
```
ABSORB MODEL XYZCORNER 4,4,4,0
```
        16grid points along X Y and Z axes. Use 5 if mu.t >50, Use 4 or 3 if mu.t <50
         The zero means no grid information printed

Here are the coordinates of the corners of the crystal
Origin is at the center of the I-beam anvil
+Y is along the beam, +Z is up at circles all zero (Busing-Levy)

The crystal is a flat plate, 30micron thick, lying on the
surface of the anvil on the diffracted-beam side of the DAC
Note that the y-coords of the corners are all 80 or 110 to describe this.
ABSORB CORNER   0.0,110.0, 90.
ABSORB CORNER   0.0,110.0,-90.
ABSORB CORNER 90.0,110.0,-90.
ABSORB CORNER 90.0,110.0, 90.
ABSORB CORNER   0.0,80.0, 90.
ABSORB CORNER   0.0,80.0,-90.
ABSORB CORNER 90.0,80.0,-90.
ABSORB CORNER 90.0,80.0, 90.
And we need the absorption coefficient of the crystal
ABSORB MU 12.1
DAC description. This is the 'Bragg Mini' cell, Boehler-Almax seats, so no Be plates
The anvils are equal, and are defined by thickness and absorption coefficient
DAC TYPE 1
DAC ANVIL 1.43, 0.2
The following cards are optional
DAC open will cause the program to reject reflections with higher psi angles
DAC OPEN 40.
The gasket card is only required if the user selects gasket shadowing corrections
DAC GASKET 60., 150., 200., 0.2

DATA FILE FORMATS

Input Data Files

Intensity data for correction is supplied in the *input data* file. All input file formats must contain F^2 and $\sigma(F^2)$ – that is intensity data that has already been corrected for Lorentz-polarisation effects and for decay of intensities during the experiment. The formats recognised by the program are:

- o RFINE "int" format, as produced by the WinIntegrStp program (Angel 2003). The file contains one line per reflection with: *hkl*, setting angles, F^2, $\sigma(F^2)$, a sequence number, flags, and continuation counter set to zero. The setting angles must be in the order 2θ, ω, χ, ϕ as defined by Busing and Levy (1967) with ω defined as the deviation from bisecting. The input angles will be converted to Busing-Levy positive parities following the information provided on the PARITY card.

- o RFINE extended format. The first line is the same as the RFINE "int" format. The subsequent lines display all of the refined profile parameters and esd's and various indicators of fit that are ignored by ABSORB.

- o SHELX *hkl* format, with *hkl*, F^2, $\sigma(F^2)$, and direction cosines with respect to the crystal axes (*not the Busing-Levy coordinate system*). In order to use these direction cosines, the *experiment* file must contain the UB matrix. The BLAXES card will be used to rotate the UB matrix onto Busing-Levy coordinate system prior to conversion of the direction cosines to the Busing-Levy coordinate system. The conversion follows the method of Allan et al. (2000).

- o The ABSORB browser also has the 'raw' data file type listed, but the internal format is that of a SHELX *hkl* file.

Output Data Files

The absorption-corrected data, plus flags and directional data as required by the file format is written to the *output data* file. Note that standard reflections are not written to the *output data* file. The supported file formats are:

- o RFINE "abs" format. One reflection per line, including *hkl, F,* $\sigma(F)$, and β, the "weighted mean path length for absorption" $-A^{-1}\,\partial A / \partial \mu$ required for various extinction models (e.g. Becker and Coppens 1974), a flag equal to "1" for observed reflections and "2" for unobserved reflections, and the setting angles with Busing-Levy parities.

- o SHELX "hkl" format. One reflection per line with *hkl*, F^2, $\sigma(F^2)$, the sequence number, and the direction cosines of the incident and diffracted beams with respect to the crystal axes *not the Busing-Levy axes*. If the UB matrix is not available, dummy direction cosines will be written to the file.

