ABSORB V6.1

A program to calculate and apply absorption corrections to single-crystal diffraction intensity data.

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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. It can be used for data collected with either an area detector or a point detector.

History

ABSORB was originally written by Burnham (1966) and was subsequently modified, developed and ported to VAX-VMS by L.W. Finger of the Geophysical Laboratory. Further developments to incorporate the corrections for datasets collected at high-pressures in diamond-anvil cells were made during 1988 -1998 by the current author, both at University College London and at the Bayerisches Geoinstitut in Bayreuth. In the late 1990's the code was ported to run in a DOS box under Windows. Major modifications were then made in 2002 at Virginia Tech, including:

- New format for control file, compatible with WinIntegrStp integration program.
- Change all internal calculations to Busing-Levy axial and circle conventions, with the option to read input data with other conventions.
- Addition of option to describe the crystal model in terms of *hkl* and distance of surface planes.
- Addition of option to describe the crystal model defined by individual corner coordinates.
- Addition of option to describe DAC absorption by either a table of measured absorption values, or by a single parameter curve.
- Removal of *Lp* corrections to data; input data is now assumed to be F^2.
- Incorporation of corrections for spherical crystals.

The resulting version of ABSORB was designated 5.2 and was distributed as a "beta-test" version. Further developments resulting from feedback from users and further work is presented as version 5.3 in February 2003. Version 6.0 was developed in summer 2003 and was the first version to be run from a Windows dialogue box, although most controls are still set by editing the control file. Version 6.1 released in May 2006 includes a number of accumulated bug fixes and minor new features. The program runs on Windows-2000, Windows-NT, Windows-XP and Win-98 machines. There were some Win-98 systems on which the file browser does not work quite as well as it does on the other systems.

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 (Burnham 1966) and the current description as follows:

Angel R.J. (2004) Absorption corrections for diamond-anvil cells implemented in the software package Absorb 6.0. *Journal of Applied Crystallography*, 37:486-492

If you would like to receive program updates (including bug fixes), please register with me as a user by e-mail (rangel@vt.edu). If you discover apparent bugs in the program, please send me the input files, the output file and a full description of the problem by e-mail. Other suggestions for improvements and modifications will also be considered. Further information will be posted on the web site http://www.crystal.vt.edu/crystal/.

Acknowledgements

Thanks are due to Charles W. Burnham for his original coding of the ABSORB program, and Larry Finger for developments of the code. Recent developments of this software were supported by NSF grant EAR-0105864 to NL Ross and RJ Angel. Many users have provided significant feedback and undertaken testing of the program, especially David Allan, Jason Burt, Ronald Miletich, Tiziana Boffa-Ballaran, Demelza Hugh-Jones, Simon Parsons, Jing Zhao and Nancy Ross. Thankyou!

Disclaimer

While I try to ensure that the ABSORB software is free of bugs and errors, people use it at their own risk. I cannot accept any responsibility whatsoever for either incorrect results or for any physical, mental or other damage arising from use of ABSORB or from errors in this manual.

MANUAL AND SOFTWARE REVISIONS

August 2002: Release and draft of manual for v5.2

September 2002: Corrections to v5.2

- Correction to handling direction cosines in Shelx files. The direction cosines are now Shelx-standard, that is with respect to the crystal axes. The UB matrix is required in the exp file to convert these to the Busing-Levy cosines used within ABSORB.
- Corrections to code to ensure proper functioning when no absorption by the crystal.
- More tests added to check for consistency of info in exp file.
- If output format is over-flowed by a structure factor (or F^2) the dataset is rewound and the 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.
- Manual revised to explain DAC options better.

October/November 2002: Further corrections to v5.2

- Introduction of UBL cards to handle entry of UB scaled by wavelength.
- Introduction of 2THETA card to restrict 2θ range of data.
- Fixed bug causing incorrect β values for spherical crystal model.

December 2002/January 2003: Modifications and developments resulting in v5.3

- Crystal filling gasket as a new model for DAC's.
- Bug in shadowing correction because sign of ψ was ignored - corrected.
- Shadowing calculation restructured to reduce calculation times: beams with either $\psi > 80^o$ are considered completely shadowed.
- Rejected reflections not included in min/max transmission statistics.
- Free format read from experiment file.
- Restructuring of common blocks within code.
- Calculation of unit-cell from UB and cross-checking with CELL entry.
- Gasket code reduced to circular gasket hole only from ellipse.
- Absorption coefficient of crystal can be calculated from listed cell contents.
- Introduction of option for absorbing pressure media in DAC.

July 2003: Modifications and developments resulting in version 5.4:

- Introduced possibility of two halves of DAC having different absorption parameters
- Removed possibility of psicurve having negative angles – this forces the cell absorption to be cylindrically symmetrical.
- Output of DAC psi angles to print file changed – now shows absolute angles and the anvils through which the beams pass.
- Grid output now sent to absorb_grid.lst, not the print file.
- Shadowing code thoroughly checked for algebraic correctness

Summer 2003: Version 6.0 for Windows with file browser GUI, plus

- Introduced writing of cif
- Added option to keep input reflections marked as rejected.
- Fixed signs of conversion between *hkl* and *ABCD* equations for bounding planes.
- Fractional stoichiometery coefficients now read from chemistry card.
- Confirmed that program reproduces test values of Cahn and Ibers (1972) and Alcock (1974).

6 May 2004: bug fix

- Fixed bug that stopped program with error message saying det(gstar) = 0, when unit-cell volume was > 4000A^3.

28 Oct 2004: bug fixes

- Fixed bug that prevented using $\mu < 0.1$ cm^{-1} for either anvils or Be plates
- Fixed handling of errors on opening grid list, prt, exp, input and output data files and cif .
- Restructured logic to correctly handle cases when either no μ or no crystal model given in exp file.

16 February 2005: Create version 6.1

- Cleaned up code files
- Added tables of I/sig(I) to output
- Added view utilities to main dialogue

17 May 2006: bug fixes

- Trapped case of no UB input when SHELX hkl used as input. Now returns error message and halts program.
- Trapped case of large psi angle in DAC leading to infinite absorption and math overflows. Reflections with psi > 70 are now set to F = 0.

