ABSORB V7.2

with

ABSORB-GUI

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

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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.

CONTENTS

INTRODUCTION

Overview

ABSORB is a program to correct single-crystal X-ray intensity datasets for the effects of absorption by the crystal and by environmental devices including diamond-anvil pressure cells. It can be used for data collected with either an area detector or a point detector from any type of diffractometer. It handles a variety of data file formats, including SHELX *hkl* files and incommensurate data.

The program runs on Windows-2000, Windows-NT, Windows-XP Windows-7 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 (Burnham 1966) and the paper describing the current version of the program:

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

Further information about the methods used in the program is also available in:

Angel RJ (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 as a user by sending an e-mail to rossangelsoftware@gmail.com. If you discover apparent bugs in the program, please send the input files, the output file and a full description of the problem by e-mail. Suggestions for improvements, modifications, and development can be considered on both a commercial and non-commercial basis. Contact us via the web site www.rossangel.com.

How to use this manual

The manual is organised so that you can start with simple examples, and then use the more complex and subtle features of ABSORB later. ABSORB is not just a program for routine data processing, but it is also a research and development tool for single-crystal diffraction, especially under non-ambient conditions. Therefore it has a lot of features and modes of operation that are not normally used. So….

- **New users:**
  - Read and perform the installation following the section ‘Installation’.
  - Try to run a couple of the examples with the help of ‘Running Absorb Interactively’
  - Use ABSORB-GUI to make your own experiment files. For guidance for ‘normal’ experiments, read the section ‘Describing the Experiment’.
  - For further details and for unusual experiments, read ‘The Experiment File’. You may have to manually edit the *experiment file* to activate some of the less-used features of ABSORB.
- **Users of Absorb 6:**
  - Read the new features section, below this one. Your old *exp* files will not work!
  - Read and perform the installation following the section ‘Installation’.
  - Edit your old *exp* files and use the new ABSORB-GUI to repeat some runs you did with ABSORB-6.

- **Programmers:**
  - Do as suggested for 'new users'
  - Full documentation of the program methods, file formats, and how to call ABSORB from another program are given in the *Programmers' Guide* available from the website.

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. See the *Programmers Guide* for details if you want to write your own interface to run ABSORB.
- 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).
- Ag mass absorption coefficients added. And one can now specify wavelength 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.

Version 7.2

Version 7.2 was released in December 2014. If you are using an earlier version please upgrade to this version; it includes bug fixes, as detailed in the last section of this manual.

Acknowledgements

Thanks are due to Charles W. Burnham for his original coding of the ABSORB program, Larry Finger for developments of the code over many years, and Javier Gonzalez-Platas for writing the GUI to build *experiment* files. Many users have provided significant feedback and undertaken testing of the program, especially David Allan, Jason Burt, Diego Gatta, Ronald Miletich, Tiziana Boffa-Ballaran, Andrzej Grzechnik, Clivia Hejny, Demelza Hugh-Jones, Simon Parsons, Nancy Ross, Elinor Spencer and Jing Zhao. Thankyou!

INSTALLATION

There are three ways in which you can download and install the program and documentation. The methods provide exactly the same version of the ABSORB program itself.

Absorb GUI

This provides the ABSORB program along with a GUI written by Javier Gonzalez-Platas that allows you to create or edit the description of the crystal (and DACs), and then runs the program.

Download and run the installer from www.rossangel.com. After installation a system restart is performed in order to ensure that the environment variable ABSORB is correctly installed in your system. This variable points to the location of the ABSORB executable.

We recommend that you install the programs in a separate folder, and not in the folders where you work on data. The installer will create two sub-folders, one with the full users' manual and copies of publications, and one with some example files.

We recommend that you **do not** install the program to a folder in C:\Program Files (x86) because this can lead to problems arising from restricted permissions (e.g. to delete files) in this folder.

Absorb standalone

Use this method if you want to run the ABSORB program from another program. This provides the ABSORB program without a browser and without any installation being performed.

1. The absorb.zip file contains: the executable, some test datasets, and *pdf* files of Angel (2004), Angel and Gonzalez-Platas (2013) and this manual.
2. Unzip the *absorb.exe*. It is recommended that this folder is not used for data files. You will have to provide the location of the *absorb.exe* to programs that call it.
3. Unzip the remainder of the files into a working directory. These contain example datasets and corresponding *experiment* files that are described later in this manual.

See Programmers manual for information as to how to run Absorb in this way.

External Distribution

Absorb may also be distributed with other software, for example with other data reduction programs. Follow the instructions for installation provided by that software. Absorb can then be run from the other software, but the *experiment* file can still be edited manually by the user, either with a normal editor, or with ABSORB-GUI.

RUNNING ABSORB INTERACTIVELY

To run Absorb you need two files:

- The *input data* file containing the reflection data to be corrected in either SHELX *hkl* or *raw* format or WinIntegrStp *int* format.
- An *experiment* file. This is a text file that 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.

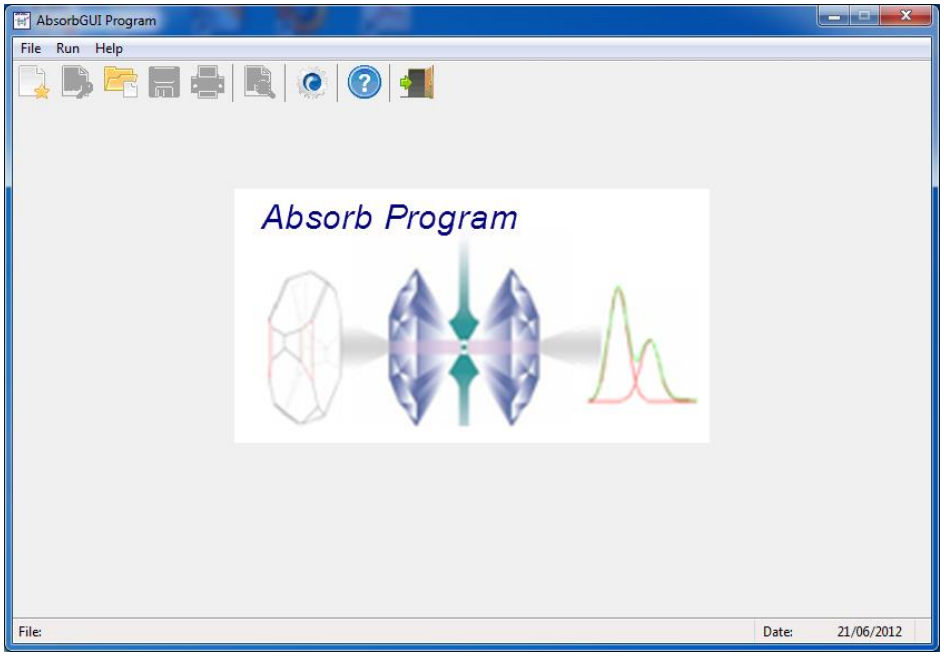
You can create or edit an *experiment file* in several ways:

- With a text editor (e.g. Notepad, WordPad etc),
- You can use the ABSORB-GUI to create and save an *experiment file.*
- You can use the editor from *View Files* icon on the main window of ABSORB-GUI
- Through third-party data reduction software.

Once the experiment file is created, you can use ABSORB-GUI to run ABSORB.

Using ABSORB-GUI

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



If you just want to run ABSORB with a pre-existing *experiment* file, you can go straight to the *Run* menu and select the files. For more details see below.

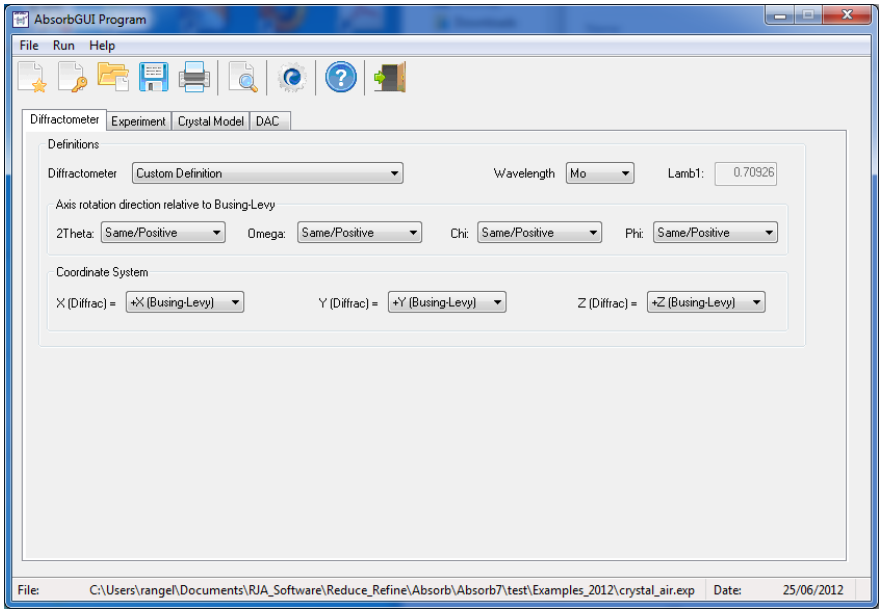
If you want to load and edit a pre-existing *experiment* file, use the *File* menu. If your diffractometer control software or data reduction software has produced a description of your crystal in a suitable file format (Agilent, Stoe and Bruker systems), you can import the information from the file with *File|Import.*

ABSORB-GUI provides 4 pages on which to set up and edit the description of your experiment. Not all information is required for all experiments. The pages are illustrated here with the help of example files included in the distribution.

Example: Crystal in air

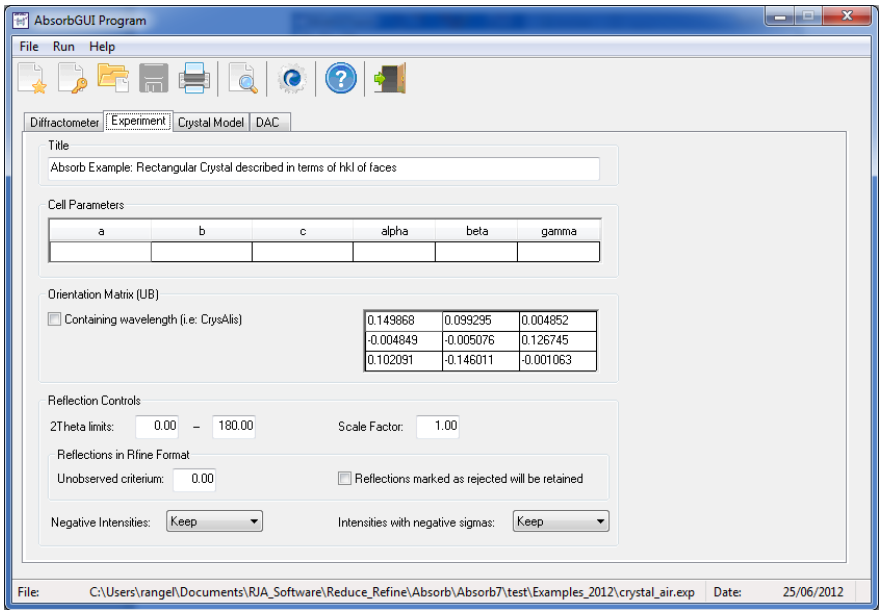
Start ABSORB-GUI if you have not yet done so. Use the file menu to load *crystalair.exp* from the examples folder. This file contains the instructions for absorption corrections for a crystal in air.