For both output file formats the values of F and $\sigma(F)$, or F^2 and $\sigma(F^2)$, are dynamically formatted to fill the output field. If the output format is over-flowed by F^2 the dataset is

rewound and the entire output re-scaled to fit the format. Values of $\sigma(F)$ or $\sigma(F^2)$ that overflow the format are set equal to the maximum value allowed by the format.

Scales File

The absorption-corrected data plus the correction factors calculated by ABSORB are written to a *scales* file, given the same name as the *output data* file, but with an extension "*abs_scales*". This enables the absorption corrections calculated by ABSORB to be used or applied by other programs.

The file contains the information for one reflection on each line, in the same order as given in the *input* datafile.

All reflections from the input file are present in the *scales* file, including those reflections marked for rejection by ABSORB, and therefore that are not present in the *output data* file. Rejected reflections have the *Total correction factor* set to zero in the scales file. If required, this total factor can be reconstructed from the component scale factors in the file. These rejected reflections can also be identified either by the rejection flags.

The format of each line of this file is similar to a SHELX *hkl* file: 3I4,1X,F7.*,1X,F7.*,I4,8F10.3,5X,6A1. The variables are:

- Indices: *hkl*
- Corrected Fsq
- Sig(Corrected Fsq)
- Frame number (copied from *input* datafile)
- Total correction factor (the scale factor to be applied to a reflection),
- The scale factor due to crystal absorption alone
- The scale factor due to dac absorption alone (anvils and backing plates)
- The scale factor due to dac gasket absorption alone
- The scale factor due to dac pressure medium absorption alone
- Reserved for future use
- Reserved for future use
- The scale factor due to illuminated volume for the small beam case
- Reflection flags with the same codes as in the *print* file. See 'Users manual'.

PROGRAM DESCRIPTION

Methods

This is a brief version of the information provide in Angel (2004).

The intensity of an X-ray beam passing through a distance *t* of a material with absorption coefficient μ is reduced by a transmission factor $T = \exp(-\mu t)$. The absorption coefficient therefore has units of inverse length (e.g. cm^{-1}). The value of the absorption coefficient depends on the elements present in the sample and the density; the higher the density for a fixed chemistry, the higher the absorption coefficient. The coefficients used in the ABSORB program for calculating the absorption coefficient from the chemistry are taken from the *International Tables*, Vol C (1992). Note that they depend on the wavelength of the radiation. The value of the absorption coefficient can, instead, be specified independently by the user.

The transmission factor, often called the "transmission coefficient", is different for different reflections from the same crystal because the path lengths of the incident and diffracted beams within the crystal are different. This is the case even for spherical crystals. The transmission factor for a crystal reflection is given by the integral over the crystal volume of the path lengths of the incident (t_I) and diffracted beams (t_D):

$$T = \frac{1}{V} \int \exp(-\mu(t_I + t_D))dV \tag{1}$$

This integral can only be calculated analytically for a small number of regular shapes, as tabulated in the *International Tables*, Vol C. For more complex shapes, the integral can be approximated by a summation over a number of points within the crystal:

$$T = \frac{1}{V} \sum \exp(-\mu(t_I + t_D)) \tag{2}$$

The crystal volume *V* can be recovered as the sum over the grid points multiplied by the volume of crystal associated with each grid point. If a grid of equally-spaced points is employed for this calculation, a very large number of points is required in order to ensure a reasonable approximation (say within 0.1%) of the integral. Therefore ABSORB is coded to set up a Gaussian grid of unequally-spaced grid points over which the path length calculation is performed. The summation becomes:

$$T = \frac{1}{V} \sum_{i,j,k} w_i w_j w_k \exp(-\mu(t_I + t_D)) \tag{3}$$

in which the w_i, w_j, w_k are weights pre-assigned to each grid point. Such summations usually converge to within 0.1% of the true value of the integral with 16 points or less along each of the three axes. In this case the volume of the crystal model can be back calculated as the sum $V = \sum_{i,j,k} w_i w_j w_k$. Further details about the absorption corrections made by this method of calculation can be found in the original paper describing the original ABSORB program (Burnham 1966) and in *International Tables*, Vol C, section 6.3.3.4.