INSTALLATION

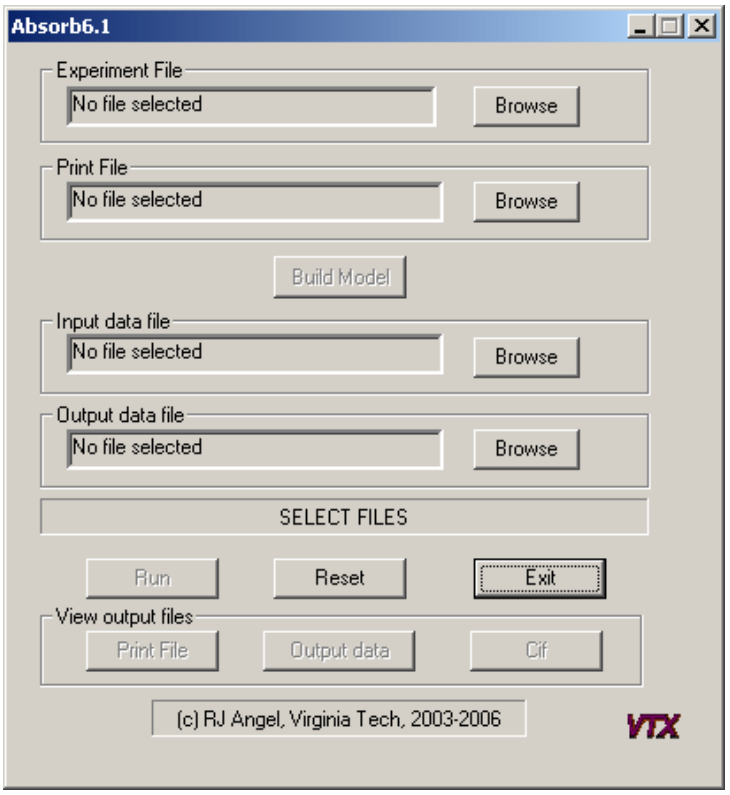
1. The absorb61.zip file contains the executable, some test datasets with all input and output files, and this manual as a pdf file.
2. Unzip the absorb61.exe and the pdf file containing the manual into one folder. It is recommended that this folder is not used for data files.
3. Unzip the remainder of the files into a working directory. These contain example datasets and corresponding experiment files and output files.
4. Create a shortcut to absorb61.exe either in the working directory, or on the desktop, by right-clicking on the file, dragging to the working directory or desktop and then selecting "create shortcut". Right-click on the shortcut, select "properties" and *either* put the full path of the working directory into the line "Start in" *or* clear this entry. Version 6.1 of Absorb includes a file-browser so the location of the shortcut is not critical.
5. Test the installation by running the program (see below) and using the example datasets and control files provided in the distribution. Each example is provided with an annotated *experiment file*, e.g. *example1.exp*, and an *input data file*, e.g. *example1.int* to be used in testing the program. The output from the test should be compared to the other three files, e.g. *example1.prt* (program log file) *example1.abs* (datafile of corrected data) and *example1_absorb.cif* (cif). The examples are chosen to illustrate the common modes of operation of ABSORB. The *experiment files* are extensively annotated, and further notes on them are provided after the next section

RUNNING THE PROGRAM

The normal procedure is to first create an *experiment file*. This is an ASCII file which can be edited by any normal editor (e.g. Notepad, WordPad etc). It contains all of the information about the crystal, the diffractometer geometry, diamond-cells etc. Details of the content of the *experiment file* are given later in this manual. For testing the program use the example files provided in the distribution.

You also need the *Input data file* containing the reflection data to be corrected in either Shelx *hkl* format or WinIntegrStp *int* format. For testing the program use the example files provided in the distribution (but read the next section *before* proceeding!).

Start the program by double-clicking on the shortcut. The main Absorb dialogue box will appear:

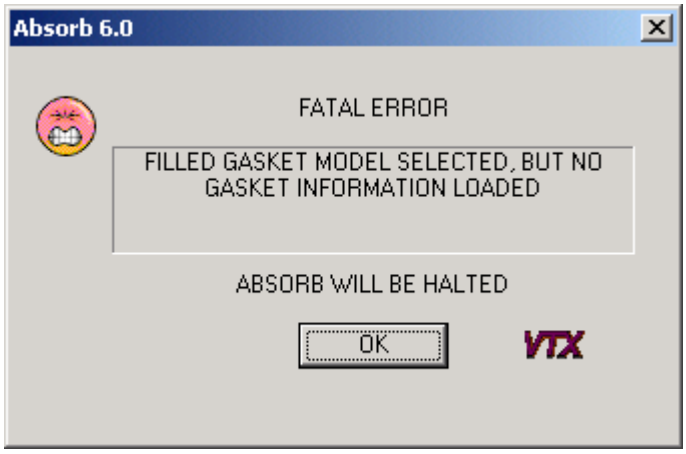


Some guidance as to what to do at each step is provided in the message window (that says “Select Files” in the example shown here).

Use the *Browse* buttons to select an *Experiment file* (must exist) and a *Print file*. The print file will contain details of the calculations and results. It may exist – if it exists the new information will be appended to it. The file names will appear in the dialogue box.

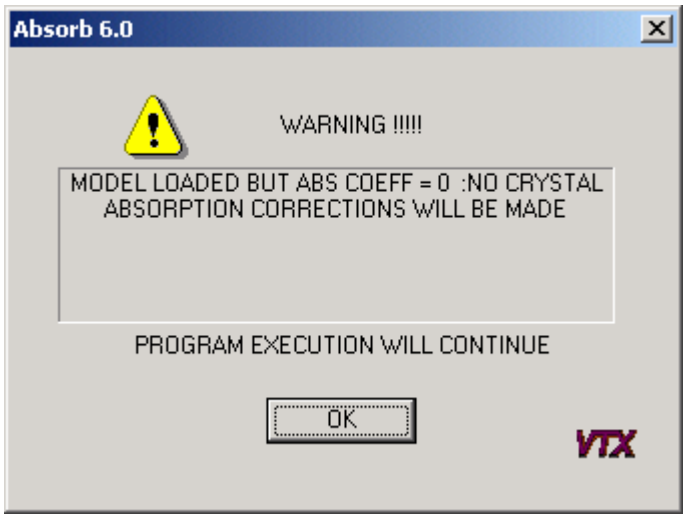
Select *Build Model* on the dialogue box. This will cause the program to read the *experiment file* and to construct the mathematical model of the crystal. If there is an error

in your *experiment file* (e.g. some inconsistency, or a format error) you will see the error box with an explanation, for example:



