

**CRYSCON**

**for Windows**  
**and**  
**Macintosh**

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**CRYSCON**  
**for Windows and Macintosh**  
**Version 1.1**

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# 1 Introduction

Preliminary topics:

[Capabilities](#)

[General Procedure](#)

[Types of Windows](#)

## 1.1 Capabilities

CRYSCON is a general crystallographic conversion program, with the following capabilities. See [General Procedure](#) for an overview of the main possibilities.

- 1) **Data Entry.** Data can be [imported](#) from several popular crystallographic file formats, read in through a "[free-form](#)" file input, or entered manually.
- 2) **Transformation of unit cell and atomic coordinates.** You can convert to a sub-cell or super-cell or simply translate to a different origin; or any combination of these. When converting to a sub-cell the positions of presumably coincident or superimposed atoms are averaged, and when converting to a super-cell the extra symmetry-unique atoms which may be required are generated. In any case the result is a set of symmetry-unique atoms for the target cell and symmetry, suitable for entry into crystallographic software such as Fourier analysis, least-squares refinement or structure drawing ([Control Window](#), [Transformation Parameters](#) dialog).
- 3) **Change of symmetry in the same or different unit cells.** You can convert to a sub- or super-symmetry group, or even a non-related space group. As in the case of cell transformation, new atoms are generated and/or old atoms are averaged as necessary, and the result is a set of symmetry-unique atoms for the target cell and symmetry ([Control Window](#), [Transformation Parameters](#) dialog).
- 4) **Transformation of anisotropic temperature factors and atomic vectors** (e.g. magnetic vectors).
- 5) **Computation of bond lengths and angles** in either the original or transformed structures ([Bond Lengths and Angles](#)).
- 6) **Conversion of temperature factors** among the different common isotropic and anisotropic forms ([Export file](#)).
- 7) **Conversion of atomic parameters among several different crystallographic database and structure refinement formats** ([Export file](#)).
- 8) **Transformation of hkl index data**, such as diffraction data ([Transformation Parameters](#) dialog).

9) **Computation of powder diffraction** intensities and simulation of powder diffractograms ([Powder Diffraction](#)).

10) **Simulation of precession photographs** ([Precession Pattern](#)).

11) **Expansion of layers**, leaving the layers themselves unchanged, creating space in between ([Expand Layers](#)).

## 1.2 General Procedure

The first step is to enter or import the data for the crystal to be transformed. To import from one of several file formats, choose **Import** from the File menu. After selecting the format, you will see the [Import File](#) dialog. The 3-letter file extension ".xxx" in the edit box will be used to filter the files (that is, the **Open File** dialog will show only the files with this extension). Any changes you make in file extensions will be saved for future runs. Some formats may offer a choice of symmetry option; if the file actually lists symmetry "as XYZ", that is in the form of the positions of the general equipoint for the space group in the *International Tables for X-ray Crystallography*.

To enter the data manually, choose **New** from the [File menu](#).

In the first dialog which appears, [Title/Axes](#), supply an 80-character title, and specify the unit-cell parameters.

The two [Symmetry](#) options are [Space Group](#) and [Custom](#). The Space Group option lists almost all standard orientations and origins, so this is usually the first choice. You can type in a Hermann-Mauguin or Hall symbol, or give the *International Tables* number, but it is normally safest to select the space group in the scrolling list and double-click on it or click the **Select** button (be sure the symbols/number for the selected group appears in the edit boxes above). If you type in the H-M symbol, it is interpreted either according to Volume I of the 1952 edition of the *International Tables*, or Volume A of the 1983 edition. The main difference between the two is that in Volume I the default orientation for monoclinic crystals is a-axis unique, and in Volume A the default is b-axis unique. That is, if you type in "P2/m" the orientation will be different. Of course to be certain you can also type in the long form "P112/m" or "P12/m1", or select one of these in the list.

If the space group is a non-standard one, such as C-1 (Cbar1), it will be necessary to use the [Custom Symmetry](#) option. Often you can start with the Space Group option and then switch to the Custom option (**Change Symmetry Option** button) and make modifications as necessary. In the list of operations you must supply (if they are not there already), the coordinates of the equivalent positions of the general equipoint as listed in the *International Tables*, one per line. If the space group is centrosymmetric and the origin is on a center of inversion, select the **Centric** radio button and supply only half the operations – the center will be supplied by CRYSCON. If the origin is not on a center of inversion, you must supply all the operations and select the **Acentric** radio button.

In the [Input Atom \(Site\)](#) dialog, supply the standard atomic parameters. The type is normally the atomic number, but it could also be an arbitrary number. If there is only one occupant of the site or position it is not necessary to enter the data in the list box. If there is multiple occupancy, click on **Add** and supply the parameters as necessary in the [Atom Sharing a Site](#) dialog. For a cell/symmetry transformation such multiple occupancies are seldom used - they are simply carried over for possible [Export](#). The label and type of the main entry will be those of the first occupant.

When the atom list is complete you are done with the "Old" crystal. The atom list is shown in the [Control Window](#). You can save this file or document at any time with the **Save** or **SaveAs** options in the **File** menu.

### General Procedure for Cell/Symmetry Transformation

Now click on the **Transform** button to specify the parameters of the "New" crystal. In the [Transformation Parameters](#) dialog, click on the [Symmetry](#) button if the symmetry of the New crystal is to be different from the old symmetry. Specify the symmetry as above. The symmetry specified here pertains to the New orientation, not the Old. The default symmetry is the same as the Old.

Three types of transformation can be carried out - **Translation only**, **Input atoms only**, and **Full unit cells**. **Input atoms only** is the only option which will transform anisotropic temperature factors and/or atomic vectors (magnetic, displacement, etc.). See [Transformation Parameters](#) for more details.

The parameters specified in the [Transformation Parameters](#) dialog, going downward in the dialog, correspond to the operations successively carried out by CRYSCON.

First, translations may be applied to the input atom coordinates (**Pre-symmetry translations**). If the origin for your atom coordinates does not correspond to that of the standard symmetry specified for the Old crystal, corrections must be made here. If you select **Translation only**, this is all that will be done – the remainder of the parameters are ignored.

#### **Input atoms only** option:

CRYSCON applies the **Pre-matrix translations**, transforms the coordinates of the Old input atoms only, and applies the **Post-matrix translations**. (**Pre-symmetry translations** are not used). This gives a set of input atoms for the New structure, and the transformation is complete. Anisotropic temperature factors and atomic vectors are transformed to the new unit cell.

#### **Full unit cells** option:

CRYSCON now generates all the atoms in the Old unit cell. If the origin of the New unit cell differs from that of the Old, with respect to the common symmetry elements, you must make corrections in the **Pre-matrix translations** edit boxes. Such differences among sub/supergroups are common, and it may be necessary to study the diagrams and coordinates in the *International Tables* to get these translations.

CRYSCON now transforms the coordinates according to the matrix supplied. Now it has the contents of the Old unit cell, expressed in coordinates of the New unit cell.

In order to fill out the contents of a supercell, or to shift the contents for a reorientation, CRYSCON now systematically adds and subtracts the New unit-cell vectors.

Next, in order to average atom positions for a subcell or an increase in symmetry, CRYSCON similarly adds and subtracts the Old unit-cell vectors. If the position of a new atom generated in this way falls within the specified distance, or **Tolerance**, the atomic positions are averaged. CRYSCON keeps a running count of the number of atoms averaged in this way. The tolerance should be large enough to avoid having quasi-superimposed atoms in the result, but of course it must be less than the smallest bond length in the structure. Setting this may take some trial and error. A value of 0.4-0.5 seems to be large enough for even rather extreme cases of atomic shifts in sub/supercells and sub/supergroups.

**Post-matrix translations** may be applied here if the standard origin for the New space group is different from that of the Old space group. This is an alternative to the **Pre-matrix translations** - it should not be necessary to use both.

At this point, there should be a complete and hopefully realistic set of atoms for the New unit cell. Depending on the symmetry change, the new set may or may not conform to the New symmetry. CRYSCON now applies the New symmetry to eliminate symmetry-equivalent atoms. Again a tolerance is applied to decide if atom positions are "coincident". This generates a standard set of symmetry-unique atoms, or the "asymmetric unit". However, in many cases when generating a subcell or increasing the symmetry the averaging process does not put the new atoms exactly on special symmetry positions.

CRYSCON now applies the new symmetry to the supposed asymmetric unit, to generate a complete set of atoms for the New unit cell. You should know, based on simple volume considerations, how many total atoms are expected in the New unit cell. If the number of atoms in the unit cell generated in this step does not agree with that generated by transformation (before symmetry consolidation), CRYSCON now prints out the number it has generated and asks if you want to recycle to refine the location of atoms on special positions. If the atoms in special positions were not located within tolerance (.0001??) in the previous step, extra atoms will be generated, and the total generated will be greater than expected. If so, "recycling" will repeat the previous step of reducing to the asymmetric unit, and hopefully averaging will place the atom positions closer to the symmetry elements, if not on them (within tolerance). It may take several cycles of no change in number before the number of atoms generated comes down to the number expected. If there appears to be no improvement after 3 or 4 cycles, inspection of the results is in order - the correction to the atoms in special positions may be obvious, or it may appear that the matrix and/or translations are not valid.