For data collected from crystals held within a diamond-anvil pressure cell (DAC) there are two further corrections that need to be considered. First, there is the absorption of the incident and diffracted beams by the diamond anvils and by their backing plates. Second, there is the

potential for shadowing of part of the crystal by the gasket. These can be treated separately. Note that ABSORB is only currently coded to handle transmission diamond-anvil cells in which the incident and diffracted beams pass through the anvils close to the cell axis. ABSORB does not currently handle transverse geometry cells in which at least one of the beams enters or exits the cell in a direction that is close to perpendicular to the cell axis.

Absorption by the DAC

The general expression for the transmission coefficient of the beam becomes (Santoro et al. 1968):

$$ T = V^{-1} \int_V \exp\left(-\sum_i \mu_i t_i\right) dV \tag{4} $$

where the integration is over the crystal volume V and $\exp\left(-\sum_i \mu_i t_i\right)$ is the transmission factor associated with a volume element dV of the crystal. In the summation, the μ_i are the linear absorption coefficients, and the t_i are the path lengths for the X-ray beam in each different material i traversed by the beam. In ABSORB it is assumed that the correction for absorption by the cell components is the same for every point in the crystal. The term $\exp(-\mu t)$ for each of these components can then be removed as a constant of multiplication from inside the integral in Equation (4) and applied as a multiplier to the separately calculated absorption correction due to the crystal (Santoro et al. 1968).

The ABSORB program provides a number of different functions and methods for calculating this absorption correction. Note that all of these assume that the correction is cylindrically symmetric about the cell axis, and is therefore only a function of the angle ψ between the beam direction and the cell axis. Further, it is assumed that the two halves of the DAC have identical absorption curves.

If the optical access hole in the beryllium plates is filled with a Be plug during data collections (e.g. Allan et al. 1996) the contribution of each half of the DAC to the absorption correction for each beam then becomes simply that for two infinite flat plates, one made of diamond, one of Be:

$$ I = I_0 \exp\left(-\left(\mu_{Dia} t_{Dia} + \mu_{Be} t_{Be}\right)/\cos\psi\right) \tag{5} $$

This is coded into ABSORB as DAC TYPE 1. The values of μ_{Dia} and μ_{Be} and the thickness of the components must be entered with the DAC PLATE and DAC ANVIL cards in the *experiment* file. It is recommended that the absorption of the Be plates be measured experimentally, because the material may include alloying elements, and because transmitted intensities are also reduced by diffraction. Thus the measured absorption coefficient can be 10-20% higher than that calculated for pure Be (Angel et al. 2000). An alternative method of applying the same correction is provided in ABSORB by DAC TYPE 5. The absorption curve is expressed in terms of a single parameter $\xi = \left(\mu_{Dia} t_{Dia} + \mu_{Be} t_{Be}\right)$, and the relative absorption of a beam inclined at an angle ψ to the cell axis is given by:

$$ \frac{I(\Psi)}{I(\Psi = 0)} = \exp\left(\xi\left(1 - 1/\cos\psi\right)\right) \tag{6} $$

The parameter ξ can be determined by fitting an experimentally-measured transmission curve for a half-cell, and is provided to the program on the ABSORB PSI CURVE card. Note that

this method provides a *relative absorption correction,* with the beams with ψ = 0 having no correction applied. Two of these terms from either Equation (5) or Equation (6), one for the incident beam and one for the diffracted beam, are multiplied with the absorption correction due to the crystal to obtain the total absorption correction. If X-ray opaque seats are used to support the diamond anvils, then only correction for absorption by the anvil is necessary.

That is the simplest case. In the original design of a Merrill-Bassett DAC and its derivatives (see Miletich et al. 2000 for a review), the Be backing plates were drilled with cylindrical optical access holes that were left unfilled for data collection. At high inclination angles, when the beam does not pass through the access hole, the absorption correction reduces to that given in Equation (5). But at smaller values of ψ the beam passes partly or completely through the hole, producing a sharp step in the absorption as a function of ψ (Angel et al. 2000). In other cells the backing plates are not flat plates. The absorption curve for these cells can be described in terms of a specific absorption function and a few parameters, as coded in ABSORB for DAC TYPE 2, 3, and 4 (see section on *experiment* file input). Alternatively, DAC TYPE 5 can be specified and the measured absorption curve expressed (with card DAC ABSPSI) as a series of points of absorption coefficient as a function of Ψ angle.