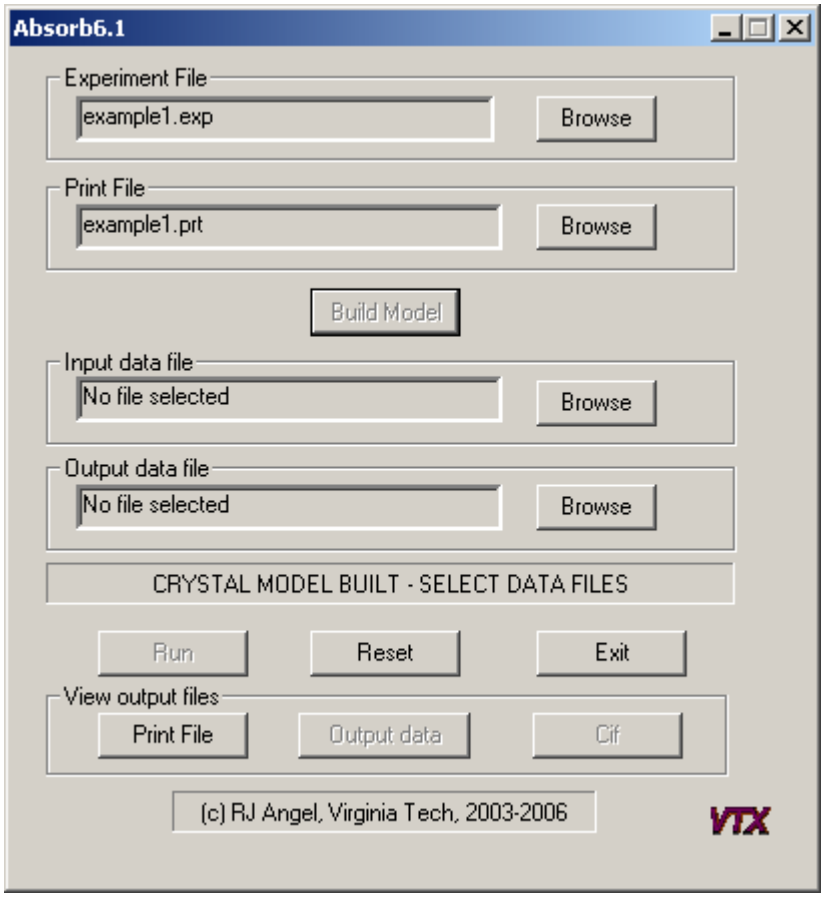
After you select *OK* you will be forced to exit the program because the error will prevent the program from processing your data. You will need to correct the error in your *experiment file.*

You may also see a warning box (the following example is from the *example6.exp* file):



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. In this case, the file describes a non-absorbing crystal in a diamond-anvil cell, so corrections for pressure cell absorption will still be made and the program will execute normally.

After you select *OK* on the warning box you will be returned to the main dialogue box. If the *experiment file* could be interpreted without errors, you will see the message “Crystal model built”:



Use the *browse* button to select the *Input data file* (must exist) containing your *h,k,l, and* F^2 data. The file extension *int* is interpreted as a file produced by WinIntegrStp, the extension *hkl* is interpreted as a Shelx file. Other extensions can be used.

Use the *browse* button to select the *Output data file* to contain your absorption-corrected data. The file extension *abs* is interpreted as a file to be produced in the RFINE format, the extension *hkl* is interpreted as a Shelx file. Other extensions can be used. If the file exists you will be asked if you want it to be over-written.

The *Run* button should now be enabled. Select it and Absorb will start processing your data, as indicated in the message window at the bottom. You may see a fatal error if there are problems reading your *input data file*.

When the data are processed, the program writes the information about the corrections to the *print file* and also to a *cif file*, given a name based upon the name of the *output data file*, together with "_absorb.cif".

TEST DATASETS

Run the program with the test datasets, creating *new* names for the *print file* and the *output datafile*, e.g. *test1.prt* and *test1.abs*. Do not use *example1.prt* as this will overwrite the file provided in the distribution!

Carefully compare the output from your test run with the *prt*, *cif* and *abs* files provided in the distribution. Report any discrepancies to the author at rangel@vt.edu. Please send copies of the files, a full description of the problem especially noting the *first discrepancy* from the example output, and details of your operating system.

The examples are designed to show the new user how to employ most types of absorption model calculation available within ABSORB.

1. Spherical crystal in air.

   The dataset is a dummy one with 2θ values set at exact multiples of 10 to allow you to compare the absorption coefficients with those given in Table 6.3.3.3 of Vol. C of the *International Tables*.

2. Rectangular crystal in air, described by *hkl* of the faces.

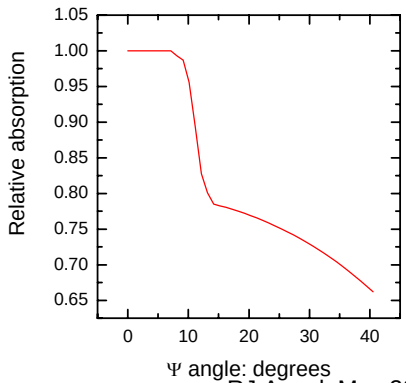
3. The same rectangular crystal described by *xyz* of the corners forming the faces.

4. The same rectangular crystal described by *xyz* of the corners.

   Models 2, 3, and 4 are alternative ways of describing the same crystal and should therefore give identical output within the limits of numerical rounding errors (less than 1 part in 10,000 for *F*). The data for these three models is supplied in two file formats, *example234.int* is RFINE format, *example234.hkl* is the same data in SHELX format. The transmission coefficients for the same reflection in both files should be identical. Note, however, that the SHELX file format does not allow standard reflections or rejected reflections to be labelled and ABSORB therefore treats both types of reflections as "normal" reflections. Hence the reflection totals at the end of the respective *prt* files named e.g. *exercise2R.prt* (from RFINE) and *exercise2S.prt* (from SHELX) differ. Output datafiles are all in the *abs* format and labelled similarly.