You will then see the first page of the GUI which describes the diffractometer configuration:



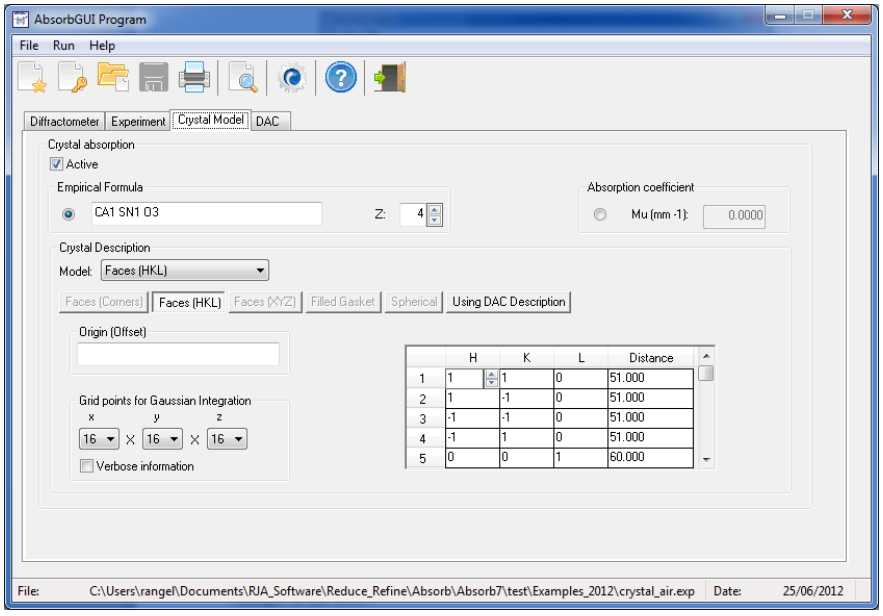
This *experiment* file describes the configuration of a Stoe diffractometer. This is important because the interpretation of the orientation matrix depends on the choice of coordinate system here. You will get the same results if you select *Stoe Instrument* from the pull-down list of diffractometer definitions. You must also specify the correct wavelength for your experiment here. If you used synchrotron radiation, select *custom* and input the wavelength value.

The *Experiment* page holds the orientation matrix, which is always required if your reflection data is in SHELX *hkl* file format:



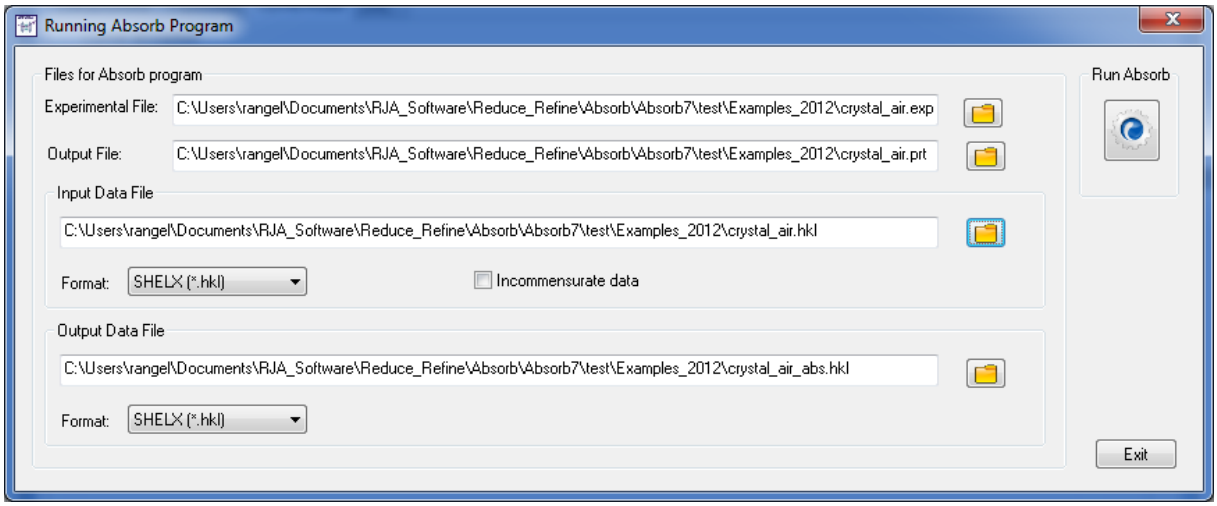
The boxes in *reflection controls* at the bottom allow you to limit the reflections that are output by the program; either by 2θ range, or if they have negative intensities or negative $\sigma(F^2)$. The parameters in the box *Rfine format* only apply to input data provided in the RFINE data format.

The *Crystal Model* page holds information about the crystal size, shape and absorption coefficient. There are many ways to specify the crystal shape and position, and they interact in a complex manner with the parameters for DAC experiments. For this example, we have a crystal in air, whose size, shape and orientation has been specified by the Miller indices of its faces:



The information described above is all that is required to perform an absorption correction for a crystal in air. If you changed any of the information with the GUI, save the changes to the *experiment* file with the *File* menu, or the *Save* icon on the main GUI. You can also edit the *experiment* file directly at any time with the *View Files* icon. If you change the *experiment* file with an external editor, including the one from *View Files*, you need to reload it in to the GUI if you want to see the changes in the GUI.

Once you have created and saved the *experiment* file, you can just run the ABSORB program by selecting *Run* from the dialog and selecting the input and output files to be used, for example:



You can change the file names and formats for the output files.

Once you have selected the files, run ABSORB by pressing the *Run* icon at the right.

Program output

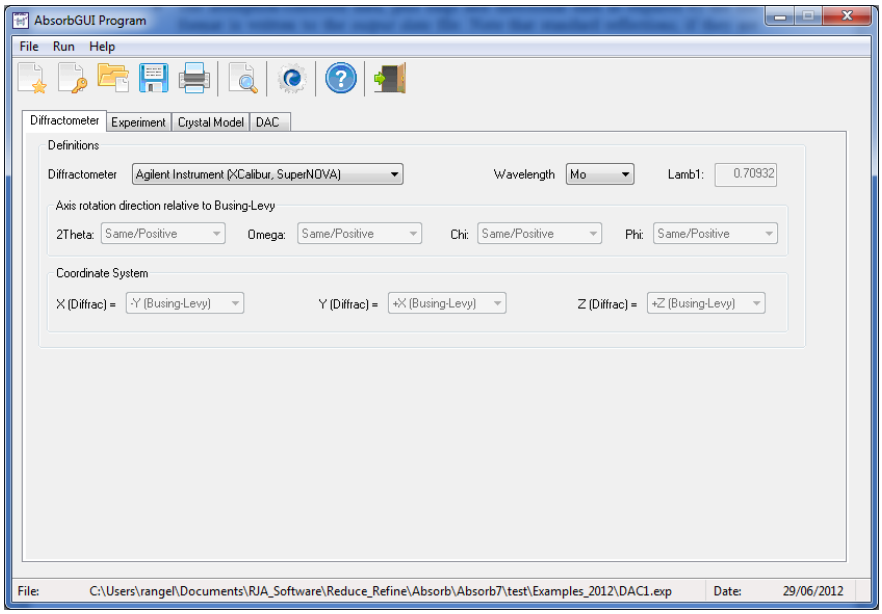
Once ABSORB finishes (with or without errors or warnings) you will see a short message to confirm that the program has finished.

When the data have been processed, the program writes several output files:

- 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 'The Print File' below. The *print file* is the place to look for information if you do not get the results that you expect. You can look at the output *print* file with the full information about the calculations with the editor available with the *View Output Files* icon on the main GUI. *Whether or not the program runs without an error, you are strongly encouraged to always check the print file. Always!*
- 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, if they are marked as such in the *input data* file are not written to the *output data* file. The supported file formats are:
    - SHELX "hkl" format.
    - RFINE "abs" format.
- 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*".
- The information about the corrections is also written to a *cif* file, given a name based upon the name of the *output data* file, together with "*_absorb.cif*".

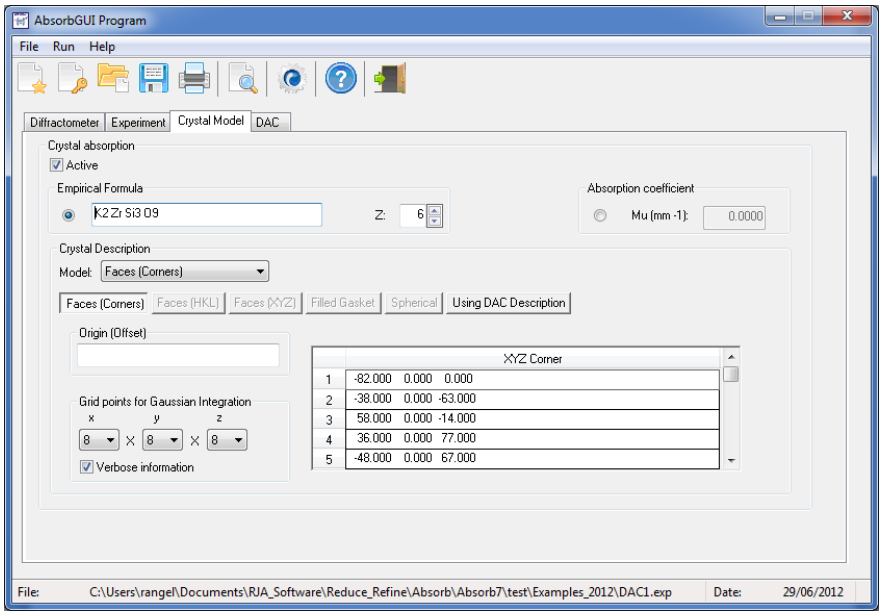
Example: Crystal in DAC

Start ABSORB-GUI if you have not yet done so. Use the file menu to load *DAC1.exp* from the examples folder. This file contains the instructions for absorption corrections for a crystal in a DAC that is backed with beryllium plates to support the diamonds. You will then see the first page of the GUI which describes the diffractometer configuration:



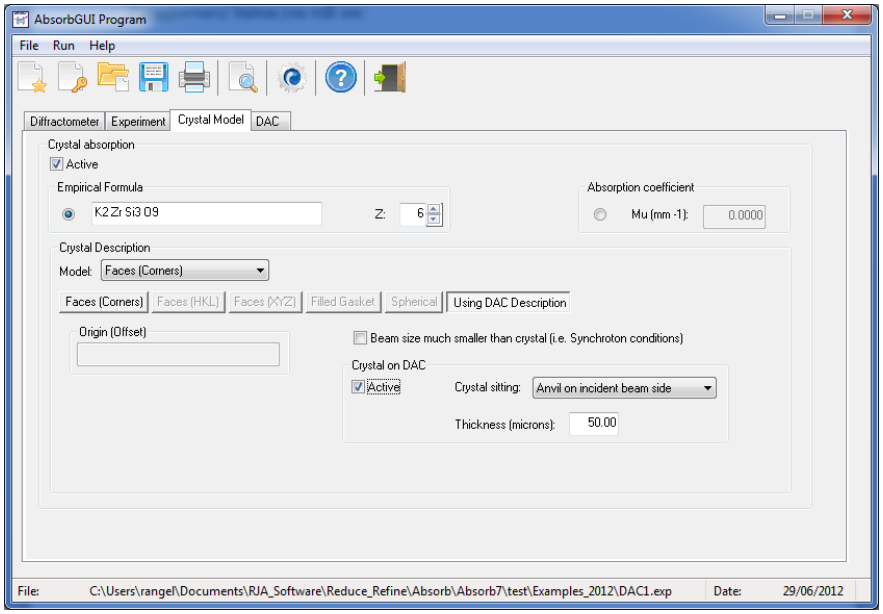
The information on the *Experiment* page is similar to that found for the crystal in air, just a title, the orientation matrix and the controls for output of reflections.