Gasket shadowing corrections

When X-ray beams enter or leave the transmission DAC at high angles of ψ, part of the beams may pass through the gasket, further reducing the measured diffracted intensity. This effect has become known as "shadowing by the gasket".

Santoro et al. (1968) developed the general equations for the simpler case of an absorbing crystal that completely fills a right-cylindrical hole made in partially-absorbing gasket material, a situation applicable to crystals formed by condensing gases or fluids *in-situ* in the DAC (e.g. Miletich et al. 2000). Von Dreele and Hanson (1984) developed the equations for the simplified case of a non-absorbing crystal filling a circular hole in a totally opaque gasket material. Kuhs et al. (1996) implemented the methodology required to address the more common situation of normal crystals that do not fill the gasket hole of a partially-absorbing gasket. The important point about shadowing corrections is that only part of the X-ray beam intersects, or passes through, the gasket. Therefore, while the absorption by the gasket becomes an additional term in Equation (4) it cannot be removed as a constant of integration, as is done for the absorption by the anvils and backing plates. Instead, the path of the beam within the gasket must be calculated for each point of the grid used to calculate the absorption by the crystal. Similarly, corrections for absorption by the pressure medium must also be calculated separately for each point on the crystal.

The assumptions made in ABSORB concerning gasket shadowing are that:

- the gasket hole is a cylinder with an axis parallel to the axis of the DAC – it has the same radius at all depths through the gasket. The latter, of course, cannot be measured and calculations are forced to assume that "gasket barrelling," in which the radius of the gasket hole is greater towards the centre of its thickness than at the surfaces in contact with the diamonds, does not occur.

- the anvil surfaces are parallel and coincident with the surfaces of the gasket. There is no allowance for "bulging" of the gasket around the anvils because this should only affect beams at very high values of Ψ which will be obscured by the other components of the DAC.

- Reflections with $\Psi > 80^\circ$ are considered totally obscured by the gasket in order to reduce time spent on computations.

In ABSORB the calculations proceed as follows. The coordinate system for the crystal model is based upon an origin located at the centre point of the surface of the anvil on the incident-beam side of the cell (when the diffractometer angles are all zero). Thus all of the *y*-coordinates of the crystal model are zero (on the incident anvil face) or positive and less than t_g, the thickness of the gasket. If the crystal sample fills the gasket hole (DAC MODEL FILLED GASKET) then the Gaussian grid is set to represent the entire volume of the gasket hole. The gasket hole is described in terms of its radius and thickness (DAC GASKET card).

For each reflection an initial calculation is performed to determine whether all of the corners of the crystal model are illuminated by both the incident and diffracted beams without passing through the gasket. If they are, then there is no shadowing by the gasket. If one or more corners are shadowed by the gasket, the path length of both beams in the gasket is calculated for each grid point in the crystal absorption model, and the transmission factor adjusted accordingly following Equation (4). If the pressure medium is also absorbing (DAC MUMEDIA card) then the path length in the medium is also calculated for each beam by subtracting the path lengths on the crystal and the gasket from the total path length in the cell.

There is an option in ABSORB to consider the gasket material to be completely opaque, in which case the transmission coefficient for the gasket shadowing alone is either 0 (beam intersects gasket) or 1 (beam does not intersect gasket). It should be noted that the assumption of an X-ray opaque gasket might be reasonable for tungsten or rhenium gaskets which absorb ~90% of MoKα radiation within a distance of ~13 μm and 99% within twice this distance, but it is not justified for steel gaskets for which the optimal diffraction size 2/μ is 60μm, a typical gasket thickness! Nor is it true for shorter X-ray wavelengths such as AgKα radiation.