5. Crystal in a DAC with minor shadowing. Both halves of the cell are identical.

6. A non-absorbing crystal filling the entire gasket hole of a DAC with a totally opaque gasket. The DAC absorption is provided as a curve for the case of a cell with conical holes, but no plugs, and is shown in the figure. The



controls are set to limit reflections to $2\theta < 60^o$ and $|\psi_I| < 30^o$ and $|\psi_D| < 40^o$.

7. Another crystal in a DAC with unequal anvils of the cell. The absorption of the cell is described in terms of the thicknesses and absorption coefficients of the diamond anvils and the beryllium backing plates. Absorption by the pressure medium is also calculated. The crystal is located to one side of the centre of the gasket hole, and is located on the surface of the diffracted beam anvil. Note that the gasket thickness has to be set slightly greater (for example 110.1) than the *y*-coordinates of the corners of the crystal (in example 110.0) in order to avoid rounding-errors halting the program.

8. In addition the *exp* and *int* files labelled *CahnIbers.** and Alcock_Irregular.* allow the user to perform the tests described in the papers by of Cahn and Ibers (1972) and Alcock (1974).

PROGRAM DESCRIPTION

Methods

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):

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

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:

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

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:

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

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 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):

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

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 and 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;

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

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:

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

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 $\Psi > 80^{o}$ 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 $2/\mu$ 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 initiated by *Build Model* on the main dialogue:
    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. Note: for a spherical crystal model only, a Gaussian grid is calculated subject to the constraint of the crystal radius. This grid is then used to pre-calculate a table of absorption factors as a function of 2θ, which are then used in correcting the data.
    g. The results of these calculations are written to the *print file*.

2. Processing of the data initiated by the *Run* on the main dialogue:
    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.*

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.

Conventions

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.

Internally the ABSORB program uses the axial conventions and circle parities 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 (2θ = 0)
- the plane of the χ circle is perpendicular to the direct beam (ω = 0)
- the ϕ-axis is perpendicular to the diffraction plane (χ = 0)
- the choice of ϕ = 0 is arbitrary.

These conventions also define the "normal-beam equatorial geometry" of Arndt and Willis (1966) subsequently generalised by Dera and Katrusiak (1998). In these zero positions the Cartesian basis of the "ϕ-axis" coordinate system (Busing and Levy 1967) has its axes defined as follows:

- the origin is at the centre of the diffractometer. Note that ABSORB does not require that the origin lies within the crystal; any convenient origin point can be used for describing a model for a crystal in air. For DAC corrections, the origin is defined as lying on the middle of the culet face of the anvil on the incident-beam side of the DAC.
- the positive *y*-axis extends from the crystal towards the detector (i.e. along the undiffracted direct beam),
- the positive *z*-axis is parallel to the ϕ axis, perpendicular to the diffraction plane, and away from the ϕ-axis carrier,
- the positive *x*-axis makes a right-handed set, and corresponds to an imaginary diffraction vector at 2θ = 0.

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*.

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

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

This information is also given in the section describing the *experiment file.*

Files

Absorb uses six files:

- Information about the crystal model, diamond-anvil cell, and diffractometer are provided by the user in the *experiment file*. Details of the format of this file are provided in a separate section below.
- Output from the program about the crystal model, the data corrections applied to each reflection, and some statistics for the whole dataset are provided in a *print file*. Further explanation of the output is provided in a separate section below.
- Intensity data for correction is supplied in the *input data file.* All input file formats must contain F^2 and esd(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:

    - RFINE "int" format, as produced by the WinIntegrStp program (Angel 2003). The file contains one line per reflection with: *hkl*, setting angles, F^2, esd(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.

    - 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.

    - SHELX hkl format, with hkl, F^2, esd(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).

- 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:
    - RFINE "abs" format. One reflection per line, including *hkl*, *F*, esd(*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.
    - SHELX "hkl" format. One reflection per line with hkl, F^2, esd(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 esd(*F*), or F^2 and esd(F^2), are dynamically formatted to fill the output field. If the output format is over-flowed by a structure factor (or F^2) the dataset is rewound and the output re-scaled to fit the format. Values of σ(F) or σ(F^2) that overflow the format are set equal to the maximum value allowed by the format.

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. Comparisons with other absorption codes for crystals in air have not revealed any discrepancies greater than those expected from rounding errors and limitations in the numerical methods.

"Back of the envelope" calculations suggest 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 next section.

THE EXPERIMENT FILE

The experiment file is an Ascii text file that can be edited by any text editor, such as Notepad. 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). 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.

There are two basic types of information that are provided in the experiment file. First, there is basic information about the diffractometer. If you are using WinIntegrStp (Angel 2003) to integrate step-scanned intensity data you can use that program to create these entries in a file to which you can add the second type of information, about the crystal and diamond-anvil cell, with any suitable editor. The recognised labels and information are listed below, complete with examples:

DIFFRACTOMETER INFORMATION

WAVEL 2, 0.709316, 0.713606, 0.50

Variables:		
	nwave	number of wavelengths, 1 or 2
	wave(1)	wavelength in Angstrom of α_1 component
	wave(2)	wavelength in Angstrom of α_2 component (if nwave=2)
	wratio	Intensity ratio of α_2/α_1 (if nwave=2)

Only the first wavelength value is used by ABSORB.

PARITY 1, 1, -1, 1
Default: 1,1,1,1

Parities for the four diffractometer circles in the order 2θ, ω, χ, ϕ as defined by Busing and Levy (1967). This example has the χ axis rotating in the opposite direction to that defined as positive by Busing and Levy (1967). These parities are applied to the angles in RFINE *int*-format datafiles. They are not used if the input data is in a SHELX format file.