When you decline another cycle, the process is terminated and the results appear in a special Output Text or Edit window (see [Types of Windows](#)). This window has a separate menu bar, with standard entries for text editing. This text document or output file can be saved separately from the input data (which is in files with extension .cco) using the **Save** and **SaveAs** option in this menu bar.



Note that when different input atoms are consolidated during a transformation, for example super-to sub-cell or on increasing the symmetry, CRYSCON does not attempt to combine the two sets of occupancies; it simply takes the list of occupants from the first atom generated.

In the **Full unit cells** option, CRYSCON does not attempt to transform anisotropic temperature factors; if there are anisotropic temperature factors they are converted to isotropic B's in the New structure. Atomic vectors are not transformed either - the New atoms will have vectors which are simply copied from the first Old input atom which was used to generate the New atom.

To go back to the main data input, click on the [Control Window](#) or use the [Window menu](#) to switch. The process or transformation can be repeated without removing the Output window, but its contents will be replaced. If you want to save successive results files, use the SaveAs option (when the Output file is active or has the focus) to give the file a different name (eg *myfile1.ccd*) before recalculating.

The transformed (New) input atoms (symmetry-unique atoms) can be converted into the original (Old) input atoms with the Transformed to Input option in the Input menu.

### Other Operations

There are several things which can be done without Transformation. All these operations may be done on the transformed atoms, as well as the original atoms, after a transformation has been carried out.

*Bond Lengths and Angles.* The [Bond Lengths and Angles](#) button in the [Control Window](#) will call up a special dialog for this.

*Powder and Precession diffraction simulation.* See the [Powder Diffraction](#) and [Precession Pattern](#) dialogs.

*Exporting Files.* You can write files containing either the Old data or the New data in most of the same format as are available for import. Select [Export](#) in the **File** menu. In the case of input files for structure refinement programs, such as SHELX, RIETAN, DBWS/LHPM, etc. CRYSCON cannot supply all of the required parameters, only the symmetry, unit cell and atomic positions and temperature factors. Non-essential information such as comments is also not necessarily passed on, but in most cases the relevant lines can simply be copied from the import file (Old crystal) to the export file (New Crystal).

## 1.3 Types of Windows used in CRYSCON

CRYSCON uses four types of windows besides dialogs and alerts; the Startup window, the Control window, Text windows and Graphics windows. In Windows, each window has its own menus; in Macintosh, the menus are at the top of the screen. The menus and commands therein depend on which type of window is active.

When starting up CRYSCON, the menus displayed include only a [File menu](#) and a standard Help menu. Use the commands in the [File menu](#) or the buttons in the window itself to start a new CRYSCON data set, or read an old one from a file.

After you have entered or read in the data for a CRYSCON file, the [Control Window](#) opens. This is actually a kind of dialog, but it cannot be dismissed without closing the current data set. Only one data set at a time is allowed in CRYSCON, and there is only one Control Window. When this window is active, the [File Menu](#) has additional commands such as [Export](#), the View Menu has [Powder Diffraction](#) and [Precession Pattern](#) options and there is an [Input Menu](#) for data input and modification. Note that the [Print](#), [Print Preview](#) and [Metafile](#) options in the File menu are inactive - they are active only when a Graphics window (below) is active.

The **Transform** button in the [Transformation Parameters](#) dialog lists the transformed atom parameters and other data to a separate **Text window**. The **Listing** option in the [Powder Diffraction](#) dialog ([File Menu](#)) lists the data to a Text window, as does the [Bond Lengths and Angles](#) dialog (called from the Control Window). When any of these Text windows is active, the menu bar contains standard menus for saving, printing and editing the contents. Each window actually displays the contents of a file, called respectively Powder1.dat, Powder2.dat and BONDS.DAT. These files are written over again each time the respective option is called, so if they are to be preserved they should be saved with the **Save As** command in the [File Menu](#) using a different name.

The [Powder Diffraction](#) and [Precession Pattern](#) dialogs ([Diffraction Menu](#)) present output in **Graphics Windows**. When a Graphics menu has the focus, the [Print](#), [Print Preview](#), [Raster](#) and [Metafile](#) or [PICT](#) options in the [File Menu](#) produce graphics output, essentially what is shown on the screen. There are four possible Graphics Windows, for Powder Pattern Old and New atoms, and Precession Pattern Old and New atoms.

## 2 Menus and Dialogs

[Startup Window Menus](#)

[Control Window Menus](#)

[Text Window Menus](#)

[Diffraction Windows](#)

### 2.1 Startup Window

Startup Window (see [Types of Windows](#)).

This window appears when CRYSCON is first started, or when a data set ([Control Window](#)) is closed.

It has its own menu bar, and the following buttons for getting a data file into CRYSCON.

**New** - Step-by-step input of a new CRYSCON data set.

**Open** - Open an old CRYSCON data file.

**Import File** - Shows a pop-up menu with the file types currently supported. This includes:

- CCDC FDAT files from the Cambridge Crystallographic Data Centre.
- SHELX .INS files from the program system of Prof. G. Sheldrick.
- CIF - Crystallographic Information Files.
- DBWS/LHPM Rietveld input files.
- ICSD Inorganic Crystal Structure Database files.
- ORTEP Original or ORTEP II atom information.
- XTLVIEW Drawing program.
- VIBRAT (.MOT) Graphic output files from VIBRATZ.
- PDB Protein Data Bank files.
- RIETAN Rietveld program files.
- GSAS Data files (.EXP) files from the Los Alamos Lab system - may include magnetic vectors.
- AM MINERAL. Data files from the American Mineralogist structure data base.
- FULLPROF. All-purpose refinement program - may include magnetic vectors.
- Free-form (.inp). This allows input of atomic coordinates and other information from almost any source.

**Exit/Quit** - Quit the CRYSCON program.

### 2.1.1 File Menu - Startup Window

**New** - Step-by-step input of a new CRYSCON data set.

**Open** - Open an old CRYSCON data file.

**Close** - Close the current graphics window.

**Save** - Save a CRYSCON data file.

**Save as** - Save a CRYSCON data file with a new name

**Import File** - Shows a pop-up menu with the file types currently supported. This includes:

**--Free-form (.inp)** This allows input of atomic coordinates and other information from almost any source.

--**CCDC FDAT** files from the Cambridge Crystallographic Data Centre.  
--**SHELX .INS** files from the program system of Prof. G. Sheldrick.  
--**CIF** - Crystallographic Information Files.  
--**DBWS/LHPM Rietveld** files.  
--**ICSD** Inorganic Crystal Structure Database files.  
--**ORTEP** Original or ORTEP II atom information.  
--**XTLVIEW** Drawing program.  
--**RIETAN** Rietveld program files.  
--**GSAS** Data files (.EXP) files from the Los Alamos Lab system - may include magnetic vectors.  
--**AM MINERAL** Data files from the American Mineralogist structure data base.  
--**FULLPROF** . All-purpose refinement program - may include magnetic vectors.  
--**ATOMS** Atomic structure plotting program (Shape Software).  
--**VIBRATZ** Normal-coordinate calculation program for crystals and molecules (Shape Software).

**Quit** - Quit CRYSCON.

### 2.1.1.1 Import Data File

**Dialog Box: Import File** [ [File Menu](#) ]

If there is a data set in memory which has been modified, you are asked if you want to save the changes.

If there is more than one data set or phase in the file, the [Data Sets...in Import File](#) dialog will present you with a list. The name of the CRYSCON data file will be taken from the name of the file, and the title ( [Control Window](#) or [Title/Axes](#) dialog in the [Input Menu](#)) will be taken from the data set or phase. The extension .CCO will be appended to the structure file.

**File Extension** The three-letter extension (.XXX) which identifies the file type under Windows may be specified here - only files of that type will be shown in the **Open File** dialog. To show all files, enter ".\* ".

**Source of symmetry** (some formats lack this option). If you select **Use positions as xyz**, in which symmetry operators are given in the form of positions in the general equipoint as in the *International Tables*, the symmetry option (Input Menu) will be [Custom Symmetry](#). After import, you may need to check the [Symmetry](#) option to be sure the centric/acentric choice and the Bravais lattice type are correct (some formats include a center of inversion and/or lattice centerings in the operators and some do not). If you select **Space group symbol**, the [Space Group](#) symmetry option will be used. The Hall symbol, the Hermann-Maughtin symbol, and then the *International Tables* number will be used in that order if present. If you select **Use positions as xyz** and the information on operations is not present, the symmetry option will default to **Space group symbol**. The H-M space-group symbol, Hall symbol, and space-group number are always read if present.