Execution

The overall sequence of program operations is as follows:
1. Preliminary calculations:
    a. The contents of the *experiment* file are read and checked for consistency.
    b. The equations describing the plane faces of the crystal are calculated from the information provided in the *experiment* file.
    c. The coordinates of all of the corners of the crystal are calculated from the face equations.
    d. The coordinates of all of the points on a Gaussian grid within the crystal when all the diffractometer angles are zero are calculated and stored. An integration over these points provides the volume of the crystal.
    e. If requested, the grid points are written out to the file *absorb_grid.lst*.
    f. The results of these calculations are written to the *print* file.

2. Processing of the data:
    a. The process_data subroutine is entered.
    b. Statistical counters for the dataset are zeroed.
    c. Each reflection is read in turn from the *input data* file. Reflections marked as "rejected" in the file are discarded unless requested otherwise in the *exp* file.
    d. The setting angles or the direction cosines associated with the reflection are transformed to be consistent with the conventions used by the program. The value of F^2 and its estimated standard deviation are rescaled by the user-supplied factor.

e. The absorption correction is calculated by enumeration of the absorption-weighted path lengths over the Gaussian grid that was calculated from the crystal model. DAC corrections are calculated and applied as required.

f. Statistics are accumulated from this reflection provided it has not been rejected by the program, for example because 2θ or Ψ are outside the user-specified limits.

g. If the reflection is not marked as a standard reflection, *hkl,* the corrected structure factor, its estimated standard deviation, and other information as required by the file format are written to the *output data* file. The correction factors for each reflection are also written to the *scales* file.

3. At the end of the *input* file:

a. several statistical measures of the dataset and the standard reflections are printed to the *print* file.

b. A *cif* is created with information regarding the absorption corrections.

Code Validation

As noted by many authors (including Cahn and Ibers 1972; Alcock 1974; Flack et al. 1980) it is very difficult to validate the correct operation of all parts of a computer code for calculating transmission functions, especially because the calculations are based upon numerical approximations to integrals. The ABSORB code provides values for the transmission function of crystals in air that agree to within rounding error with the standard test values tabulated by Cahn and Ibers (1972) and Flack et al. (1980), provided the integral is approximated by a fine-enough Gaussian grid. As an approximate guide, a grid of 8 or 16 points along each axis is sufficient up to $\mu t \approx 10$, but 32 point grids are required for accuracy at the 0.1% level for $\mu t \approx 100$. Alternative descriptions of the same model of faceted crystals provide values of the transmission function that agree to about 1 part in 10,000 which is the expected level of uncertainty and indicates that the conversion routines for the various types of crystal description are at least internally consistent. The transmission functions for a spherical crystal calculated with 16 grid points per axis agree to within 1 part in 1,000 with those calculated analytically and listed in Table 6.3.3.3 of Maslen (1992) for µR from 0.1 to 2.5. "Back of the envelope" calculations for other crystal shapes suggest that the resulting corrections are "reasonable". For highly-absorbing crystals the application of an absorption correction consistently leads to lower *Rint* values upon averaging and more reasonable refined displacement parameters for atoms. Comparisons with other absorption codes for crystals in air have not revealed any discrepancies greater than expected from rounding errors and limitations in the numerical methods.

Some simple and limiting cases for DAC data can be compared to analytic solutions. The author has attempted to do his best with respect to testing (as he uses the code!) and these attempts are summarised here. He nonetheless remains interested in any proposals for further tests and validation methods.

- *Crystal filling hole of opaque gasket.* The shadowing corrections for a non-absorbing crystal that completely fills a cylindrical hole in a perfectly absorbing gasket can be calculated analytically (Von Dreele and Hanson 1984). When the gasket is specified as opaque in ABSORB (by setting the absorption coefficient of the gasket to be negative on the GASKET card) the shadowing factors are within 1.0% of those calculated analytically. The same agreement is obtained when one sets the absorption coefficient of the gasket to 9999999 cm^{-1}. The discrepancy is less at normal inclination angles,

but increases to around 1% for $\Psi > 50^o$ presumably because of the limitations of both the numerical integration and also the way in which the path length through the gasket is calculated. The latter could be improved at the expense of greatly increased computation time. Note that the gasket shadowing is set to complete for $\Psi > 80^o$.