On the *crystal model* page is the description of the crystal in the DAC. When you press the *Faces(corners)* button you will see:

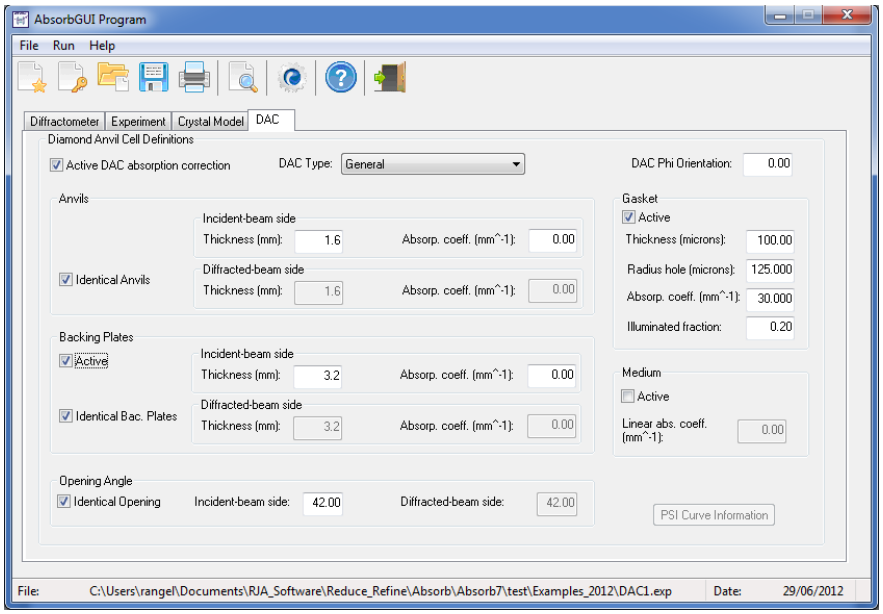


It is recommended for high-pressure work to input the unit-cell contents and let the ABSORB program calculate the absorption coefficient, because this changes with pressure.

There are several ways to describe a crystal in a DAC, as discussed in detail below. This example has the simplest method. It assumes that the crystal is a flat plate sitting on one of the diamond anvils. The crystal is defined in terms of the *x* and *z* micron coordinates of it's corners, as shown above. This crystal has five corners. If you press the *Using DAC Description* button, you can then specify which anvil the crystal is sitting on, and how thick it is:



There are also several ways to describe the DAC, on the *DAC* page. For this example, the components are specified in terms of their dimensions, and the opening angle is given at the bottom. The ABSORB program will reject reflections calculated to have paths that exceed the opening angle of the cell.



In this example, the absorption coefficients of the diamonds and Be plates are not given, so the program will calculate them from the wavelength specified on the *Difffractometer* page.

For a synchrotron dataset you will have to calculate the absorption coefficients for the cell components and your sample crystal yourself. This DAC is symmetric – both sides have the same dimensions – but it is possible to make corrections for asymmetric cells. Lastly, the parameters of the gasket dimensions are specified on the right hand side.

You can run this example just as for the crystal in air. Go to the *Run* page, select the files, run the program and look at the output files.

Warnings and Errors

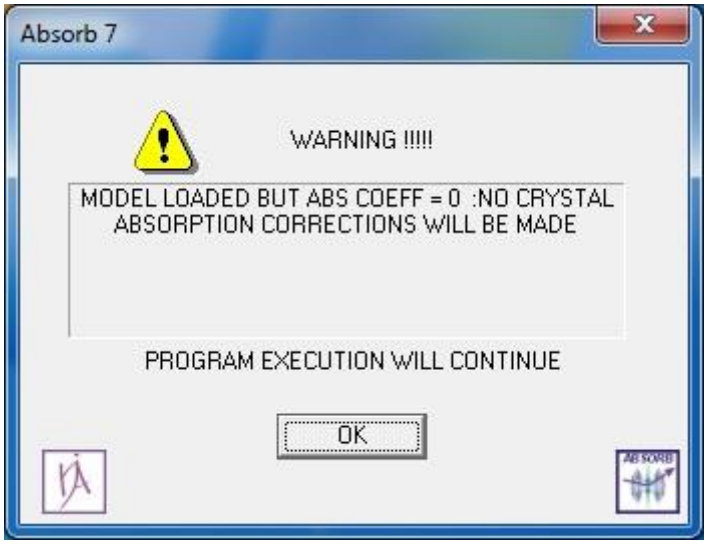
If there is an error in your description of the experiment (e.g. some inconsistency) you will often be warned by the GUI. If the ABSORB program detects an error from the data given in the *experiment* file you will see the error box with an explanation, for example:

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, either by editing it directly, or by modifying it with ABSORB-GUI.

Errors will also occur if you do not supply enough information in the *experiment* file to allow the program to perform the corrections that you have requested. For example, if your *input data* file is a SHELX *hkl* file, then you have to supply the program with the orientation matrix in order for it to perform the geometry calculations. If you forget, then you will see an error message:

Error messages are also written to the *print* file, along with as much information as possible. Use the information to correct the problem in your *experiment* file and try running the program again.

You may also see a warning box, for example:



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.

DESCRIBING THE EXPERIMENT

Introduction

ABSORB allows you to describe the size and shape of the crystal, and the diamond-anvil cell if you have one, and the diffractometer, and to make all sorts of absorption corrections. You provide this information to the program in the *experiment* file. ABSORB-GUI will create the *experiment* file from the information you input.

In this section some of the different methods are listed and examples of *experiment* files are given as a way of getting started. Full details of all possible descriptions are given in the section 'The Experiment File'. So, if you are a new user, start by using ABSORB-GUI and the information in this section to set up your *experiment* file.

Note that the ABSORB-GUI program can also import files from some diffractometer control software that include the descriptions of the crystal shape and the diffractometer. In addition, some commercial data reduction software provides GUIs to set up the *experiment* file and run ABSORB for 'normal' experiments, so you don't have to worry about the format and details of the *experiment* file until you have an unusual experimental configuration.

Format

The *experiment* file is a 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). Comment lines can also be marked with an #. 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 but *not* tabs.

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 or the ABSORB-GUI.

Conventions

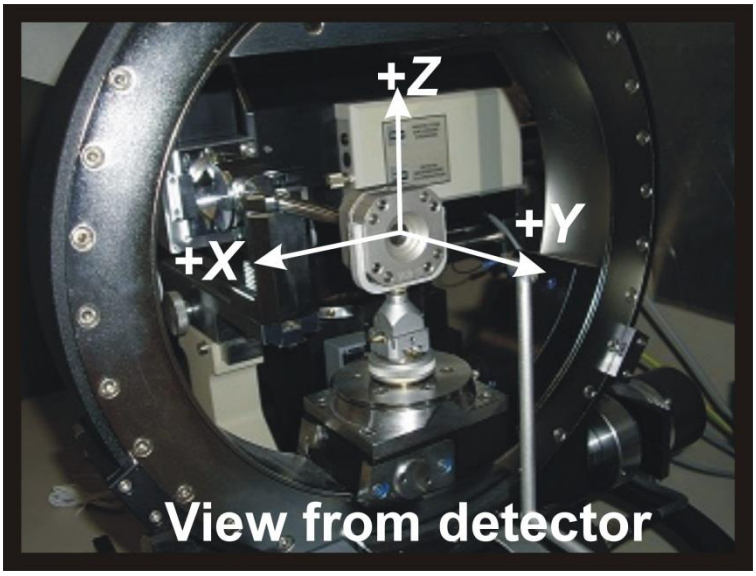
In order for the program to calculate the correct path lengths for the incident and diffracted X-ray beams in both the crystal and the DAC (if present), the reflection data, the crystal shape, and the DAC must all be described on a self-consistent set of coordinate axes, diffractometer circle parities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

Internally the ABSORB program uses the axial conventions 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 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 un-diffracted direct beam to the beamstop),
- 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 the diffraction vector at $2\theta = 0$.



This coordinate system can also be used to describe the position, size and orientation of the crystal.

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}.

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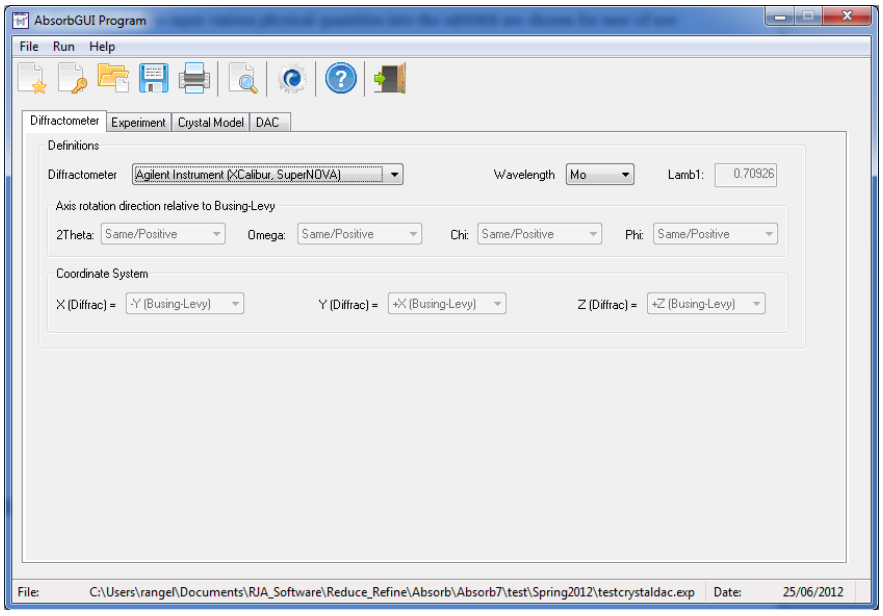
Describing the diffractometer

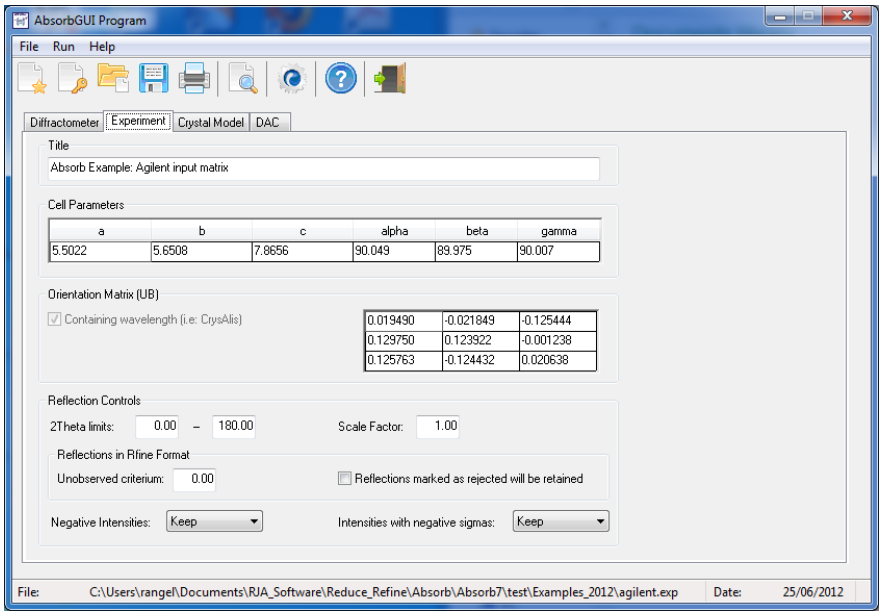
It is almost always necessary to provide basic information about the diffractometer, the wavelength, and the conventions used in the diffractometer software for describing the orientation matrix of the crystal. You input this information on the first page of the GUI. The example below describes an Oxford Diffraction/Agilent Technologies diffractometer with a Mo radiation source:



The selection from the *diffractometer* pull-down menu sets the description of the Cartesian axis system. Note that the axis parities are not needed if your input data file is a SHELX *hkl* file. If you data was collected with a point detector instrument and the data format includes the diffractometer angles, you have to select 'custom definition' for the *diffractometer*, and then input the parities of the circles. This is *not* needed if your data is in a SHELX *hkl* file.