If symmetry is present in the "xyz" or operation form, this is usually the safest option. However, this option does not give information on systematic extinctions or true d-spacings, which are required for the [Powder](#) and [Precession](#) options. It is usually possible to derive the correct space-group symbols from the operations using the **Get Symbol** option in the [Custom Symmetry](#) dialog.

**Atom types** (some formats lack this option). If a distinct atom type number is not present in the input, CRYSCON will try to assign an atomic number to each input atom either from the first one or two characters of the atom label itself, or from a separate atom type label if that is present. In diffraction refinement file formats, this separate atom type label typically identifies the scattering factor, and it may be a matter of operator preference whether this or the atom label (if either) will identify the element.

Note that in the case of multiple atoms with the same coordinates, that is multiple occupancies for a site, CRYSCON consolidates them into one input atom, but preserves the information on the site occupants (see [Input Atoms](#)).

File types supported, with the default extension:

\*\*\*\* **Free-Form - .inp**. This imports files in the free-form format described elsewhere ([Atom Parameter Files](#)). Note that this format has been expanded, so that essentially all relevant data for a crystal may be entered.

\*\*\*\* **CCDC (Cambridge Crystallographic Data Centre) FDAT - .fdt**. The files normally contain a unique set of input atoms, which are the same as those required for input of a crystal in CRYSCON, plus in many cases some extra symmetry-derived atoms necessary to complete the molecule; CRYSCON will use only the unique set of atoms, omitting the extra ones.

\*\*\*\* **SHELX-93 - .ins**. CRYSCON is programmed only for SHELX-93 files, although it may also be possible to read SHELX-76 files.

*Symmetry* . The [Custom Symmetry](#) option will be used. Typically the true space-group symbol can be recovered from the title. CRYSCON will read the SYMM lines in the SHELX file only if they are in standard *International Tables* format - the translational part must precede the positional part (i.e.  $1/2+x$ , not  $x+1/2$ ). If the symmetry was copied from the *Tables*, there should be no problem. You can edit the symmetry operators after they are read in.

*FRAG instruction* . Atoms listed between this instruction and the FEND instruction will be ignored.

*RESI instruction* . Atoms listed after this instruction will be included, but not treated in any special way.

*Hydrogen atoms* . SHELX has several sophisticated ways of locating hydrogen atoms which are not duplicated by CRYSCON. Frequently, the positions of the hydrogen atoms are not in the .INS file, and must be taken from the output. The output lines giving the hydrogen positions can be copied into the .INS file. If this is done, a type or SFAC number must be inserted after the label and before the coordinates. The hydrogen lines can also be put into a separate file and read in with the SHELX *+filename include-file* instruction.

Most of the instructions in a SHELX file will be ignored. However, CRYSCON may not know all the current instructions. If it cannot identify an instruction, it tries to read the line as an atom line (this is the way SHELX works). If this fails, you are asked if you want to add the first four letters of the line to the list of instructions to be ignored. These instructions-to-be-ignored are at the end of the SCRPTTR setup file, separated by spaces and preceded by the number of instructions. You can edit this list if necessary.

\*\*\*\* **CIF (Crystallographic Information Files) - .exp.** CRYSCON uses only a small number of the possible data items in a CIF file and recovers only the most basic information. The dictionary file, CIFDIC.SHT (a shortened version of the complete CIF dictionary), must be in the home directory (the directory containing the CRYSCON.EXE file).

\*\*\*\* **DBWS/LHPM Rietveld - .dbw/.lhp.** The DBWS and LHPM formats are very similar.

In the **Atom type numbers from:** box, the **Type label** option will select the NTYP field which usually contains the elemental symbol for recovery of the scattering factor.

Three different versions of DBWS file are recognized: 9002, 9411 and 9807. Trying to read a 9002 file may cause an error on the first pass, as CRYSCON tries to read according to the later formats, and in that case you will have another chance to read again according to the 9002 format. Files with only one phase are more likely to be read correctly (but please report any problems reading valid DBWS files).

\*\*\*\* **ICSD ( Inorganic Crystal Structure Database) - .ret/.cry.** Three types of ICSD file are supported:

- 1) Files from the current CD-ROM database, accessed by the program RETRIEVE. The RETRIEVE files must be written from the DATA window using the PRINT option, not as export files (if there is sufficient demand, export files may be supported). That is, the file should be a copy of what is shown on the screen in the RETRIEVE program.
- 2) Files from the Canadian Scientific Numeric Database System (CAN/SND). This service may no longer be available. The files are referred to as CRYSTIN.
- 3) Files in the original CRYSTIN format (or close to it), available from the Netherlands CAOS information system, from ETH (Switzerland) and perhaps other sources. These files are also referred to as CRYSTIN.

Please contact Shape Software if you have ICSD files which cannot be read by one of these options. The best procedure is to send samples of the files by email or on a floppy diskette.

In CAN/SND files, CRYSCON will use the "NA:" line for the title; in RETRIEVE and original CRYSTIN files, CRYSCON will use the first "MINR" line if present, otherwise it will use the "NAME" line.

\*\*\*\* **ORTEP - .ort.** This imports the unit-cell parameters, symmetry, atomic positions and thermal data from original or ORTEP II files. It does not read the boundary and plotting

instructions.

\*\*\*\* **XTLVIEW** - **.xtl**. CRYSCON may need to shift the fractional coordinates to insure that the origin is placed on a center of inversion.

\*\*\*\* **FULLPROF** - **.exp**. The "User-supplied" non-magnetic and magnetic options (JBT = +-4 or +-5) are not directly supported - crystallographic and magnetic parameters in files using these options will be read as if one of the standard options were used. Magnetic information is always read as vectors in the crystallographic axes (not as polar or other coordinates), and FULLPROF-specific magnetic symmetry is not currently used.

\*\*\*\* **American Mineralogist Structure Database** - **.amc**. The American Mineralogist structure database is currently available on the Internet at [www.geo.arizona.edu/xtal-cgi.test](http://www.geo.arizona.edu/xtal-cgi.test). This may change, but the database should be locatable by searching for American Mineralogist.

\*\*\*\* **GSAS** - **.exp**. The General Structure Analysis System (Los Alamos) can give magnetic moment vectors.

\*\*\*\* **RIETAN** - **.xyz**. This format gives complete symmetry operations, including a center of inversion and lattice centerings if present, as numeric matrices. CRYSCON will convert the matrices to "xyz" form and use the Custom Symmetry option. It will also attempt to identify the center of inversion and lattice centerings and will remove them with your approval.

\*\*\*\* **ATOMS (Shape Software)** - **.str**. CRYSCON will read and store data on atom colors and radii from these files. Such data will be written into free-form (.inp) files when exported, and can then be read back into ATOMS.

\*\*\*\* **VIBRATZ (Shape Software)** - **.vbr**. CRYSCON will read the main data files (.vbr) from the Windows version.

### 2.1.1.2 Data Sets in Import File

**Dialog Box: Data Sets...in Import File [ Import File Command - [File Menu](#) ]**

When you open an [Import File](#), CRYSCON will search through it to find all the data sets within it, up to a limit. If there is more than one data set, this dialog will present you with a list. The name of the CRYSCON data file will be taken from the name of the file, and the title ([Control Window](#), or [Title/Axes](#) dialog in the [Input](#) Menu) will be taken from the data set, phase or crystal selected. The extension.cco will be appended to the structure file.

## 2.2 Control Window

This window, which has controls like a dialog, is present whenever a data set is in memory. It lists the input atoms and allows easy modification of them and access to the main operations in CRYSCON.

The **Symmetry** button allows specification or modification of the current symmetry for the original or old atoms - it calls up the [Symmetry](#) dialog, if an option has not been selected, and either the [Space Group Symmetry](#) or [Custom Symmetry](#) dialogs if the option has been selected.

The **Transform** button brings up the [Transformation Parameters](#) dialog, which allows specification of the parameters for the new crystal. The unit-cell and atomic coordinates of the new crystal are displayed in an output text window which is called from the [Transformation Parameters](#) dialog. If you want to carry out certain operations on the old crystal only, such as [Export](#) ([File](#) menu), [Powder Diffraction](#) or [Precession Patterns](#) ([Diffraction Menu](#) menu), it is not necessary to [Transform](#).

The **Expand Layers** button brings up the [Expand Layers](#) dialog - this will expand a crystal structure on certain planes, increasing the length of the selected axis, but leaving the actual short-range dimensions of most of the structure (bonds, etc. within layers) unchanged.

The **New to Old** button will replace the current Old or input atoms, cell and symmetry with the the New or transformed atoms, cell and symmetry. You will have the option of saving the current file and assigning a new name to the transformed data.