BLAXES -2, 1, 3
Default: 1,2,3

Defines the sense of the axes of the orthogonal coordinate system used by the diffractometer control software in calculating the UB matrix, relative to the positive axial system defined by Busing and Levy (1967). The three digits refer to the *x,y,z* axes of the diffractometer coordinate system. In the example

- the –2 in the first position indicates that *+x(diffractometer) = -y(Busing-Levy)*
- the 1 in the second position indicates that *+y(diffractometer) = +x(Busing-Levy)*
- the 3 in the third position indicates that *+z(diffractometer) = +z(Busing-Levy)*

Note that when the diffractometer circles are all at zero, *+x(Busing-Levy)* is along the diffraction vector (towards $2\theta = +90^{o}$), *+y(Busing-Levy)* is along the X-ray beam, *+z(Busing-Levy)* makes a right-handed set.

This information is used to rotate the UB matrix provided in the experiment file to the Busing-Levy axial system. The converted UB matrix is then used for two purposes by ABSORB – to convert direction cosines associated with shelx datafiles, and to convert crystal models expressed with ABSORB MODEL HKL to internal representation. See also description of the UB cards.

For data collected with the Crysalis software and Xcalibur diffractometers of Oxford Diffraction, use -2,1,3.

MISCELLANEOUS INFORMATION AND CONTROLS

CELL 7.5, 5.2 ,6.7 ,90., 113.7, 90.,
Default: none

Unit-cell parameters a, b, c, α, β, γ, and Volume. If the volume is not given, then it is calculated from the cell parameters. Not needed if the UB matrix is input.

UB 0.019490 -0.021849 -0.125444
UB 0.129750 0.123922 -0.001238
UB 0.125763 -0.124432 0.020638
Default: none

UB matrix. If the entries of the UB matrix contain the wavelength (ie. UB(input) = UB(Busing-Levy).λ) then the UBL cards should be used instead.

On input, the UB matrix is rotated to the Busing-Levy coordinate system by use of the information provided on the BLAXES card. The rotated UB matrix is used to –

- determine the unit-cell parameters.

- determine the face equations of the crystal in the Busing-Levy coordinate system when ABSORB MODEL HKL is used.
- convert the direction cosines in Shelx data files to the Busing-Levy ϕ-axis coordinate system.
- to convert the Busing-Levy direction cosines used by ABSORB to the crystal system for output to a shelx–format output data file.

If the cell parameters have been specified by the CELL card and none of these other operations are required, the three UB cards can be omitted.

UBL 0.019490 -0.021849 -0.125444
UBL 0.129750 0.123922 -0.001238
UBL 0.125763 -0.124432 0.020638
Default: none

UB matrix input if the entries of the UB matrix contain the wavelength (ie. UB(input) = UB(Busing-Levy).λ). This is the case for UB matrices used by the Crysalis software system of Oxford Diffraction.

On input, the UB matrix is rescaled by λ and then used as described by the UB cards.

TITLE example title
Default: none

Title written onto output files.

2THETA MIN 5. MAX 60.
Or
2THETA MIN 5.
Or
2THETA MAX 60.

Default: 0.,180.

Restricts the dataset to the specified 2θ range (in degrees). Reflections lying outside the specified range will not be processed by the program. It is not necessary to specify both MIN and MAX, one only can be specified if desired. But if both limits are required then they must both appear on one line as in the first line above, not on two separate lines.

Reflections which exceed these limits are flagged with a "T" in the *print file* and are not written to the *output data file*.

SCALE 1.65
Default: 1.0

The values of F^2 and esd(F^2) are multiplied by this scale factor. If the card is not present, no rescaling is applied.

ABSORB LESSTHAN 2.0
Default: 0.0

Reflections with F^2/esd(F^2) less than this value are marked as "unobserved" in the output datafile.

ABSORB REJECT KEEP
Default: DISCARD

Reflections in the *int* file marked as rejected by the Integration program are normally discarded by ABSORB. If ABSORB REJECT KEEP is specified these reflections will instead be retained.

CRYSTAL ABSORPTION MODEL

There are a number of entries starting with ABSORB that define the crystal model for the absorption correction. Note that there are several valid combinations of these cards, and many invalid combinations! Examine the output carefully to check the validity of your absorption model.

ABSORB MU 122.7
Default: 0.0

The absorption coefficient of the crystal in cm^{-1}. If no absorption coefficient is given or the absorption coefficient is zero, and no CONTENTS card is present, no crystal absorption will be performed.

CONTENTS Ca1 Al2 Si2 O8 Z=8

Instead of specifying the absorption coefficient by value on the ABSORB MU card, it can be calculated from the unit-cell contents as specified on this card and the wavelength as given on the WAVEL card. Note that values can only be calculated for Mo, Cu, Fe, Cr and Co Kα radiations. Mass absorption coefficients for this calculation are taken from the 1992 edition of International Tables, Vol. C, and the density is calculated from the specified cell contents and the unit-cell volume. The number of formula units within the unit cell is specified by the "Z=" entry: this example specifies a unit-cell content of Ca8 Al16 Si16 O64.

ABSORB MODEL
There are five possible types of absorption model, specified as follows. Only one of these alternatives should appear in the file:

ABSORB MODEL XYZFACE	Model specified by faces, each face defined by the Cartesian coordinates of three points (usually corners) within the face on ABSORB FACE cards.
ABSORB MODEL XYZCORNER	Model specified by the Cartesian coordinates of all of the individual corners on ABSORB CORNER cards.
ABSORB MODEL HKL	Model will be described in terms of the Miller indices of the faces of the crystal, and the distance of the face from a common point within the crystal by ABSORB FACE cards. This method may not work with DAC data, for which one of the two previous methods is recommended.

ABSORB MODEL FILLED GASKET	Crystal fills the volume of the gasket hole in a DAC. The crystal size is therefore specified by the dimensions of the gasket, as given on the DAC GASKET card.
ABSORB MODEL SPHERE	Model is a spherical crystal, centred at the origin of the coordinate system, of specified radius. Not valid for DAC data.

For all except the SPHERE option the string should be followed by four integer values:

- The first three integer values specify the number of grid points along each axis to be used in the Gaussian integration. A value of *n* means 2^n points will be used; thus a value of 4 means 16 points will be used. Default is 8 points along each axis, maximum value is 5, for 32 points per axis.

- The last integer specifies how much information about the grid for the absorption model is printed into the file *absorb_grid.prt*. Default is 0 for none, 3 for maximum information.