Experiment information

If your data is in a SHELX *hkl* file, you must provide the orientation matrix that indexes your dataset, and the *hkl* file must contain the direction cosines of the incident (i.e. primary) and diffracted beams. The orientation matrix can be input or edited on the *Experiment* page:



The example shows a matrix from a system run by the Crysalis software, which includes the value of the wavelength in the orientation matrix.

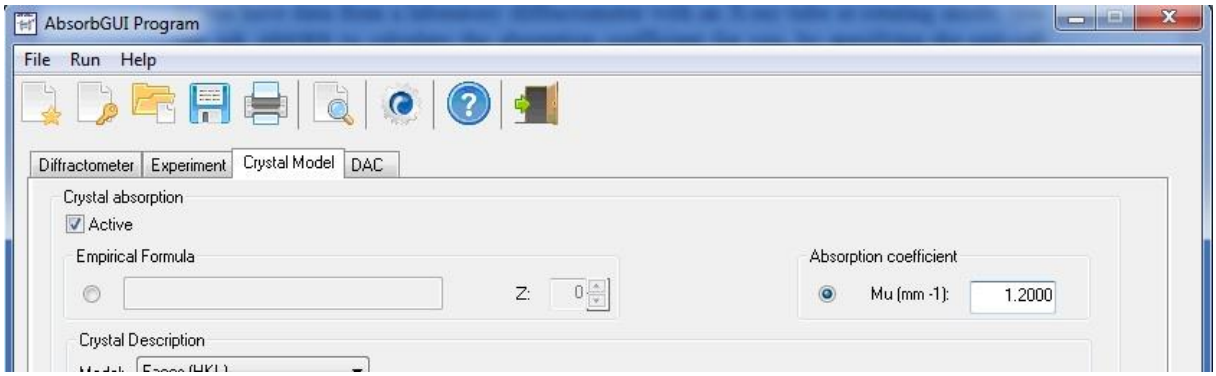
Other controls on this page allow you to control which reflections are processed. Reflections that are written to the *output data* file can be limited by the 2θ value. In addition, you can tell

the program to keep or reject reflections with either negative intensities or negative $\sigma(F^2)$. The controls in the *Rfine format* box only apply to *input data* files with the RFINE format because this format includes extra information from the integration process.

CRYSTALS IN AIR – EXAMPLES

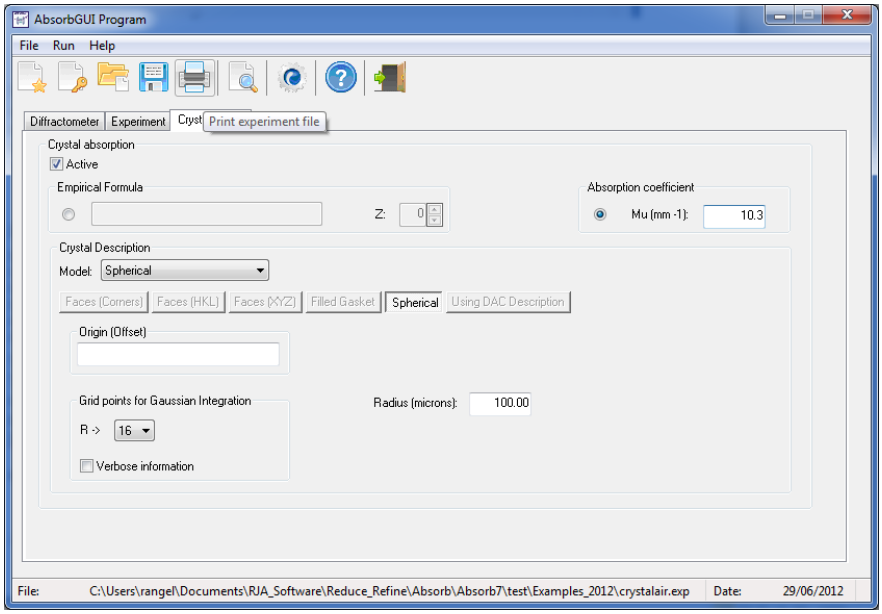
If you want to make corrections for absorption by the crystal, you can specify the absorption coefficient by one of two methods. If you have data from a laboratory diffractometer with an X-ray tube or rotating anode, you can ask ABSORB to calculate the absorption coefficient for you, by specifying the unit-cell volume either explicitly or by giving the orientation matrix, both on the *experiment* page. Note that values can only be calculated for Mo, Cu, Fe, Cr and Co Kα radiations (as specified on the *Diffractometer* page.

If you have synchrotron data, you must calculate the absorption coefficient yourself and specify it on the *Crystal Model* page, for example:



For crystals in air, there are four possible types of crystal absorption model, and one example of each of three types of models is given here (the fourth is not often used). The choice of type of absorption model is made with the pull-down menu *Model* on the *crystal model* page. Once the type of model is selected, the appropriate input boxes are activated with the labeled buttons in *Crystal Description.*

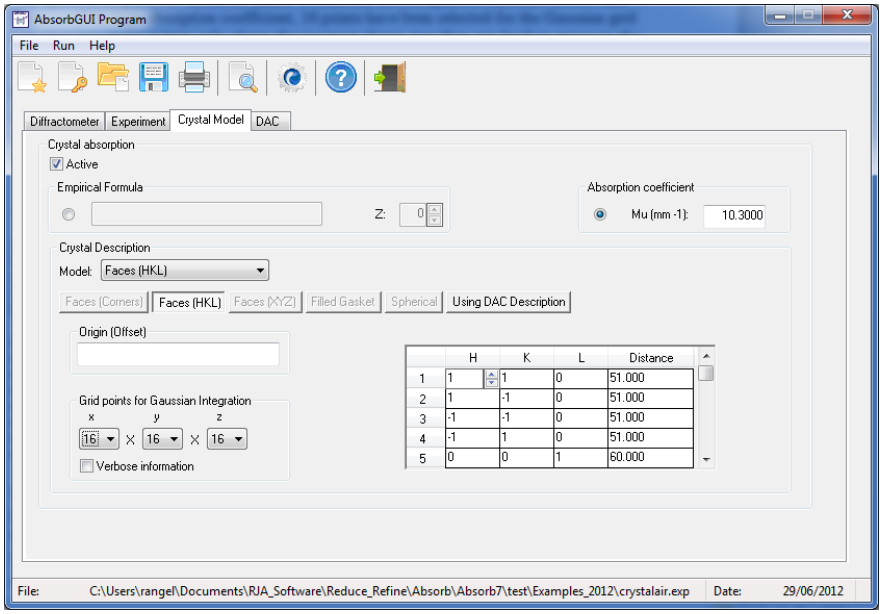
Spherical Crystal



This specifies a spherical crystal of radius 100um and an absorption coefficient of 10.3 mm^{-1}. Because of the high absorption coefficient, 16 points have been selected for the Gaussian grid. Selecting too many points only slows the program down, too few can lead to errors in the calculated transmission coefficients. As an approximate guide, a grid of 8 or 16 points along each axis is sufficient for values of $\mu t < 10$, but 32 grid points are required for accuracy at the 0.1% level for $\mu t \sim 100$ (Angel, 2004).

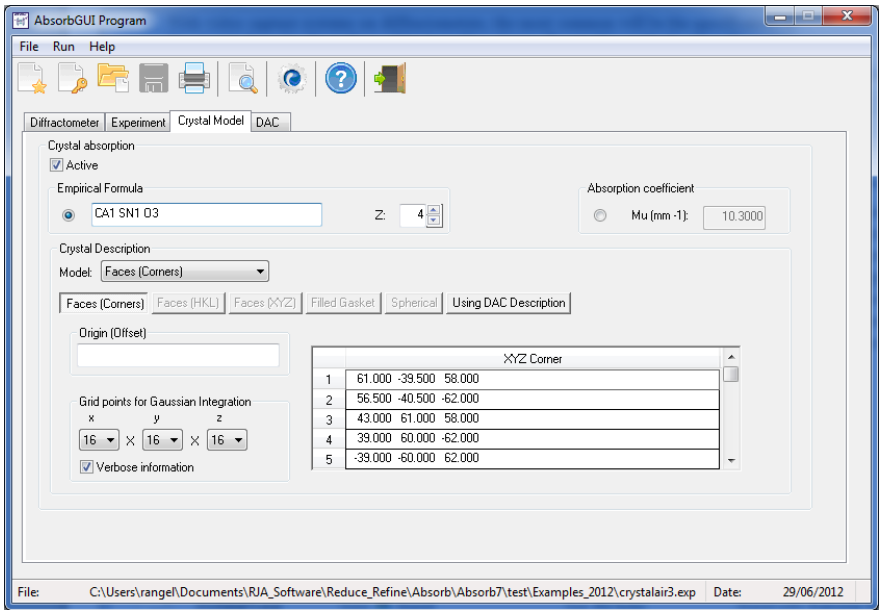
Crystal by faces

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, select *Faces(hkl)* from the pull-down *model* menu, and then enter the faces information in the box that appears when *Faces(hkl)* button is selected:



Crystal by corners

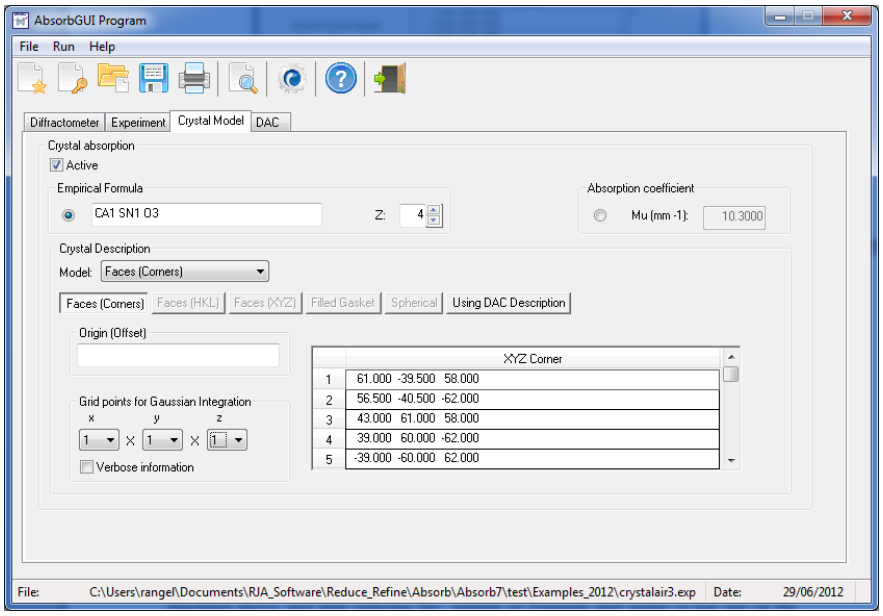
It is also possible to describe the crystal by the coordinates of the corners of the crystal, as measured in microns relative to the centre of the diffractometer, using the ϕ-axis coordinate system described in the 'conventions' section above. For this type of description select *Faces(Corners)* from the pull-down *model* menu:



The coordinates are then input in to the box that appears when *Faces(Corners)* button is selected. An example is in the *crystalair3.exp* file, which describes exactly the same crystal as *crystalair.exp*.