The large list window gives the current Old or original input atoms, which can be modified or deleted with the buttons below the list. Atoms can also be modified by double-clicking on the selection, which brings up the [Input Atom \(Site\)](#) dialog.

CRYSCON lists only distinct atomic positions, or sites, in this dialog. These sites may have multiple occupants, which are listed in the [Input Atom \(Site\)](#) dialog. The site occupancy (SOF) for each input atom shown in this dialog is the sum of the individual occupancies, which can be accessed through the [Input Atom \(Site\)](#) and [Atom Sharing a Site](#) dialogs.

B(equivalent) is equal to Biso or derived from Uiso if the site is isotropic, or calculated according to the formula below for anisotropic sites.

$$B_{eq} = 2\pi^2 (1/3) \sum(i) \sum(j) U_{ij} a^*(i) a^*(j) A(i) A(j)$$

where a\*'s are the reciprocal axis lengths and A's are the direct axis lengths.

The [Bond Lengths/Angles](#) button brings up a dialog allowing calculation of bond lengths and angles for all atoms or a selected atom - you can choose either the old or new crystal.

### 2.2.1 Input Atom (Site)

**Dialog Box:** **Input Atom (Site)** [ [Control Window](#) ]

**Label.** Each atom may be assigned a label of up to 6 characters. Labels in CRYSCON may not contain any embedded blanks. Any embedded blanks or leading blanks in labels in import files will be converted to underscores. Trailing blanks will be stripped.



**Fractional coordinates.** For crystals, the  $x$ ,  $y$  and  $z$  coordinates should be in fractions of the unit cell.

**Type.** It is usually expedient to enter the same type for all atoms which are bonded similarly (e.g. all carbons, all silicons, all six-coordinated cations, all oxygens, etc.) to save effort in defining bonds and polyhedra. The atomic number can usually be used for the type, although there are situations in which different type numbers should be used for the same element.

In a transformation, if atoms are found to be superimposed the type and other parameters are simply taken from the initial atom generated in this position. Thus if it is known that atoms are going to be consolidated, for example in a super- to sub-cell transformation, it may be a good idea to use a single type for those which will be consolidated.

Any change in the **Label** or **Type** for the site will be transmitted to the *first* site occupant.

The list box gives the current occupants of the site. To modify individual occupants, double click on the selection or click the Revise button.

In the **Temperature Factor** group, the type number as used in ORTEP must be specified. The temperature factors are given below (in abbreviated form). The common type numbers are given in the dialog; other types are rarely used nowadays. Supply the b, B or U double-subscripted coefficients as required - in type 0, the b coefficients are usually called betas. If the type is isotropic, the single value (B or U) is given in the (11) box.

#### ORTEP Types of Temperature Factors

Type 0 -  $e^{(-b_1h^2\dots+2b_{12}hk\dots)}$  \*\*\* Beta aniso

Type 1 -  $e^{(-b_1h^2\dots+b_{12}hk\dots)}$

Type 2 -  $2^{(-b_1h^2\dots+2b_{12}hk\dots)}$

Type 3 -  $2^{(-b_1h^2\dots+b_{12}hk\dots)}$

Type 4 -  $e^{(-.25(a^{*2}B_{11}h^2\dots+2a^*b^*B_{12}hk\dots))}$  \*\*\* B aniso

Type 5 -  $e^{(-.25(a^{*2}B_{11}h^2\dots+a^*b^*B_{12}hk\dots))}$

Type 6 - ISOTROPIC -  $e^{(-B(\sin(\theta)/\lambda)^2)}$  \*\*\* B iso

Type 7 - sphere of arbitrary radius

Type 8 -  $e^{(-2\pi^2(a^{*2}U_{11}h^2\dots+2a^*b^*U_{12}hk\dots))}$  \*\*\* U aniso

Type 9 -  $e^{(-2\pi^2(a^{*2}U_{11}h^2\dots+a^*b^*U_{12}hk\dots))}$

Type 10 - ISOTROPIC -  $e^{(-2\pi^2U(\sin(\theta)/\lambda)^2)}$  \*\*\* U iso (not a standard ORTEP)

type)

## 2.2.2 Atom Sharing a Site

**Dialog Box: Atom Sharing a Site** [ [Input Atom \(Site\) dialog](#) ]

This lists the properties for each occupant of a site.

Site occupancies in CRYSCON do not include space-group multiplicities and the total for a fully-occupied site should be 1.0. If [Import](#) or [Export](#) files include multiplicities CRYSCON should convert as necessary.

The **Type** and **Site Occupancy** will be used in the intensity calculations for [Powder](#) or [Precession](#) patterns. For this purpose, the type number should be a valid atomic number, unless the SCATFAC.DAT file (containing the scattering factors) is modified.

Any change in the **Label** or **Type** of the *first* occupant will be transmitted to the main entry for the site in the **Input Atom (Site) dialog**

The **Element**, **Charge** and **Scattering Number** are parameters specific to some import/export file types, and are not used by CRYSCON. They may not be meaningful unless the data is exported in the same format in which it was imported.

## 2.2.3 Bond Lengths and Angles

**Dialog Box: Bond Lengths and Angles** [ [Control Window](#) ]

This supplies the parameters for the computation of the list of bond or interatomic distances and angles centered on one or all of the input atoms. You can select either original (Old) or transformed (New) atoms. The radio buttons determine whether distances and angles are computed for all input atoms or only the one currently selected in the [Control Window](#) or in the edit box.

Only 36 atoms in addition to the central atom are allowed, so the **distance limit for central-ligand** should normally not be more than about 4 Angstroms. Angles are only calculated for ligand pairs at less than the **ligand-ligand limit**; if you want to determine angles for atoms on opposite sides of the central atom, the ligand-ligand limit should be twice the central-ligand limit.

The results of the distance and angle calculations are written to a file called either Bonds1.ccd (original atoms) or Bonds2.ccd (transformed atoms) in the home directory (see [Files used by CRYSCON](#)), and then shown in a Text window (see [Types of Windows](#)). This window has its own menus for editing and saving the text file. From this Text window, return to the [Control window](#) and the ordinary operating mode of CRYSCON by clicking in the Control Window, or with the **Window** menu.

Errors in bond lengths and angles are not calculated by CRYSCON. This is because sufficient data are seldom available for accurate calculation - it would be necessary to have the complete variance-covariance matrices for both the unit-cell and atomic-parameter refinements. The difference between the correct error values and those calculated using only the standard deviations of the parameters is usually not large, but discrepancies between values in the original publications and those calculated by CRYSCON could create confusion.

## 2.2.4 Expand Layers

**Dialog Box: Expand Layers** [ [Control Window](#) ]

This option will expand a crystal structure on certain planes, increasing the length of the selected axis, but leaving the actual short-range dimensions of most of the structure (bonds, etc. within layers) unchanged. It operates on input atoms (original crystal), leaving the symmetry unchanged.

Any atoms which are exactly on the expansion plane (for example K atoms in a mica structure) will remain on the expansion plane, and thus bonds from these atoms to other parts of the structure will be lengthened. Bonds connecting structural layers will also be lengthened.

The **Expansion factor** is the amount by which the selected axis is increased. For example, if the c-axis is 10.0 Angstroms before conversion, an expansion factor of 1.5 will change it to 15.0 Angstroms.

**Expand on axis.** This selects the axis to be lengthened. Fractional coordinates of most atoms on this axis will be changed. The other two axes, and fractional coordinates on these axes, will be unchanged.

**Number of planes.** There are often several symmetrically identical planes cutting the selected axis. For example, there may be identical mirror planes at 0.0 and 0.5. You must determine this number from examination of the space-group symmetry.

**Expand at zero.** There may be a choice of location of the expansion planes. Normally this will be a choice between the set of planes at fractional coordinate zero (on the expanded axis) and another set at some rational fractions. For example, if the **Number of planes** is 2, there may be a set at 0.0 and 0.5 and another at 0.25 and 0.75. If the **Expand at zero** box is checked, the expansion will be at the first set.

At the moment an arbitrary location of the expansion plane is not supported, and for low-symmetry crystals, or those which have a choice of more than two locations, it may be necessary to adjust all coordinates so that the expansion plane is at zero. If this situation is common, support for arbitrary location will be added.

**Tolerance.** This is used to decide if an atom is exactly on the expansion plane, in which case its coordinate on the expansion axis will not be changed - that is, it will remain exactly on this plane. Tolerance is in fractional coordinate units (not Angstroms). If you want atoms which are exactly on the expansion plane to remain in continuity with the remainder of the structure, their fractional coordinates on the expansion axis should be changed by greater than the tolerance. Usually this

will result in duplication of the atoms.