For ABSORB MODEL SPHERE, the string should be followed by:
- a real number being the crystal radius in microns
- a single integer to specify the number of grid points to be used along all three axes (as described above)
- an integer value for the print control (as above).

ABSORB FACE

There are two options for input of the crystal model in terms of faces, as specified by the ABSORB MODEL card. In either case, one card is required for each of the faces of the crystal. The cards are not allowed for "ABSORB MODEL SPHERE", "ABSORB MODEL XYZCORNER", or "ABSORB MODEL FILLED GASKET"

For "ABSORB MODEL HKL", each face is specified in terms of its Miller indices (corresponding to the given UB matrix) and the perpendicular distance of the face in microns from a common point within the crystal. For example:
ABSORB FACE 1,-2,0,57.3
This specifies a face parallel to the crystallographic plane (1,-2,0) at a distance of 57.3 microns from an origin point within the crystal. The choice of origin is arbitrary, except when making DAC corrections.

For "ABSORB MODEL XYZFACE", each face is specified in terms of the Cartesian coordinates in microns of three points that lie within the face. It is usual to use the coordinates of the corners. For example:

ABSORB FACE 73.0,0.0,32.0,-44.0,0.,61.0,-69.0,0.0,-32.0
This specifies a face that passes through the three Cartesian points (73.0,0.0,32.0), (-44.0,0.,61.0), and (-69.0,0.0,-32.0). In this case the face is perpendicular to the y-axis (and thus the X-ray beam when the diffractometer is zero) and passes through the origin.

Note that in both cases the *areal extent* of the faces is controlled by their intersection with the other faces.

ABSORB CORNER

Only valid if the model is specified as "ABSORB MODEL XYZCORNER".

These cards are used to define the *corners* of the crystal in terms of their Cartesian coordinates in microns. One card is required for each corner of the crystal, and the equations to describe the equations of the crystal faces are constructed from them. For example:

ABSORB CORNER 73.0,0.0,32.0
This specifies a corner at 73 microns along the x-axis and 32.0 microns along the z-axis from the origin.

DIAMOND-ANVIL CELL

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! Examine the output carefully to check the validity of your absorption model.

DAC TYPE 1
Default: 0

Specifies the type of corrections to be made for absorption by the anvils and Be backing plates of a DAC. The valid numbers are:

0: No DAC corrections. All other DAC cards are ignored. If 0 is intended, the card DAC TYPE can be omitted.

1: DAC with plugs filling the optical access hole in the platens, so the absorption correction simplifies to that of an infinite flat plate. Requires cards DAC ANVIL and DAC PLATE to specify the thickness and absorption coefficients of both the diamonds and the platens. Can also be used for any backing plates without holes. The absorption by diamond-cells with backing plates made of X-ray opaque material drilled with an access hole can also be modelled with this type by setting the thickness of the platen on the DAC PLATE card to zero, and using the DAC OPEN card to limit the data to that which passes through the access hole.

2: DXR-4 cell from Diacell Products with curved Be platens and the optical access holes filled with Be plugs. The parameters were derived from a drawing provided by the company. Requires cards DAC ANVIL and DAC PLATE to specify the thickness and absorption coefficients of the diamonds and the absorption coefficient of the platens. *Probably obsolete but retained just in case!*

3: Merrill-Bassett cell with cylindrical optical access holes and 1.6 mm diamonds. Derived from PDP-11 code written by Larry Finger for Geophysical Lab MB cells. No adjustable parameters, and probably obsolete.

4: Cell with conical optical access holes of 8^{o} half-angle, without plugs. Requires cards DAC ANVIL and DAC PLATE to specify the thickness and absorption coefficients of both the diamonds and the platens. *Not sure about the reliability of this one !*

5: User-supplied absorption curve for a half-cell. Requires DAC ABSPSI card to specify curve. *Recommended method.*

DAC ANVIL 0.16, 2.0
or
DAC ANVIL 0.16,2.0,0.14,2.0
or
DAC ANVIL 0.16

Thickness of the anvils in cm, and their absorption coefficient in cm^{-1}. Only used for DAC TYPEs 1, 2 and 4.

If two numbers are given, as in the first example above, then the two anvils are assumed identical.

If four numbers are given, as in the second example above, then the first pair refer to the anvil on the incident-beam side of the cell when the diffractometer is zero, and the second pair to the other anvil.

If no absorption coefficient is given, as in the third example above, it is set by the program to 2.025 cm^{-1}.

DAC PLATE 0.32, 0.47
or
DAC PLATE 0.32, 0.047,0.4,0.47
or
DAC PLATE 0.32

Thickness of the backing plates in cm, and their absorption coefficient in cm^{-1}. Only used for DAC TYPEs 1, 2 and 4.

If two numbers are given, as in the first example above, then the two backing plates are assumed identical.

If four numbers are given, as in the second example above, then the first pair refer to the anvil on the incident-beam side of the cell when the diffractometer is zero, and the second pair to the other anvil.

If no absorption coefficient is given, as in the third example above, it is set by the program to 0.473 cm^{-1}, for beryllium.

If no correction is required for backing-plate absorption, then set the thickness of the plates to 0.0, e.g. DAC PLATE 0.32

DAC OPEN 40., 30.
Default: 80., 80.

Maximum opening angle Ψ in degrees for the incident and diffracted beam sides of the DAC. They can be set unequal. If only one value is given both limits are set equal to this value. Reflections which exceed these limits are flagged with a "D" in the *print file* and are not written to the *output data file*.

DAC GASKET 60., 300., 2000., 0.2
Default: no gasket

Parameters for the gasket, in order:

- Thickness of the gasket in microns.
- Radius of the gasket hole in microns.
- Absorption coefficient of the gasket material in cm^{-1}. If this parameter is set to a negative value, then the gasket is treated as being completely opaque. If this parameter is set to zero, the gasket is non-absorbing.
- A minimum fraction of illuminated volume of the crystal for the data to be used. Reflections with less than this fraction of their volume illuminated (i.e. not shadowed) are flagged with an "O" in the *print file* and are not written to the *output data file*.