The small beam case for crystals in air.

The normal mode of calculation in ABSORB (see Angel, 2004) is based upon the assumption that the incident beam intensity is constant across the crystal, and that the beam diameter is therefore much greater than the maximum dimensions of the crystal. This is true for most laboratory X-ray measurements with conventional sealed-tube sources. At synchrotrons it is possible to collimate the beam down to a size *much smaller* than the crystal. In this case the relative absorption for each crystal reflection can be approximated by specifying the crystal as described above, and then reducing the number of Gaussian grid points to just one (at the crystal centre) as shown here:



CRYSTALS IN DAC – SIMPLE EXAMPLES

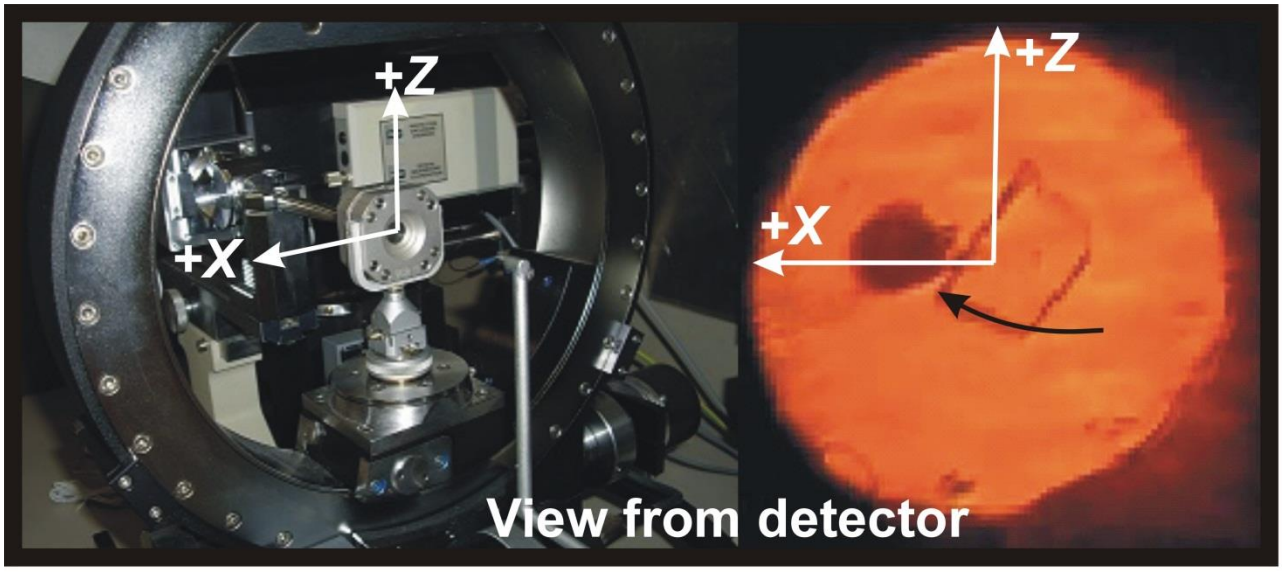
Diffractometer and Crystal

For a crystal in a DAC the entries for the diffractometer and the orientation matrix are the same as for a crystal in air. The crystal can, in general, be described by three methods:

- By the micron coordinates of its corners
- By the indices of its faces
- If it fills the gasket hole, by specifying the dimensions of the gasket.

For the crystal description, 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 is 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.

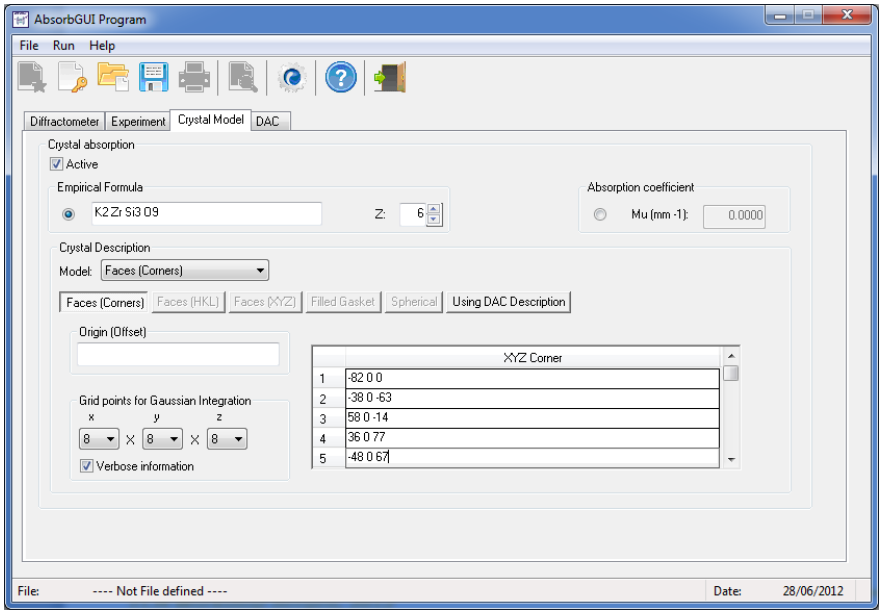
Thus, whether the DAC is rotated or not, the coordinates of the crystal corner indicated by the black arrow in the picture are x = 37um, z= -16um (the gasket has a radius of 150um).

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.

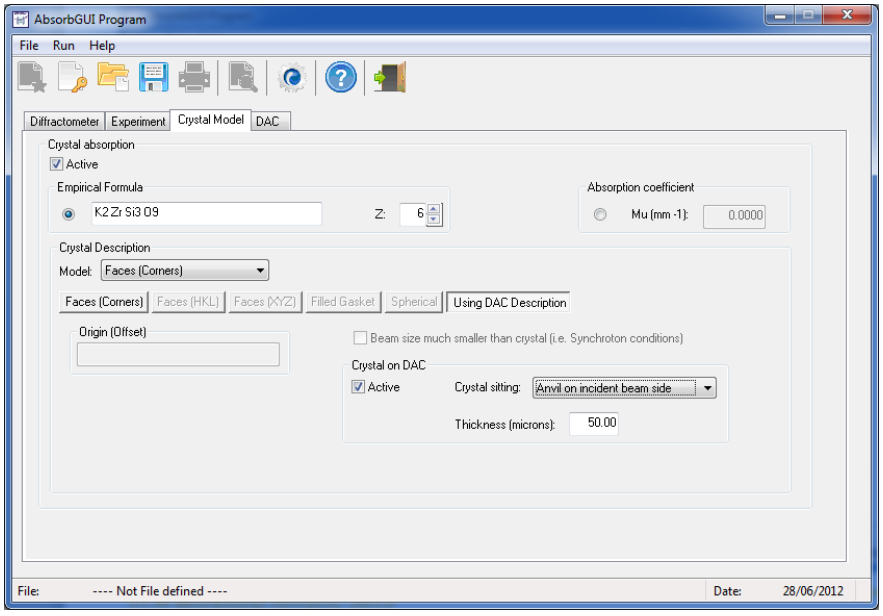
If the crystal is on the other anvil (the diffracted-beam anvil or anvil 2), the *y*-coordinates of one face of the crystal will be equal to the thickness of the gasket, and the other face will have coordinates equal to the thickness of the gasket minus that of the crystal.

Thus, the crystal in a DAC can always be described in terms of the coordinates of its corners, as for crystals in air. However, it is easier to have the program calculate the *y*-coordinates of

the crystal for you. To do this, select the *Faces(Corners)* model and enter the coordinates of the corners, but with the *y*-coordinate set to zero:



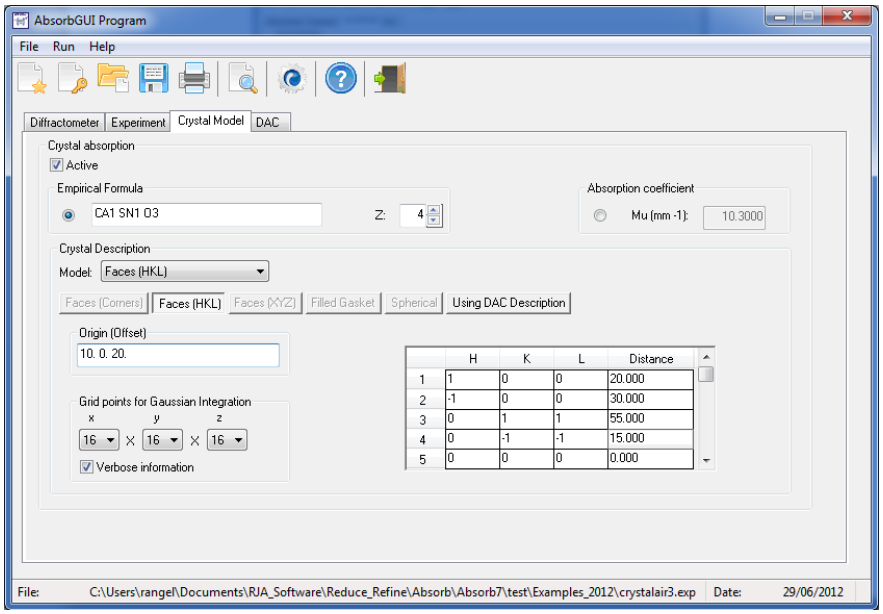
Now push the *Using DAC Description* and enter the information about which anvil it sits on and its thickness:



Remember that if the crystal is on the diffracted-beam anvil, you must specify the thickness of the gasket on the *DAC* page.

It is also possible to specify the crystal in the DAC in terms of the *hkl* indices of its faces when the DAC is set face-on to the incident beam when the diffractometer is at zero. However, in order to avoid ambiguities, this is not allowed when the DAC is rotated, and you must use the corner coordinates.