### 2.2.5 File Menu - Control Window

**New** - Step-by-step input of a new CRYSCON data set.

**Open** - Open an old CRYSCON data file.

**Close** - Close the current graphics window.

**Save** - Save a CRYSCON data file.

**Save as** - Save a CRYSCON data file with a new name

**Import File** - Shows a pop-up menu with the file types currently supported. This includes:

**--Free-form (.inp)** This allows input of atomic coordinates and other information from almost any source.

**--CCDC FDAT** files from the Cambridge Crystallographic Data Centre.

**--SHELX .INS** files from the program system of Prof. G. Sheldrick.

**--CIF** - Crystallographic Information Files.

**--DBWS/LHPM Rietveld** files.

**--ICSD** Inorganic Crystal Structure Database files.

**--ORTEP** Original or ORTEP II atom information.

**--XTLVIEW** Drawing program.

**--RIETAN** Rietveld program files.

**--GSAS** Data files (.EXP) files from the Los Alamos Lab system - may include magnetic vectors.

**--AM MINERAL** Data files from the American Mineralogist structure data base.

**--FULLPROF** . All-purpose refinement program - may include magnetic vectors.

**--ATOMS** Atomic structure plotting program (Shape Software).

**--VIBRATZ** Normal-coordinate calculation program for crystals and molecules (Shape Software).

**Export File** - This will write unit-cell, symmetry and atomic-coordinate information in most of the Import formats above.

**Quit** - Quit CRYSCON.

#### 2.2.5.1 Export Data File

**Dialog Box: Export Data File** [ [File Menu](#) ]

You have the choice of exporting the original (Old) or transformed (New) data. Note that the transformed data is not otherwise saved except in the .ccd file which is written on transformation, although it can be recalculated easily enough.

Most of the import/export formats supported by CRYSCON fall into one of two categories; archival formats and refinement formats. The archival formats, such as CIF, ICSD and CCDC tend to give only basic crystallographic information, including space group, unit cell parameters, atomic coordinates and thermal parameters. The refinement file formats, such as DBWF, SHELX and GSAS generally contain much more information, such as scattering factors, weighting factors and refinement flags. CRYSCON generally cannot provide all this latter information, and it cannot be expected that a refinement-format file written by CRYSCON will be successfully read in by the target refinement program (e.g. DBWF, SHELX or GSAS) without many additions and even some editing of the lines which are written by CRYSCON, since even these lines may contain some refinement-specific data.

Space groups symbols may be written in many ways, for example space group number 116: P-4c2; P -4 c 2; P\_-4\_c\_2; P4-c2. CRYSCON does not generally change the symbol - it is usually exported in the form it was imported or entered. The SgInfo routines used by CRYSCON can interpret many of the variations, but export target program may not be able to interpret some forms, and it may be necessary to edit the space group symbol after exporting a file.

You can convert the type of the temperature factors, e.g. from beta's to U's; and/or you can convert from isotropic to anisotropic and vice versa. Of course not all export formats allow a choice. If the **Keep current form** radio button is checked, the current temperature factors will be kept, *if possible*. However, the export format may not support the current form, in which case the temperature factors will be converted to a type which is supported.

The equivalent isotropic temperature factor, if converting from anisotropic to isotropic, will be computed according to the formula:

$$B_{eq} = 2\pi^2 (1/3) \sum(i) \sum(j) U_{(ij)} a^{*(i)} a^{*(j)} A(i) A(j)$$
 where a\*'s are the reciprocal axis lengths and A's are the direct axis lengths.

If the **Remove multiple occupancies** box is checked, only a single atom will be written for each site, using the relevant data for the first atom in the list of occupants. If not, in most file formats a new atom will be written for each site occupant - that is, the number of atoms in the export file will be larger than the number of sites listed by CRYSCON.

Note that when different input atoms are consolidated during a transformation, for example super-to sub-cell, CRYSCON does not attempt to combine the two sets of occupancies; it simply takes the list of occupants from the first atom generated.

## 2.2.6 Input Menu

[Title/Axes](#) - Input of the 80-character title, selection of crystal system and specification of unit-cell parameters

[Symmetry](#) - Selection of space-group or custom symmetry

### 2.2.6.1 Title/Axes

**Dialog Box: Title/Axes** [ [Input Menu](#) ]

The title may have up to 80 characters of identifying information.

You should supply the axis lengths and interaxial angles appropriate to the crystal system you selected. Axis lengths should be in Angstroms, and angles in degrees and fractions (not minutes and seconds).

Although standard crystallographic nomenclature gives the same letter (usually a) to symmetry-equivalent axes, after the initial input CRYSCON may call all axes, whatever the system, "a, b, and c" and angles "Alpha", "Beta" and "Gamma".

### 2.2.6.2 Symmetry

**Dialog Box: Symmetry** [ [Input Menu](#) - [Control Window](#) - [Transform Dialog](#) ]

The authority and source of information for crystal symmetry is normally the *International Tables for X-ray Crystallography*. However, any space-group symmetry may be used for the atoms. There are two options for selecting or entering symmetry information.

[Space group from table](#) - Choose a space group by symbol or number.

[Custom Symmetry \(xyz\)](#) - Enter all the individual operations as fractional x,y,z coordinates in the unit cell.

Each choice calls up a sub-dialog.

#### 2.2.6.2.1 Space-Group Symmetry

**Dialog Box: Space Group Symmetry from Table** [ [Symmetry dialog](#) ]

Space-group symmetry is obtained using licensed excerpts from the SGInfo program of Ralf Grosse-Kunstleve.

You can specify the space group in any of three ways: 1) the Hermann-Mauguin (H-M) or International symbol; 2) the Hall symbol (S.R. Hall: Acta Cryst., A37, 517, 1981); or 3) the number of the group in the *International Tables for X-ray Crystallography*.

**International Tables Volume** You have the option of using the older version of the *Tables* (called the *Second Edition*: various revisions and reprints from 1952 to 1979) in which the symmetry information was in Volume I, or the newer version (1983 onwards) in which it is in Volume A. The principal difference between the two versions is that in the older one the unique axis of a monoclinic group is assumed to be the c-axis, whereas in the newer one it is assumed to be the b-axis. Thus entering the symbol P2/m gives two different orientations depending on the volume selected. You can always specify the orientation by entering the long form of the symbol,

i.e. P 2/m 1 1, P 1 2/m 1 or P 1 1 2/m.

The H-M or Hall symbol can be typed into the appropriate edit box in either short form or long form, with or without spaces between positions. However, it is usually safer to select the symbol from the list box at the bottom, which gives the standard-form symbols for all the space-groups. Clicking the **Select** button copies the relevant data to the edit boxes at the top; it does not actually generate the symmetry. Symmetry generation is done after you click OK - this may take a few seconds.

If the space group you select does not appear to be consistent with your choice of axes, a warning box appears, but in most cases consistency is not required. However, if you selected trigonal rhombohedral axes in the [Title/Axes](#) dialog, only a rhombohedral space group may be selected. This is done by adding :R to the end of the symbol in the case of H-M symbols, or asterisk (\*) in the case of Hall symbols. If you select the rhombohedral setting and then switch to the [Custom Symmetry](#) option, the lattice type will be P; it will be R if the axes are hexagonal.

**Origin of coordinates.** In the *International Tables*, 24 space groups in the orthorhombic, tetragonal and cubic systems are given with a choice of origin: 1) not on a center of inversion or 2) on a center of inversion. These two origins are selected by adding :1 or :2 respectively to the end of the H-M symbol or the number. Although the origin on the center is second in the *Tables* and in the list, if the number is omitted this will be the default. This difference in origin is explicit in the Hall symbol, and other choices of origin may be specified for any space group with the Hall symbol. Note also that the origin may be shifted before transformation (see [Transformation Parameters](#)).

#### 2.2.6.2.2 Custom Symmetry

**Dialog Box: Custom Symmetry** [ [Symmetry Dialog](#) ]

CRYSCON can access all the standard orientations for space groups in the *International Tables* but there are still a few possibilities for alternate settings of symmetry elements with respect to structure axes which are not listed in the *Tables*. In some cases displacement, rotation or permutation of atomic coordinates may not be convenient, and it may be easier to enter the symmetry operations for the non-standard setting. These are sometimes given in reports on structures (e.g. Wyckoff, *Crystal Structures*). Note however that often only the operations for special positions are given: CRYSCON needs all the operations for the general position.

Some [Import](#) formats do not give a space-group symbol, and symmetry is supplied in the form of operations as xyz, or as actual numerical matrices. CRYSCON converts numerical matrices to xyz form.

The **Symbol** is not used by CRYSCON for transformations, unless you switch to the [Space Group Symmetry](#) option. However, the [Powder](#) and [Precession](#) options require a valid space-group symbol - they must use the symmetry from the symbol rather than the custom symmetry.