IMPORTANT: Gasket shadowing calculations will only be performed if a crystal model is defined or a "Filled gasket" is specified.

DAC MUMEDIA 8.3
Default: 0.

The linear absorption coefficient of the pressure medium in cm^{-1}. The medium is assumed to completely fill the space within the gasket hole not occupied by the crystal. Cannot be used with the "Filled gasket" model! The medium is assumed non-absorbing unless a value is specified by this card.

DAC ABSPSI CURVE 0.605
Or
DAC ABSPSI CURVE 0.605, 0.510

Default: 0.

Only used for DAC TYPE 5. Specifies that the *relative* absorption by the backing plate and anvil of each half of the DAC will be calculated as $\exp(\xi(1-1/\cos\psi))$. The value on the card is the dimensionless parameter ξ, equal to the summation $\sum \mu t$ for a beam passing through the half cell at $\Psi = 0$.
If only one number is given, as in the first example above, then the two halves of the cell are assumed identical.

DAC ABSPSI TABLE

Only used for DAC TYPE 5. Specifies that the absorption by the backing plate and anvil of each half of the DAC will be calculated by interpolation between a table of values. The card must be followed by a series of data pairs being the Ψ angle and the absorption factor for that angle. One data point per line. Terminate the data with the card DAC ABSPSI END. For example:

```
DAC ABSPSI
0.  ,1.0
1.  ,0.999
2.  ,0.980
3.  ,0.965
….etc….
39. ,0.672
40. ,0.663
DAC ABSPSI END
```

If the two halves of the cell have different absorption curves, then two values must be given for each Ψ angle in the list, e.g.

```
DAC ABSPSI
4.  ,1.0   ,1.000
5.  ,0.999,0.995
6.  ,0.980,0.97
7.  ,0.965,0.96
….etc….
DAC ABSPSI END
```

Some hints for DAC data.

There are a number of different combinations of corrections that you may wish to apply to the data. Individually the corrections are:

1. Absorption by the crystal.
2. Absorption by the cell components (anvil and backing plate).
3. Shadowing by the gasket.
4. Absorption by the pressure medium.

Here are some suggestions for how to set up some possible combinations. First, for a normal crystal in a non-absorbing pressure medium....

Crystal absorption only	Do not use any DAC cards – describe the model just as you would a crystal in air.
Crystal, cell and gasket shadowing.	Use DAC TYPE to specify cell and appropriate cards (DAC PLATE, DAC ANVIL or DAC ABSPSI) to specify the cell absorption. Use DAC OPEN to limit reflections by Ψ_I and Ψ_D. Describe gasket with DAC GASKET. Set up crystal model with ABSORB MODEL XYZ CORNER or XYZFACE, and ABSORB MU or CONTENTS card.
Crystal and cell only, no gasket shadowing.	Use DAC TYPE to specify cell and appropriate cards (DAC PLATE, DAC ANVIL or DAC ABSPSI) to specify the cell absorption. Use DAC OPEN to limit reflections by Ψ_I and Ψ_D. Set up crystal model with ABSORB MODEL XYZ. CORNER or XYZFACE, and ABSORB MU or CONTENTS card.
Cell and shadowing, no crystal.	Use DAC TYPE to specify cell and appropriate cards (DAC PLATE, DAC ANVIL or DAC ABSPSI) to specify the cell absorption. Use DAC OPEN to limit reflections by Ψ_I and Ψ_D. Describe gasket with DAC GASKET. You must still set up crystal model with ABSORB MODEL XYZ CORNER or XYZFACE (for shadowing), but omit the ABSORB MU card (or set μ=0) and CONTENTS card.
Crystal and shadowing, no cell.	Use DAC TYPE 5 and set the parameter on the DAC ABSPSI CURVE card to 0. Use DAC OPEN to limit reflections by Ψ_I and Ψ_D. Describe gasket with DAC GASKET. Set up crystal model with ABSORB MODEL XYZ CORNER or XYZFACE, and ABSORB MU or CONTENTS

	card.
Cell only.	Use DAC type to specify cell and appropriate cards (DAC PLATE, DAC ANVIL or DAC ABSPSI) to specify the cell absorption. Use DAC OPEN to limit reflections by Ψ_I and Ψ_D Omit the crystal model, and/or omit the ABSORB MU card (or set μ=0) and omit the CONTENTS card.
Shadowing only	Use DAC TYPE 5 and set the parameter on the DAC ABSPSI CURVE card to 0. Use DAC OPEN to limit reflections by Ψ_I and Ψ_D Describe gasket with DAC GASKET You must still set up crystal model with ABSORB MODEL XYZ CORNER or XYZFACE (for shadowing), but omit the ABSORB MU card (or set μ=0) and omit the CONTENTS card.

To include the absorption by the pressure medium into any of the above cases when DAC GASKET has been specified, just specify the absorption coefficient of the medium with the DAC MUMEDIA card.

The case of the crystal filling the gasket hole (ABSORB MODEL FILLED GASKET) is slightly different. First, there is no meaning to specifying the absorption coefficient of the pressure medium, because there is none! Note also that the transmission coefficients for a crystal filling the gasket hole *are not* the same as those calculated for a normal crystal and a pressure medium of the same absorption coefficient, because the integrals for the absorption are carried out over different volumes!

Crystal absorption only.	Use DAC TYPE 5 and set the parameter on the DAC ABSPSI CURVE card to 0. Use DAC OPEN to limit reflections by Ψ_I and Ψ_D. Describe gasket with DAC GASKET but set the absorption coefficient of the gasket to zero. Specify the crystal absorption coefficient with ABSORB MU or CONTENTS cards.
Crystal, cell and gasket shadowing.	Use DAC type to specify cell and appropriate cards (DAC PLATE, DAC ANVIL or DAC ABSPSI) to specify the cell absorption. Use DAC OPEN to limit reflections by Ψ_I and Ψ_D. Describe gasket with DAC GASKET Specify the crystal absorption coefficient with ABSORB MU or CONTENTS cards.
Crystal and Cell only, no gasket shadowing.	Use DAC type to specify cell and appropriate cards (DAC PLATE, DAC ANVIL or DAC ABSPSI) to specify the cell