If you use a crystal description with the Miller indices of the faces, select *Faces(hkl)* as your model, and enter the indices of just the planes that describe the edges of the crystal:



And then push the *Using DAC Description* and enter the information about which anvil it sits on and its thickness. This will allow the ABSORB program to complete the crystal model for you. In addition, if the internal point in the crystal used for describing the distances of the faces of the crystal does not coincide with the centre of the gasket hole, its offset from the centre of the gasket hole must be specified in the *origin offset* box shown above.

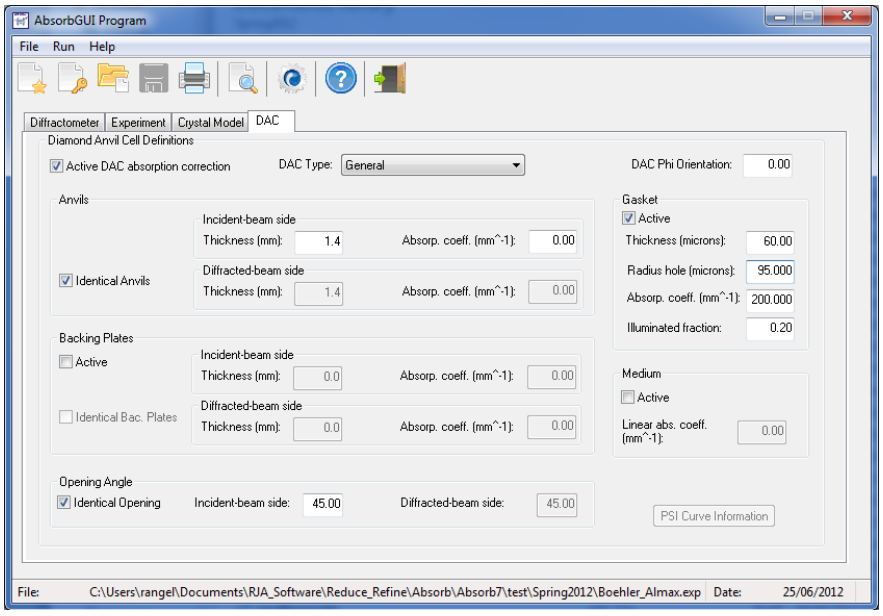
Note that if you have already measured the crystal in air, before you put it in to the DAC, you can use the same face description as you determined for the crystal in air (provided you did not break the crystal on loading it to the DAC!). But of course, you must use the orientation matrix from the DAC experiment!

Diamond anvil cell

There are a lot of different ways to describe the DAC, designed to accommodate all types of transmission-geometry DACs. Some of the options are available on the *DAC* page of the GUI, and are illustrated here.

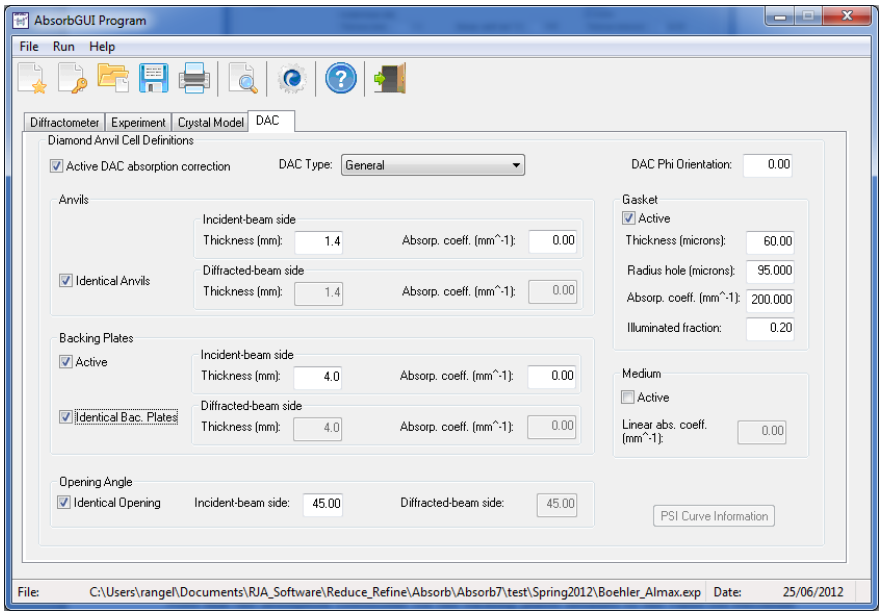
There are two basic ways to describe the absorption by the DAC components; either by specifying their sizes and absorption coefficients, or by specifying a measured absorption curve. For specification of the absorption curve parameters, read the section on *The Experiment File*, later in this manual.

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:



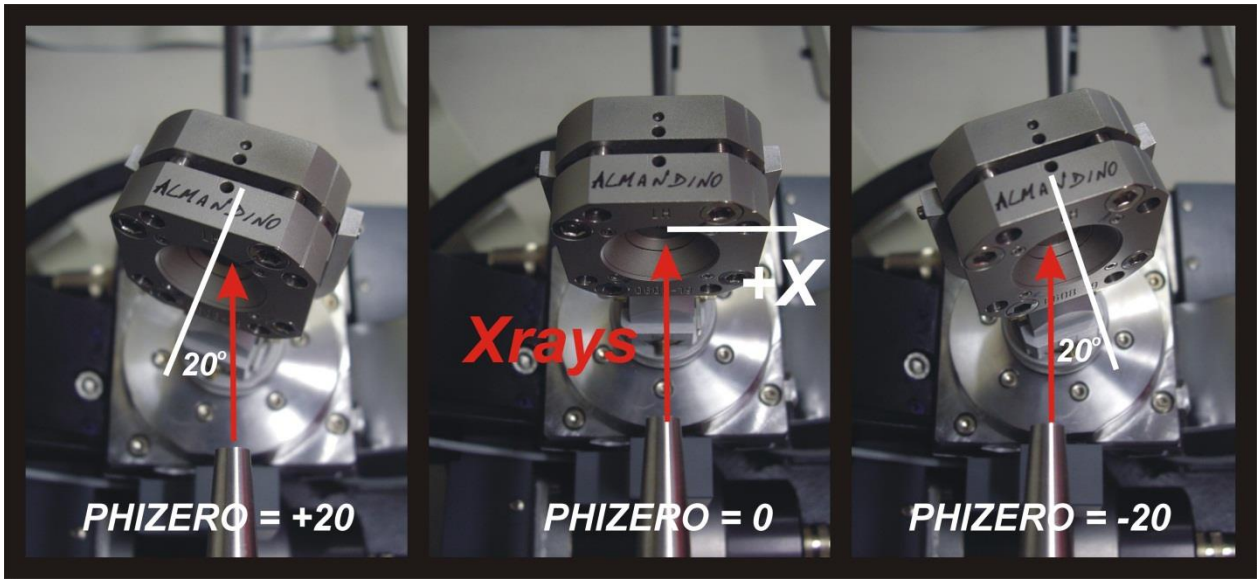
The GUI shown above describes a Boehler-Almax cell with two identical anvils, 1.4mm thick and an opening angle for X-rays of 45deg. Because no absorption coefficient is given for the anvils, it will be determined by the ABSORB program from the wavelength that is given on the WAVE card. The gasket is 60um thick between the anvils, and it has been drilled with a hole of radius 95um. 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:



Note that if you do not enter the absorption coefficient for the backing plates, it will default in the ABSORB program 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 this GUI page.

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 give the rotation angle on the *DAC* page of the GUI in the *DAC phi orientation* box. The angle you input 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 have a cell rotated in this way, you cannot describe the crystal in terms of the indices of the faces.

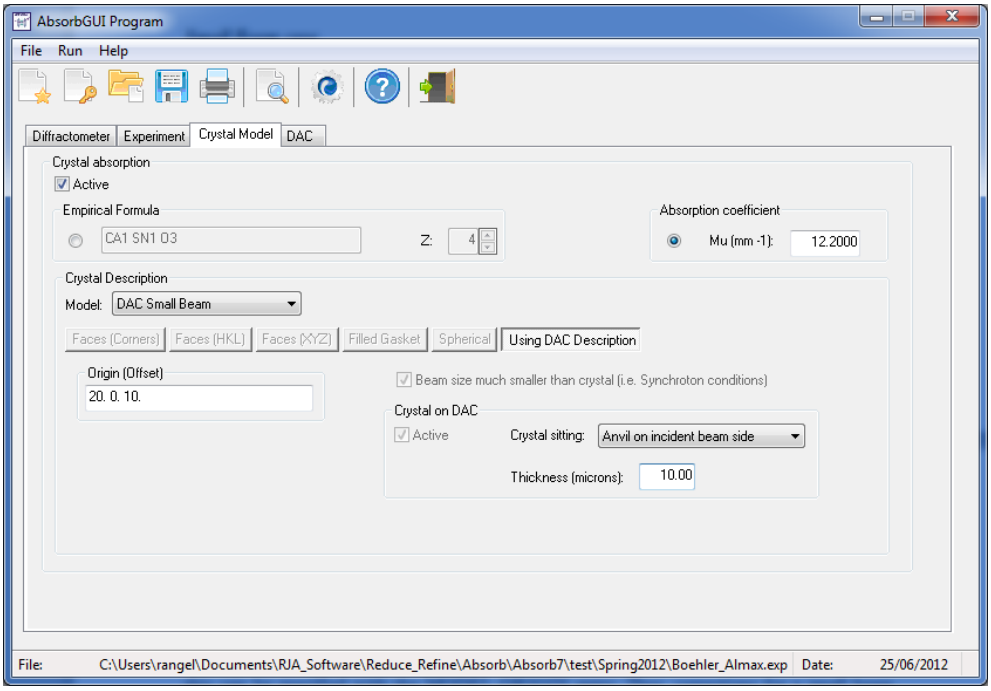
There are other ways to specify the absorption of the DAC, and to describe cells with different absorption (e.g. different sized anvils) on the two sides of the cells. For these and other details, see the full description in the section 'The Experiment File'.

Small beam case

The normal mode of calculation in ABSORB (see Angel, 2004) is based upon the assumption that the incident beam intensity is constant across the crystal, and that the beam diameter is therefore much greater than the maximum dimensions of the crystal (and indeed the gasket hole). This is true for most laboratory X-ray measurements with conventional sealed-tube sources. At synchrotrons it is possible to collimate the beam down to a size *much smaller* than the crystal, and thus avoid generating extra background in the diffraction pattern by diffraction from the gasket or backing plates of the DAC.

In this case the relative absorption for each crystal reflection can be calculated simply by specifying the thickness of the crystal and the dimensions of the DAC. Set up the DAC description as described above, and then go to the *Crystal Model* page and select *DAC Small Beam* as the Model. The crystal thickness and the anvil on which it is located can be set on

this page. If the point at which the beam hits the crystal is displaced from the centre of the gasket hole, this can be specified with the *Origin (offset)* entry:



THE EXPERIMENT FILE

This section includes the full specification of all possible entries in the *experiment* file. The *experiment* file contains all of the information about the crystal, the diffractometer geometry, diamond-cells etc. that is needed by ABSORB to perform the absorption corrections.

Normally, you can prepare and edit the entries in this file by using the ABSORB-GUI. However, for unusual experimental configurations it is sometimes necessary to edit the experiment file directly.

The *experiment* file is a 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). Comment lines can also be marked with an #. 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 Ångstrom of α_1 component
	wave(2)	wavelength in Ångstrom 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.