**Get Space Group Symbol.** This button will attempt to identify the space group from the operations, the lattice type and the centric/acentric setting. If the operations contain an inversion center or lattice centerings, CRYSCON should identify them and they can be removed at your

option. Clicking the **Change Symmetry Option** button will automatically causes an attempt to identify the space group.

If you specify **Centric**, rather than **Acentric**, you must enter only half of the symmetry operations (as given in the *International Tables*), related to any others by the center. The two sets or halves of the operations related by the center will have opposite signs on the x, y and z coordinates. The **Centric** choice implies that the origin of coordinates is on a center of inversion. If the space group is actually centric, but the origin is not on a center, select **Acentric** and enter all the operations. Note that for a transformation the atoms can be shifted (**Pre-symmetry translations**) in the [Transformation Parameters](#) dialog, to place the origin either on or off an inversion center.

The **Bravais lattice type** is in most cases the capital letter which begins the space-group symbol. However, CRYSCON uses a somewhat different convention from the standard for trigonal crystals: if you are using hexagonal axes for a rhombohedral crystal (whose standard space group symbol will always begin with "R"), enter "R" - if you are using the primitive rhombohedral axes, enter "P".

In the **Operations** group, you must enter all the "symmetry operations" for the most general position in the structure. Click on the **Add Line** button to add a line, **Delete** to remove one. Note that there should be only one operation per line. Enter or edit the line in the edit box to the right of the list.

## 2.2.7 Diffraction Menu

You can do [Powder](#) diffraction, either as a diagram or a listing, or a [Precession](#) pattern.

The **Font** item in this menu will set the font for the legends in the diagrams as well as the lettering for the indices in the powder diagram.

The font for the powder listing, shown in a [Text Window](#), is set in the [Window Menu](#) of the the Text Window.

### 2.2.7.1 Powder Diffraction

**Dialog Box: Powder Diffraction** [ [Diffraction Menu](#) ]

You can compute the pattern or list for either original (**Old**) or transformed (**New**) atoms and unit cell.

If you select a **List**, the list will appear in a Text window (see [Types of Windows](#)). There will be a line in the listing for each crystal form, or symmetry-unique set of reflections (with center of inversion assumed). If there is more than one wavelength, the 2-theta and relative intensity will be listed for each in that line.

If you select a **Graph**, you may show either **Bars** or a **Curve** - the curve will use Gaussian lines with the selected full width at half maximum (**FWHM**). For a curve, the location of individual



reflections will be shown as a short bar underneath the curve.

The **Line width** pertains to the width of all lines or "pen strokes" in the graph, not the width of each spectral peak (**FWHM**).

If the **Vertical scale factor** or magnification is 1.0, the strongest peak will just fill the plot area. If you want to see more detail in the weaker reflections, this factor can be increased and the stronger reflections will be truncated.

If the atom records include temperature factors, they will be used. If an atom has no temperature factor, the B isotropic value in the **Default temperature factor** box will be used. No absorption or extinction corrections are applied.

Scattering factors used by default are those for neutral atoms from Volume 4 of the *International Tables* (1974) edition. Atom type numbers must be atomic numbers, or must correlate with the order of the entries in the SCATFAC.DAT file. This file may be edited to supply different scattering factors (see [Files Used by CRYSCON](#)). Type numbers are taken modulo 100, that is 6, 106, 206 etc. all indicate carbon. By default number 99 is deuterium (symbol D) and 98 is tritium (symbol T).

There are five options for wavelength; averaged **K(alpha)**; separate **K(alpha)1** and **K(alpha)2**; averaged **K(alpha)** and (separate) **K(beta)**; a single **Specified X-ray wavelength**; and **Neutron - wavelength**. For the first three options, the X-ray tube target element must be selected in the **Radiation** combo box. When two wavelengths are calculated, the bars indicating the second (K(alpha)2 or K(beta)) are shown in red on the screen and in color output, and as a dotted line in black-and-white output.

In the case of **K(alpha)** and **K(beta)** the relative intensity of K(beta) must be specified. For unfiltered radiation this is in the neighborhood of 0.2. Of course it will be smaller for filtered radiation.

This option gives only a semi-quantitative calculation of powder intensity, intended for purposes of identification. For somewhat more elaborate options, including the ability to show multiple species, try the program Powder Cell. For highly quantitative reproduction of powder patterns, there are now many Rietveld programs available (see [Import](#) and [Export](#) files).

The results of the **Graph** option are shown in a graphics windows (see [Types of Windows](#)), and when this window is active, the file menu allows graphics [Print](#) and saving [Metafiles](#). There is a different window for the Old structure and the New structure.

For this option to work properly the space-group symbol entered either in the [Space Group from Table](#) or [Custom Symmetry](#) option must be valid for a standard setting. If it is not, it should be possible to transform to a valid setting. For example, the space group C-1 is sometimes used. It is possible firstly to transform to the primitive cell (use the standard matrix C->P). However, this would change the indices of the X-ray reflections. Alternatively, the transformation could be from C-1 to P-1 with the same cell. The h+k odd reflections will have zero intensity, but the other reflections will be indexed as for the original cell.

If the **Index graph** box is checked, the indices will be written above each line. The indices are displaced somewhat in a vertical direction if they are close together, but to index complex spectra it may be necessary to expand the scale using the 2-theta minimum and maximum settings. The font for the indices is 0.8 times as large as the font for the legends. This font is set in the [Window Menu](#), or the [Diffraction Menu](#) of the Control Window.

The 2-theta, d-spacing and intensity (on a scale of 0 to 100 for the strongest peak) for the point of the cursor are written at the bottom of the window.

### 2.2.7.2 Precession Pattern

**Dialog Box: Precession Pattern** [ [Diffraction Menu](#) ]

You can select either the original (Old) or transformed (New) atoms.

The **Precession angle** ( $\mu$ ) and **Crystal-Film distance** should match those of the real film to which comparison is to be made. The **Precession angle** determines the extent of the pattern in reciprocal space. If the **Fixed Scale** option (rather than **Fit in Window**) is selected, the pattern will be in true scale. This can be altered with the **Factor**, which is 1.0 by default.

The part of the reciprocal lattice shown is determined by the **Horizontal axis**, the **Other axis** and the **Level**. For example, for a 0kl pattern with  $b^*$  horizontal, the **Horizontal axis** is  $b^*$ , the **Other axis** is  $c^*$ , and the **Level** is 0.

Reflections are shown as squares whose area is proportional to the calculated relative intensity. The intensities are normalized based on the number of electrons in the unit cell (intensity of reflection 000) and the smallest reciprocal lattice spacing in this net. The **Intensity factor** scales the edge length, not area, of the squares (thus it really applies to the structure factor).

If an atom has no temperature factor, the B(iso) value in the **Default temperature factor** edit box will be used. Extinction and absorption are not considered.

Scattering factors used by default are those for neutral atoms from Volume 4 of the *International Tables* (1974) edition. Atom type numbers must be atomic numbers, or must correlate with the order of the entries in the SCATFAC.DAT file. This file may be edited to supply different scattering factors (see [Files Used by CRYSCON](#)). Type numbers are taken modulo 100, that is 6, 106, 206 etc. all indicate carbon. By default number 99 is deuterium (symbol D) and 98 is tritium (symbol T).

If the **Show grid** box is checked, the reciprocal lattice will be shown as a grid in red on the screen and color output, or as dotted lines in black-and-white output.

The results of this option are shown in a graphics windows (see [Types of Windows](#)), and when this window is active, the file menu allows graphics [Print](#) and saving [Metafiles](#). There is a different window for the Old structure and the New structure.

For this option to work properly the space-group symbol entered either in the

[Space Group from Table](#) or [Custom Symmetry](#) option must be valid for a standard setting. If it is not, it should be possible to transform to a valid setting. For example, the space group C-1 is sometimes used. It is possible firstly to transform to the primitive cell (use the standard matrix C->P). However, this would change the a and b reciprocal axes and the indices of the X-ray reflections. Alternatively, the transformation could be from C-1 to P-1 with no change in unit cell. The h+k odd reflections would be calculated and have zero intensity, but the other reflections will be indexed as for the original cell.

If the **Show extinctions** box is checked, systematically absent reflections are marked with a small circle, in red in color display and output.

Clicking on a reflection will bring up an alert box showing the indices, the d-spacing, the structure factor (|F|), the intensity (I) and the Lorentz-polarization factor.

The font for legends is set in the [Window Menu](#), or the [Diffraction Menu](#) of the Control Window.

## 2.2.8 Window Menu

The Window menu lists all the possible windows in CRYSCON - those which do not actually exist are greyed out. Select a window to make it active, or bring it to the front.

When a [Text window](#) or either the [Powder](#) or [Precession](#) graphics window is active, the first item in the menu is a **Font** selector. In the Text window, this acts on the entire text in the window and the font applies to all Text windows. The font for the powder and precession windows applies to both windows and to all text, except that the index lettering in the Powder window is 0.8 times the size of the lettering for legends.