- *Crystal filling hole of gasket.* The "filled gasket" model can be closely simulated by describing the crystal as a polyhedral prism whose edges touch the edge of the gasket hole and whose length is the thickness of the gasket. Correction factors calculated from the two approaches are usually within 1% - an offset of this order is expected because the polygonal prism does not actually fill the gasket hole. The comparison can be performed for both opaque and absorbing gaskets, absorbing and non-absorbing crystals, etc.

- *General DAC cases.* The internal consistency of the various DAC calculations has been checked by running the different combinations of corrections for DAC data described below under "Some hints for DAC data" in the *Users' Manual.*

REFERENCES

Alcock NW (1974) Absorption and extinction corrections: calculation methods and standard tests. Acta Crystallogr A 30:332-335.

Allan DR, Clark SJ, Parsons S, Ruf M (2000) A high-pressure structural study of propionic acid and the application of CCD detectors in high-pressure single-crystal x-ray diffraction. Journal of Physics C: Condensed Matter 12:L613-L618.

Allan DR, Miletich R, Angel RJ (1996) Diamond-anvil cell for single-crystal x-ray diffraction studies to pressures in excess of 10 GPa. Rev Sci Instrum 67:840-842.

Angel RJ (2003) Automated profile analysis for single-crystal diffraction data. J Appl Crystallogr 36:295-300.

Angel RJ (2004) Absorption corrections for diamond-anvil cells implemented in the software package Absorb 6.0. J Appl Crystallogr 37:486-492.

Angel RJ, Downs RT, Finger LW (2000) High-pressure, high-temperature diffractometry. In: RM Hazen and RT Downs (Ed) High-pressure and high-temperature crystal chemistry, MSA. pp 559-596.

Arndt UW, Willis BTM (1966) Single crystal diffractometry. Cambridge University Press.

Becker P, Coppens P (1974) Extinction within the limit of validity of the Darwin transfer equations. I. General formalisms for primary and secondary extinction and their application to spherical crystals. Acta Crystallogr A 30:129-147.

Burnham CW (1966) Computation of absorption corrections and the significance of end effects. Am Mineral 51:159-167.

Busing W, Levy H (1967) Angle calculations for 3- and 4- circle X-ray and neutron diffractometers. J Appl Crystallogr 22:457-464.

Cahn D, Ibers JA (1972) Absorption corrections: procedures for checking crystal shape, crystal orientation and computer absorption programs. J Appl Crystallogr 5:298-299.

Dera P, Katrusiak A (1998) Towards general diffractometry. I. Normal-beam equatorial geometry. Acta Crystallogr A 54:563-660.

Flack HD, Vincent MG, Alcock NW (1980) Absoprtion and extinction corrections: standard tests. Acta Crystallogr A36:682-686.

International Tables for X-ray Crystallography, Vol C (1992) Dordrecht, Kluwer Academic Publishers.

Kuhs WF, Bauer FC, Hausmann R, Ahsbahs H, Dorwarth R, Holzer K (1996) Single Crystal Diffraction with X-Rays and Neutrons: High Quality at High Pressure? High Pressure Research 14:341-352.

Maslen E (1992) X-ray absorption. In: A Wilson (Ed) International tables for X-ray Crystallography, Vol C Dordrecht, Kluwer Academic Publishers. pp 520-529.

Miletich R, Allan DR, Kuhs WF (2000) High-pressure single-crystal techniques. In: RM Hazen and RT Downs (Ed) High-pressure and high-temperature crystal chemistry, MSA. pp 445-519.

Santoro A, Weir CE, Block S, Piermarini GJ (1968) Absorption Corrections in Complex Cases. Application to Single Crystal Diffraction Studies at High Pressure. J Appl Crystallogr 1:101-107.

Von Dreele RB, Hanson RC (1984) Structure of NH_3-III at 1.28 GPa and Room Temperature. Acta Crystallogr C 40:1635-1638.