An alternative method for specifying the wavelength of laboratory X-ray sources is to specify the target material of the Xray tube, thus:

WAVE Cu

The program can calculate the absorption coefficient of a crystal for Co, Cr, Fe, Cu, Mo, and Ag sources. For other wavelengths do not use either of these cards, but instead specify the absorption coefficient of the crystal with the ABSORB MU card.

PARITY 1,1,-1,1

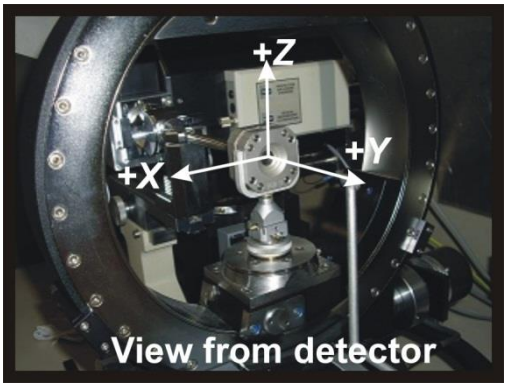
Default: 1,1,1,1

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 data files. They are not needed or 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) shown here:



- 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 orientation matrix provided in the *experiment* file to the Busing-Levy axial system. The converted orientation matrix is then used for two purposes by ABSORB – to convert direction cosines associated with SHELX data files, 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. Use the same for Bruker instruments (tested for D8).

For data collected with Stoe diffractometers, use 1,3,-2

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 orientation 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

Orientation (UB) matrix. If the elements of the orientation matrix contain the wavelength (i.e. UB(input) = UB(Busing-Levy).λ) then the UBL cards should be used instead. Use these UB entries for orientation matrices from Bruker or Stoe systems, or the SINGLE software.

On input, the orientation matrix is rotated to the Busing-Levy coordinate system by use of the information provided on the BLAXES card. The rotated orientation 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.
- convert the Busing-Levy direction cosines used by ABSORB to the crystal system for output to a SHELX –format *output data* file.

Thus the orientation matrix *must* be specified if a SHELX *hkl* datafile is used. 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

Orientation matrix input if its elements contain the wavelength (i.e. UB(input) = UB(Busing-Levy).λ). This is the case for the orientation matrices used by the Crysalis software system of Oxford Diffraction.

On input, the orientation 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 $\sigma(F^2)$ are multiplied by this scale factor. If the card is not present, no rescaling is applied.

ABSORB NEGINT KEEP
or
ABSORB NEGINT REJECT
or
ABSORB NEGINT ZERO

Default: KEEP

Specifies the handling of negative intensities by the program. For *KEEP*, the reflections are processed in the same way as those with positive intensities, the absorption corrections are applied, and the reflections are written to the *output datafile*. For *ZERO*, the reflection intensity is set to zero in the *output datafile*, with sigma(I) set to 1. For *REJECT* the reflections with negative intensity are not processed at all, and are not written to the *output datafile.*

ABSORB NEGSIG KEEP
or
ABSORB NEGSIG REJECT

Default: KEEP

Specifies the handling of intensities with negative sigmas. If *REJECT* is specified the reflections with negative sigmas are not processed at all, and are not written to the *output datafile.*

There are two instructions that apply *only* to the handling of data with the RFINE format:

ABSORB LESSTHAN 2.0

Default: 0.0

Reflections with $F^2/\sigma(F^2)$ less than this value are marked as "unobserved" in the *output data* file.

ABSORB INTREJ KEEP

Default: DISCARD

(Previously this was ABSORB REJECT in version 6 of ABSORB)

Reflections in the *int* file marked as rejected by the Integration program are normally discarded by ABSORB. If ABSORB INTREJ 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.

There are two alternative methods for specifying the absorption coefficient:

ABSORB MU 12.3

Default: 0.0

The absorption coefficient of the crystal in mm^{-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 or WAVE cards. Note that values can only be calculated for Ag, 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 $Ca_8\ Al_{16}\ Si_{16}\ O_{64}$.

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. Not normally used – superceded by XYZCORNER
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.
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

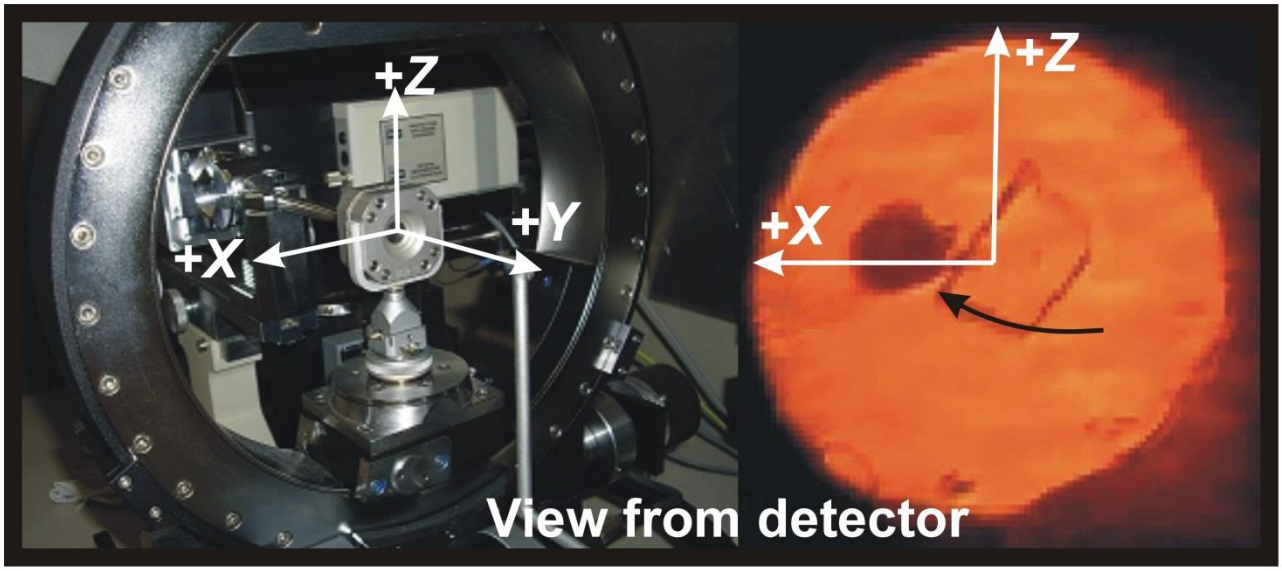
This specifies a face that passes through the three Cartesian points (73.0,0.0,32.0), (-44.0,0.,61.0), and (-69.0,0.0,-32.0). In this case the face is perpendicular to the y-axis (and thus the X-ray beam when the diffractometer is zero) and passes through the origin.

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. For crystals in air, the coordinate system is the Busing-Levy ϕ-axis system, shown below on the left. For crystals in a DAC it is always the DAC-coordinate system, shown below on the right. See the entry for DAC PHIZERO for more information..



This coordinate system is used for the crystal description, independent of the axial system used to describe the orientation matrix (which is specified by the BLAXES card).

One ABSORB CORNER 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 37.0,0.0,-16.0

This specifies the corner marked with a black arrow in the picture above at 37 microns along the x-axis and 16.0 microns along the negative z-axis from the origin.

ABSORB ORIGIN 10. 20. -30.

Default: 0. 0. 0.

Specifies the offset from the center of the diffractometer of the origin used for the description of the crystal model. Can be used in combination with any crystal description.

Especially useful when describing a crystal in a DAC with ABSORB FACE cards.

DAC SMALLBEAM

Specifies that the crystal absorption will be calculated for a beam much smaller than the crystal size. It can only be used with DACs and it requires the DAC CRYSTAL card to specify the thickness and location of the crystal. The ABSORB ORIGIN card can be used to specify the point in DAC coordinates that is under the beam.

Diamond-anvil cell components

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 corrections specified in terms of the thickness and absorption coefficients of both the diamonds and the support platens (if they are in the Xray beam paths). Absorption by diamond-cells with backing plates made of X-ray opaque material drilled with an access hole (e.g. Boehler-type seats) 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.

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

Note: Values of 2,3, and 4 specify pre-calculated attenuation curves that were implemented in earlier versions of ABSORB, but are no longer recommended.

DAC TYPE = 1

For DAC TYPE = 1 the following entries should be used to specify the absorption due to the DAC:

DAC ANVIL 1.6, 0.2
or
DAC ANVIL 1.6,0.2,1.4,0.2
or
DAC ANVIL 1.6

Thickness of the anvils in mm, and their absorption coefficient in mm^{-1}. Only used for DAC TYPE 1

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 refers 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 a value appropriate for the wavelength.

DAC PLATE 3.2 0.05
or
DAC PLATE 3.2, 0.047,4.0,0.047
or
DAC PLATE 3.2

Thickness of the backing plates in mm, and their absorption coefficient in mm^{-1}. Only used for DAC TYPE 1. Only to be used if the X-ray beams pass through the backing plate, for example in a beryllium-backed cell. If the backing plates are made of an X-ray opaque material (such as WC in a Boehler-Almax design) do not use DAC PLATE cards.

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 refers 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 DAC PLATE is specified but no absorption coefficient is given, as in the third example above, it is set by the program to a value appropriate for the wavelength assuming the plate to be made of beryllium.

If no correction is required for backing-plate absorption, then DAC PLATE should not be used at all.

DAC TYPE = 5

This allows the user to specify the absorption by each half of the DAC in terms of an attenuation curve. There are two possible methods.

The first method is by a single-parameter that 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 Ψ = 0:

DAC ABSPSI CURVE 0.605
or
DAC ABSPSI CURVE 0.605, 0.510

Default: 0.

Only used for DAC TYPE 5.

If only one number is given, as in the first example above, then the two halves of the cell are assumed identical.

The alternative is to specify the absorption by the backing plate and anvil of each half of the DAC by a table of values in terms of the inclination angle of the beam, the Ψ angle: 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 TABLE
1.0,0.999
2.0,0.980
3.0 ,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, for example:

```
DAC ABSPSI
0.0,1.0,1.000
1.0,0.999,0.995
2.0,0.980,0.97
3.0,0.965,0.96
….etc….
DAC ABSPSI END
```

In either case, the attenuation factor at any angle is determined by interpolation between the values given in the table.

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., 150., 200., 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 mm^{-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 CRYSTAL 1,30.

Default: none

If the crystal model has been specified in the DAC with ABSORB MODEL HKL this card *must* be used to specify the faces of the crystal parallel to the anvil culet surfaces. The parameters are:

Indicator of the anvil on which the crystal is sitting. '1' for the anvil on the incident-beam side of the DAC when the diffractometer angles are zero, '2' for the other anvil.

Thickness of the crystal in microns. This must be less than the thickness of the gasket, if that is specified.