## 2.2.9 Help Menu

The Help menu offers the following commands, which provide you assistance with this application:

**CRYSCON Help Topics.** This brings up the Help system. Use the Content, Index or Find tabs to locate information on a particular topic.

**About.** This gives the version number of CRYSCON. For **Macintosh**, the About dialog is either in the Apple menu (OS 8/9) or the Application menu (OS X).

## 2.2.10 Transformation Parameters

**Dialog Box: TransformationParameters** [ [Control Window](#) ]

The structure which is input and listed in the [Control Window](#) is referred to as the Old or original structure, and that derived from it is referred to as the New or transformed structure.

Click on the [Symmetry](#) button if the symmetry of the New crystal is to be different from the Old symmetry. The default symmetry is the same as the Old. The symmetry specified here pertains to the New orientation, not the Old, i.e., CRYSCON does not transform symmetry, so you must supply the correct symbol or operations for the *transformed* unit cell. The symbols for different orientations are listed in the *International Tables* Vol. 1 (1952) Table 6.2, and in the file HALL.DAT - these symbols all appear in the list box in the [Space Group Symmetry](#) dialog.

Three types of transformation can be carried out.

- 1. Translation** only simply adds the **Pre-symmetry translations** to the input atoms (Old or original atoms) and does nothing else.
- 2. Input atoms only** applies pre- and post-matrix translations and the translation matrix, but does not try to fill out the unit cell for either the old or new setting. The number of New symmetry-unique atoms will be the same as that of the Old input atoms. This is the only option which will transform anisotropic temperature factors. This option may be used for simple reorientation involving interchange of axes, and other transformations which do not involve a change of symmetry or primitive unit-cell volume. It can be used for primitive to non-primitive transformations and vice-versa, and transformations among different non-primitive Bravais cells. Again, the correct symmetry for the New orientation must be supplied.
- 3. Full unit cells** will transform all atoms in the Old unit cell to those in the New unit cell, generating new atoms when necessary (supercell or decrease of symmetry) and averaging atomic position when that is necessary (subcell or increase of symmetry). Anisotropic temperature factors are not transformed - they are converted to isotropic. Vectors are transformed, although if the symmetry is changed the new vectors are not guaranteed to be consistent with the new symmetry.

The **Tolerance** is used to decide if atoms are coincident, and their positions should be averaged (if the unit cell is decreased in volume, or the symmetry is increased). The tolerance in Angstroms is converted to fractional coordinates on x, y and z, and applied to each atomic coordinate in turn. That is, atoms are considered to be coincident if they fall within a unit-cell shaped box with edges of length equal to the tolerance.

**Use symmetry on vectors.** If this box is checked, vectors (such as magnetic spin vectors) will be operated on by the symmetry elements. If not, the atoms generated from each input atom will all have the same vector as that input atom. Note that CRYSCON, unlike ATOMS, does not apply Shubnikov symmetry.

The **Standard matrices** combo box will supply matrices for some common unit-cell transformations. These matrices should all preserve the chirality or "hand" of the structure - other combinations of signs on the coefficients are possible, particularly for the last five matrices for simple interchange of axes.

The parameters specified on the left side of the **Transformation Parameters** dialog, going downward in the dialog, correspond to the operations successively carried out by CRYSCON - see [General Procedure](#) for more detail. After setting and verifying all parameters, click on the **Transform** button, and the results appear in a new text window (see [Types of Windows](#)).

First, **Pre-symmetry translations** may be applied to the input atom coordinates. If the origin for your atomic coordinates does not correspond to that of the standard symmetry specified for the Old crystal, corrections must be made here.

---**Translation only** (origin shift) option

Nothing beyond **Pre-symmetry translations** is done – the remainder of the parameters are ignored.

---**Input atoms only** option.

The **Pre-matrix translations** are applied to the Old input atoms, they are transformed with the matrix, and the **Post-matrix translations** are applied. (**Pre-symmetry translations** are not used).

---**Full unit cells option**

CRYSCON now generates all the atoms in the Old unit cell. If the origin of the New unit cell differs from that of the Old, with respect to the common symmetry elements, you must make corrections in either the **Pre-matrix translations** or **Post-matrix translations** edit boxes. Such differences among sub/supergroups are common, and it may be necessary to study the diagrams and coordinates in the *International Tables* to get these translations. CRYSCON transforms the vectors on the input atoms with the symmetry matrices. In the case of special positions, the vector is taken from the first atom generated for that position. For subsequent atoms generated for that position, the new vector is compared and a warning message issued if the two vectors are not the same.

The transformation matrix is in the nine edit boxes. Some common standard transformation matrices may be selected in the **Standard matrices** combo box to the right. The upper three coefficients (first line) of the matrix give the New a-axis in terms of the old a, b and c axes. Likewise the second and third lines specify the new b- and c-axes.

CRYSCON now transforms the coordinates according to the matrix supplied, adding additional atoms by translation if necessary, or averaging atomic positions when necessary. The **Tolerance** is used to decide when atomic positions are "coincident", and must be averaged. The tolerance should be large enough to avoid having quasi-superimposed atoms in the result, but of course it must be less than the smallest bond length in the structure. Setting this may take some trial and error. A value of 0.4-0.5 seems to be large enough for even rather extreme cases of atomic shifts in sub/supercells and sub/supergroups.

CRYSCON does not attempt to average vectors on coincident atoms; it takes the vector from the first-generated atom and issues a warning message if vectors on subsequent coincident atoms are not the same.

**Post-matrix translations** may be applied here if the standard origin for the New space group is different from that of the Old space group. This is an alternative to the **Pre-matrix translations** - it should not be necessary to use both.

CRYSCON now applies the New symmetry to eliminate symmetry-equivalent atoms. Again a tolerance is applied to decide if atom positions are "coincident". This generates a standard set of symmetry-unique atoms, or the "asymmetric unit". However, in many cases when generating a subcell or increasing the symmetry the averaging process does not put the new atoms exactly on special symmetry positions and the calculation must be repeated in part - see [General Procedure](#)

The **Clear** button resets the transformation matrix to the identity matrix, and it also resets the [Symmetry](#) to be the same as that of the Old structure.

The [Transform HKL file](#) button will read a file containing index data and transform the indices.

### 2.2.10.1 Transform HKL File

**Transform HKL File** [ [Transformation Parameters dialog](#) ]

This option will read a file containing a list of X-ray (or other diffraction) reflections, or just a list of crystal faces, and transform them to a new axial system or unit cell.

You will be asked to specify the input file, and the output file (which must be different).

The data to be transformed must be in a text or ASCII file with one hkl per line. The data must be in fields separated by spaces.

The first three fields must be the hkl indices (integers). There may be as many as 8 additional fields, containing alphabetical or numeric information (these are read as strings).

To reach this option, click on the **Transform** button in the [Control Window](#). The only data which is used in the [Transformation Parameters](#) dialog is the transformation matrix. It is not necessary to click the **Transform** button to transform indices.

It is possible to have invalid transformed indices. For example, if the a-axis is halved, the indices (100) will be transformed to (1/2,0,0). CRYSCON will attempt to clear such fractional indices, for example changing (1/2,0,0) to (1,0,0) and (1/2,1,0) to (1,2,0). Note that such changed indices will be valid for morphology, but not necessarily for diffraction. If one of the extra fields in the file (not indices) is the d-spacing (or central distance derived therefrom) it will not be changed and thus some values may not correspond to the new indices if fractions are cleared.

The transformed data will be written line-by-line to the output file in the same order as in the input file, but column formatting will not be preserved - the fields will be separated by a single space.

## 2.3 Text Windows

When a text window is active, the menu bar contains a File Menu, for saving and printing the contents, and a standard Edit Menu for editing the contents.

To return to the main menu bar, click on the [Control Window](#) (see [Types of Windows](#)), or use the [Window menu](#)

The **Transform** button in the [Transformation Parameters](#) dialog lists the transformed atom parameters and other data to a separate [Text window](#). The **Listing** option in the [Powder Diffraction](#) dialog ([File Menu](#)) lists the data to a Text window, as does the [Bond Lengths and Angles](#) dialog (called from the Control Window). Each window actually displays the contents of a file, called respectively LIST.DAT and BONDS.DAT. These files are written over again each time the respective option is called, so if they are to be preserved they should be saved with the **Save As** command in the [File Menu](#), using a different name.

## 2.4 Powder Diffractogram Window

This is a graphics window which appears as the result of the [Powder Diffraction](#) dialog (Graph option) in the [Diffraction Menu](#). It may show either the old or original atoms, or the new or transformed atoms.

To return to the the [Control Window](#) if it is not visible, use the [Window Menu](#).

[File Menu](#). In addition to the standard Save, this has options for printing and graphics file output.

[Window Menu](#). To set the font (for all diffractogram windows) and switch between windows.