	absorption. Use DAC OPEN to limit reflections by Ψ_I and Ψ_D Describe gasket with DAC GASKET but set the absorption coefficient of the gasket to zero. Specify the crystal absorption coefficient with ABSORB MU or CONTENTS cards.
Cell and shadowing, no crystal.	Use DAC type to specify cell and appropriate cards (DAC PLATE, DAC ANVIL or DAC ABSPSI) to specify the cell absorption. Use DAC OPEN to limit reflections by Ψ_I and Ψ_D Describe gasket with DAC GASKET Omit the ABSORB MU (or set μ=0) and CONTENTS cards
Crystal and shadowing, no cell.	Use DAC TYPE 5 and set the parameter on the DAC ABSPSI CURVE card to 0. Use DAC OPEN to limit reflections by Ψ_I and Ψ_D Describe gasket with DAC GASKET Specify the crystal absorption coefficient with ABSORB MU or CONTENTS cards.
Cell only.	Use DAC TYPE to specify cell and appropriate cards (DAC PLATE, DAC ANVIL or DAC ABSPSI) to specify the cell absorption. Use DAC OPEN to limit reflections by Ψ_I and Ψ_D Use the DAC GASKET card but set the absorption coefficient to zero. Omit the ABSORB MU card (or set μ=0) and the CONTENTS card
Shadowing only	Use DAC TYPE 5 and set the parameter on the DAC ABSPSI CURVE card to 0. Use DAC OPEN to limit reflections by Ψ_I and Ψ_D Describe gasket with DAC GASKET Omit the ABSORB MU card (or set μ=0) and the CONTENTS card

THE PRINT FILE.

- The first part of the print file contains information about the crystal shape derived from the *experiment file:*

  - The equations of the planes forming the surface of the crystal in Busing-Levy phi-axis coordinate system, as calculated from the ABSORB FACE or ABSORB CORNER cards.
  - If the UB matrix was present in the *experiment file* these planes are also expressed in terms of Miller indices and distance from the origin of the coordinate system. If the crystal was described by ABSORB MODEL HKL, you may find that these numbers differ a little from the input ones due to rounding errors. Large discrepancies are an indication of a problem in the *experiment file.*
  - The coordinates of the corners of the crystal as calculated from the intersection of the planes. If the crystal was described by ABSORB CORNER cards, you may find that these coordinates differ a little from the input ones due to rounding errors. Large discrepancies are an indication of a problem in the *experiment file.*
  - The edges of the crystal are listed in terms of the intersection of the planes.

- The next part consists of a listing of instructions in, and quantities derived from, the *experiment file.* Read this carefully and compare it with the *experiment file* to ensure that the program is performing the absorption corrections in the way you want it to!

- The main part of the *print file* consists of a listing of the individual reflections and the corrections applied. There are two formats:

  - For non-DAC data, a typical section looks like:

H	K	L	TRANS	F(OBS)	SIGMA(F)	BETA	TTH	OMEGA	CHI	PHI	SEQ	
0	4	4	0.364491	55.903	0.561	2.89014	35.934	-0.052	34.019	54.774	1	S
4	0	4	0.358333	59.752	0.616	2.87115	36.604	-0.059	33.407	-33.099	2	S
4	4	0	0.334699	48.829	0.532	2.74604	42.090	-0.039	-2.248	10.043	3	S
-6	3	2	0.342365	2.830	0.077	2.20526	52.026	-0.390	12.484	119.807	4	T

    For each reflection:
    - TRANS is the overall transmission coefficient
    - F(obs) and Sigma(F) are the corrected structure factor and its esd.
    - BETA is the quantity $-A^{-1}\,\partial A/\partial\mu$ required for extinction corrections in the refinement
    - TTH, OMEGA, CHI and PHI are the setting angles. OMEGA is bisecting. If the *input datafile* was SHELX *hkl* format then OMEGA, CHI and PHI will be set to zero.
    - SEQ is the sequence number of the reflection, either from the *input datafile* or generated by Absorb.

At the end of each line may be some flags to indicate reflections that will not be written to the *output datafile*:

S indicates a standard reflection

T indicates a reflection that has a 2θ value outside of the user-defined limits.

- For DAC data, a typical section looks like:

```
 H  K  L   TRANS              F(OBS)     SIGF      BETA    THETA  OMEGA     CHI    PHI                PSII      PSID
T(XTL)T(DAC)T(GAS)T(MED) NSEQ

 2  -2   0  0.337935    20.14    0.17    4.18  20.73   4.57    98.28 -142.54 37.86[2] 38.66[1] 0.473 0.717 0.998 1.000    30
 2  -2   0  0.317440    21.28    0.18    4.21  20.73   6.86    83.55  -39.27 40.49[1] 39.79[2] 0.468 0.688 0.991 1.000   134  D
 2  -2   0  0.327503    21.08    0.19    4.19  20.73   6.75    83.43  -38.27 39.54[1] 38.82[2] 0.471 0.703 0.994 1.000   135
```

In addition to the quantities described for non-DAC data:

- PSII is the angle that the incident beam makes with the axis of the cell. The number in square brackets indicates which anvil the incident beam passes through. [1] means the anvil on the incident-beam side of the cell when the diffractometer is positioned at zero, [2] the anvil on the diffracted-beam side of the cell when the diffractometer is positioned at zero.
- PSID is the angle that the diffracted beam makes with the axis of the cell. The definition of the anvils [1] or [2] for the diffracted beam is the same as for the incident beam.
- T(XTL) is the transmission coefficient through the crystal alone.
- T(DAC) is the transmission coefficient through the anvils and backing plates.
- T(GAS) is the transmission coefficient through the gasket (i.e. the "shadowing correction").
- T(MED) is the transmission coefficient through the pressure medium.

The additional flags that may appear are:

D indicates that the reflection has at least one ψ angle larger than the user-specified limit.

O indicates that the gasket shadowing exceeded the user-specified limit.

At the end of the *print file* are some statistics on the reflections, and a summary of the corrections. These should be self-explanatory. Note that the column marked "P" in the section on standard reflections is the value of the parameter *p* derived from the standard reflections for adjusting the standard deviations of the structure factors in the refinement program according to $\sigma'^2 = \sigma^2 + (pF)^2$.

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