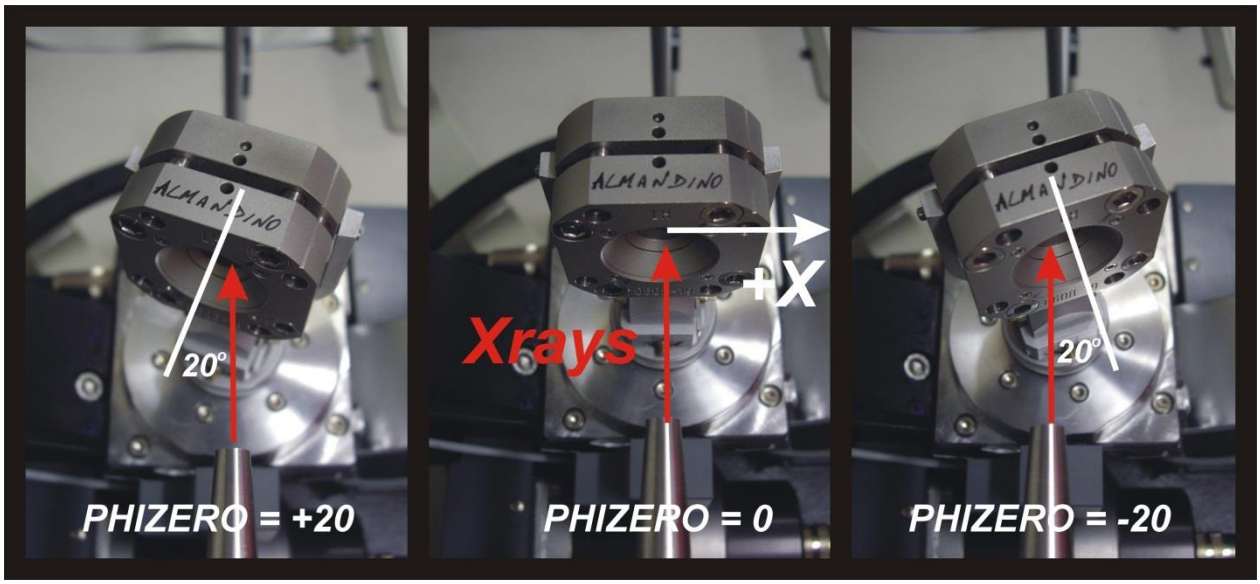
If this card is used with a model specified by ABSORB MODEL XYZCORNER, the program will take the specified corner coordinates, duplicate each corner and replace the *y* coordinates of the corners with values calculated from the parameters on this card. For example, for the example given, the *y*-coordinates would become 0.00 and 30.00

DAC CRYSTAL cannot be used with ABSORB MODEL XYZFACE, FILLEDGASKET OR SPHERE

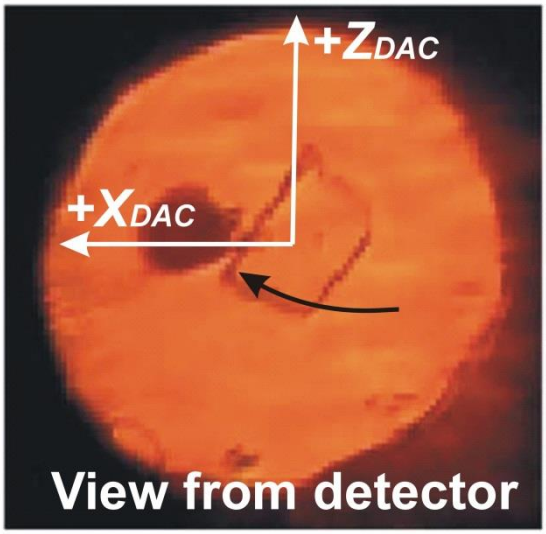
DAC PHIZERO 20.

Default: 0.

Phizero is defined as the clockwise rotation around Z (viewed from +Z and looking down on to the phi cradle) of the cell from the face-on position to the beam, when the diffractometer is at zero:



Remember that even when the DAC is rotated this way, the crystal is always described on the DAC coordinate system. That means always +Y along the cell axis, +Z up and +X to the left when viewed from the detector:



DAC MUMEDIA 8.3

Default: 0.

The linear absorption coefficient of the pressure medium in mm^{-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. Not normally used for 'normal' pressure media such as methanol:ethanol or He, or hydrogen because their absorption coefficients are small.

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:

- Absorption by the crystal.
- Absorption by the cell components (anvil and backing plate).
- Shadowing by the gasket.
- 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 orientation 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. If your input data was in a SHELX *hkl* file, for non-DAC data, a typical section looks like:

H	K	L	FSQ	SIG(FSQ)	BETA	SCALE	T(XTL)	2THETA	NSEQ	FLAGS
2	-2	3	43.64	1.06	4.697	3.012	0.332	25.97	796	
2	-2	4	4714.38	87.14	4.011	2.972	0.336	29.46	797	
2	-2	5	225.25	4.04	3.430	2.937	0.341	33.47	798	
2	-2	6	1223.62	24.49	2.964	2.910	0.344	37.85	799	
2	-2	7	30.67	1.14	2.602	2.889	0.346	42.52	800	
2	-2	8	2455.03	51.83	2.326	2.871	0.348	47.45	801	
2	-2	9	58.06	1.69	2.127	2.855	0.350	52.60	802	T
2	-3	8	6.94	0.53	2.185	2.839	0.352	50.43	803	T
2	-3	7	46.95	1.74	2.401	2.859	0.350	45.75	804	
2	-3	6	0.00	2.46	2.682	2.886	0.346	41.37	805	L

For each reflection:

FSQ and Sig(FSQ) are the corrected structure factor squared and its esd.

BETA is the quantity $-A^{-1}\,\partial A/\partial\mu$ required for extinction corrections in the refinement.

SCALE is the total correction factor by which the input F^2 was multiplied.

T(XTL) is the transmission factor through the crystal.

2THETA is twice the Bragg angle of the reflection. If your input data file included the setting angles of the goniometer for each reflection, these angles will also be printed here.

SEQ is the sequence number of the reflection, either from the *input data* file or generated by ABSORB.

At the end of each line there may be some flags to indicate the status of some reflections:

L indicates a reflection with an intensity that is less than the level set with ABSORB LESSTHAN. These reflections are still written to the *output data* file.

The following flags indicate reflections that will not be written to the *output data* file:

I indicates a standard reflection.

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

R indicates a reflection marked as 'reject' in the input file (RFINE format only)

N indicates a reflection with negative intensity (if Z appears the reflection will be output with zero intensity)

S indicates a reflection with negative sigma

For DAC data, a typical section of the print file for input data from a point detector looks like:

```
Absorb Example 5: Crystal in DAC
H   K   L    FSQ    SIG(FSQ)   BETA    SCALE T(XTL) 2THETA  OMEGA     CHI     PHI  PSII     PSID    T(DAC)T(GAS)T(MED)  NSEQ  FLAGS
2   -2   0    423.35     7.90   4.137   2.814 0.477   20.73  -4.32   81.57   35.44 36.75[1] 35.94[2] 0.746 1.000 1.000    208
2   -2   0    428.31     7.76   4.155   2.883 0.475   20.73  -4.47   81.65   36.45 37.70[1] 36.90[2] 0.732 0.999 1.000    209
2   -2   0    418.55     7.54   4.175   2.959 0.473   20.73  -4.61   81.73   37.46 38.65[1] 37.87[2] 0.717 0.998 1.000    210
2   -2   0    427.72     8.21   4.195   3.043 0.470   20.73  -4.76   81.81   38.47 39.59[1] 38.83[2] 0.703 0.997 1.000    211
2   -2   0    411.75     7.30   4.216   3.138 0.468   20.73  -4.90   81.90   39.47 40.55[1] 39.80[2] 0.687 0.995 1.000    212  D
2   -2   0    432.34     7.88   4.238   3.244 0.466   20.73  -5.04   81.98   40.48 41.50[1] 40.77[2] 0.672 0.992 1.000    213  D
2   -2   0    420.88     7.95   4.260   3.363 0.463   20.73  -5.18   82.07   41.49 42.45[1] 41.74[2] 0.656 0.988 1.000    214  D
2   -2   0    422.55     7.83   4.283   3.496 0.461   20.73  -5.32   82.16   42.49 43.41[1] 42.71[2] 0.639 0.983 1.000    215  D
2   -2   0    410.36     7.65   4.307   3.645 0.458   20.73  -5.45   82.26   43.50 44.37[1] 43.68[2] 0.622 0.978 1.000    216  D
```

In this example the input datafile had the setting angles of the diffractometer. If you use a SHELX *hkl* file, you will only see '2THETA'

SCALE is still the overall scale factor applied to correct the intensity

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 $\sigma'^2 = \sigma^2 + (pF)^2$.

MANUAL AND SOFTWARE REVISIONS

For revisions to earlier versions of Absorb, see the manuals for Absorb v6. For details of all of these changes, consult either the *Programmers Guide* or the section 'The Experiment File' in this manual, as appropriate.

Spring- Summer 2012: Version 7

- Program configuration
  - Separated the absorb program from the file browser and made changes to allow absorb to be run from other software. Introduced the *configuration* file. For details see the *Programmers Manual.*
  - There is a new GUI to set up the description of the crystal and diamond-anvil cells in the *experiment* file.
  - Removed FILES card from experiment file; the information is now provided in the configuration file.
  - Creation of error log file.
  - Write correction factors for every reflection as scale factors to a new *scales* file..
- Absorption coefficients
  - Changed all absorption coefficients to mm^{-1}
  - Sizes of DAC components are now in mm.
  - Ag mass absorption coefficients added. And can now specify wavelength by target material.
- Data Handling
  - Handling of negative intensities and sigma(I)
  - Rescaling factor now reported if applied.
  - All data reported in F^2, instead of F.
  - Handling of data internally switched to F^2 from F
- Model description
  - Added ABSORB ORIGIN to specify model origin.
  - DAC CRYSTAL defined to allow ABSORB FACE cards to be used to describe a crystal in a DAC.
  - Added DAC SMALLBEAM to handle beam smaller than crystal in DAC
  - DAC PHIZERO defined to allow the DAC to be set at an angle to the incident beam. A distinction is now made between the *sample* coordinate system and the ϕ-axis coordinate system.
  - Further improvements to the checking of the consistency of the input information about the crystal and DAC.
  - More traps of unphysical parameters for DACs
- Improved formatting of print file:
  - More information on Cartesian axes
  - On reflection listing, suppressed angle output when area detector data, and included all 6 indices for incommensurate datasets.

Autumn 2012 to January 2013: Version 7.1 to 7.13

- Minor bug fixes:
    - Corrected printing of values of absorption coefficients to *cif*
    - Minimum volume correction factor for small beam case was incorrectly reported on print file. Fixed.
    - The correction for the illuminated volume was not being calculated for the small beam case. Fixed and checked to be correct.
    - Changed reading of contents card in exp file, so that a space can be left between element symbols and the quantity.
- Changes to reflect publication of *J Appl Cryst* paper:
    - information printed on *cif*
    - provided reference in manuals

2013-2014: Version 7.2

- Ported to Intel Fortran compiler, and internal changes made to comply with new compiler.
- Minor bug fixes:
    - Fixed errors in *cif* items.
    - Fixed problem with large unit cells that caused program to complain that the unit cell volume was zero.
    - Fixed problems that caused program suite to hang up, caused by absorb.exe being launched with 'ProcSilent' attribute from the GUI.
    - Fixed problems that caused program suite to hang up when the input files could not be opened by absorb.exe
    - Changed reading of contents card in exp file, so that the number of molecules/cell can be set with 'Z = ' as well as 'Z='
    - Fixed handling of absorb_error.log, so that it now records all warnings, not just the last one.

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