### 2.4.1 File Menu (Diffraction Graphics)

The options here for graphics output ([Print](#), [PostScript](#), [Raster](#), [Metafile](#) or [PICT](#)) are for [Powder](#) or [Precession](#) graphics only.

#### 2.4.1.1 Print Graphics

**Dialog Box: Print Graphics Image** [ [File Menu \(Powder\)](#) or [File Menu \(Precession\)](#) ]

If the **Standard printer dialog on OK** box is checked, the **Print** dialog supplied by the operating system or the printer driver comes up after you click OK. Use that dialog to set the number of copies, the orientation (Portrait/Landscape) or the resolution.

**Color** output gives essentially the same image as on the screen, with the bars for a second wavelength in the [Powder](#) pattern, and the reciprocal-lattice grid in the [Precession](#) pattern being in red. If the **Color** box is unchecked, these lines are shown dotted. If you have a color printer, you may need to make a choice between color and black-and-white printing in one of the printer dialogs as well as with the **Color printing** checkbox in this dialog. This choice may be an option in the standard printer dialog above, or you may need to set it in the **Print Setup** option in the File menu.

See [Frames](#) for details of the frame and frame units.

### 2.4.1.2 Page Settings

This allows setting of the paper type or size, the standard orientation (portrait or landscape) and the paper margins. Margins will only be used in [Text Windows](#).

For Macintosh, margins are set in [Page Margins](#).

### 2.4.1.3 Page Margins

----Macintosh only----

This dialog sets the margins for [Text Windows](#). Use the [Page Setup](#) dialog to choose page size and orientation.

### 2.4.1.4 PostScript Output

**Dialog Box: Direct Postscript Output** [ [File menu](#)]

---- Windows only ----

This option can be used to write Encapsulated Postscript (EPS) files for transmission of graphics to other software, as well as for direct output to a Postscript printer. This direct output is generally superior to, as well as faster than, the output from the normal [Print Graphics](#) command in the [File menu](#) if your printer is PostScript. The **Destination** option sends output either directly to a printer or to a file in standard EPS (Encapsulated Postscript V3.0) format.

#### Screen Preview.

Most word-processing and publishing software cannot display an EPS file on the screen unless the file has a special bitmap attached, called the screen preview. This is actually a sub-file in the TIFF format. The pixel depth of this file can be set in the [PostScript Settings](#) dialog (**Settings** button). The pixel depth of the preview is set to that of the screen, and the pattern series is set to fine (see [Raster Files](#)).

---- Macintosh only ----

This option can only be used to write Encapsulated Postscript (EPS) files for transmission of graphics to other software. For direct output to a Postscript printer, use the [Print](#) option.

#### Screen Preview .

---



Most word-processing and publishing software cannot display an EPS file on the screen unless the file has a special attachment, called the screen preview. This is actually a PICT in the resource fork of the file.

---- End Windows/Macintosh only ----

**Settings** button ([PostScript Settings](#) dialog). On or before first using the **Direct PostScript Output** command, you should set or verify the settings in this dialog, especially the port to which the printer is attached.

*Fonts in PostScript output* . Depending on your system configuration (Windows or Macintosh, printer type and driver), the PostScript fonts supported by a PostScript printer may or may not appear in the dialog for selecting fonts which may be called from the xxxx dialogs. Furthermore, you may want to write EPS files for a printer which is not even connected to your computer. These dialogs thus have an option to specify a character string for the PostScript font. This string specifies the typeface, and includes the weight (normal, bold) and other attributes (italic or oblique), but does not include the size - the size is specified in the font dialog. There are certain [standard PostScript typefaces](#) which are present on most PostScript printers.

See [Frames](#) for details of the frame and frame units.

#### 2.4.1.5 PostScript Settings

**Dialog Box: PostScript Settings** [ [Direct Postscript Output Dialog](#)]

The page size, page margins and dots per inch/centimeter should be determined by the actual printer used for final output; if these are not correct, the drawing may not be scaled and/or placed on the page correctly.

**Preview Color.** If you select a screen preview (TIFF bitmap or PICT sub-file) in the [Direct PostScript Output](#) dialog, and if color output is selected, you can specify either a color or black-and-white bitmap. The **Screen** option uses the color depth of the the current screen display. Black-and-white PostScript output always uses a 1-bit or black-and-white screen preview.

---- Windows only ----

If you are using direct output to a printer you *must* select the **Port**; this will be either "LPTn" or "COMn". Also, if you are using a serial port for the printer, you must set or verify the data transmission parameters, such as baud, parity, etc., even if the port currently shown is the correct one. This is done in the **Ports** item of the Windows

**Control Panel** (not in CRYSCON).

### 2.4.1.6 Raster Files

**Dialog Box: Raster (Bitmap) Files** [ [File menu](#) ]

--Windows Only -----

This command can write files in four different formats (**File type**): Windows device-independent format (.BMP); PC-Paintbrush (.PCX); Tag-image-format (.TIF); and Portable Network Graphics (.PNG) files.

--Macintosh only-----

This command can write files in the Portable Network Graphics (.PNG) format. The [PICT/Clipboard](#) option (File menu) can also write raster or bitmap files, in the PICT format.

--End Windows/Macintosh only----

See **Selection of File Format** below for information on choosing the format.

The drawing may be either black and white or color. If black and white, the **pixel size** is 1-bit. For color files the pixel size may in some cases be selected. In **Windows**, 16-bit is only available for .bmp files. In **Macintosh**, 8-bit (256-color) is only available if the screen is currently set at this color depth.

If the **Compress** box is checked, .TIF files are compressed with run-length encoding, which is one of the required formats under the TIFF 6.0 standard. However, some applications may not support this type of compression, or may reject .TIF files for other reasons. Also, if the **Compress** box is checked, 4- and 8-bit .BMP files are compressed. 1-bit and 24-bit .BMP files are never compressed. Owing to a Windows system bug, compression of 4-bit .BMP files may not work when banding is used (see below). .PCX files are always compressed, with their own format. 24-bit .PCX files can compress well, whereas 24-bit .TIF files are only partially compressed (and then only if there are large areas of black, white or grey), and 24-bit .BMP files are not compressed at all. PNG files also are always compressed.

See [Frames](#) for details of the frame and frame units.

**Maximum memory.** Windows and Macintosh both use *virtual memory*, which means that they pretend that a hard disk can be used in place of actual hardware memory chips. For some applications this is useful, but when writing raster files it usually results a form of lingering death involving "disk thrashing", or constant reading and writing of data to

the hard disk.

CRYSCON is capable of imaging and writing raster files in segments or bands to avoid this problem. This requires repeating the entire drawing process for each band, but this usually is much faster than the reading/writing to disk involved in using virtual memory. To do this requires knowing how much actual chip memory is available. Unfortunately, at present Windows does not provide this information in a way that can be used for both 16- (standard Windows 3.1) and 32-bit (Windows 95/98/NT/XP) systems. Thus the user may need to determine this by trial and error using the **Maximum memory** parameter.

When the **Maximum memory** parameter is set to zero, CRYSCON will simply ask the system for a block of memory large enough to image the entire drawing at once. This amount of memory is printed out in the dialog which appears after starting the raster imaging: "nnnn bytes required, mmmm bytes available - will require 1 bands". If this amount of memory is greater than the amount of chip memory available, Windows will use virtual memory, which is typically manifested by constant running of the hard disk for long periods (disk thrashing). If you change the **Maximum memory** to some amount smaller than nnnn (say half), CRYSCON will only request this amount of memory from the system, and virtual memory may not come into play. A **Maximum memory** setting should be good for a given session, regardless of the size of the raster file; larger files will use more bands. However, the amount of memory available may depend on whether other applications are active.

The amount of virtual memory is determined by the available space on the hard disk. If this is insufficient, CRYSCON will automatically use bands, but since virtual memory is being used, it may still be advantageous to use a **Maximum memory** value which will increase the number of bands.

**Selection of File Format.** The choice of format depends first of all on what formats are supported by the target software (paint program; publishing program; etc.). Beyond this the first choice should be PNG, second choice PCX, and then PICT, TIF or BMP depending of what is supported and how much memory or disk space is available.

As of 1997, the preferred graphics file types for the internet were GIF and JPEG. However, GIF uses the LZW compression scheme copyrighted by Unisys Corp., which in principle charges a license fee for every application using it. JPEG files are compact but involve losses and degradation of the image and are thus not suitable for CRYSCON files.

The PNG format is intended to be a replacement for GIF, and in fact is superior to most other formats, being lossless and giving very good compression for the type of images generated by CRYSCON. Essentially all major software vendors have subscribed to the PNG convention and releases from 1998 onward should support it.

Most TIF files also use LZW compression, but CRYSCON does not use this type of compression because of the copyright problem. The run-length-encoding which CRYSCON does use is supposed to be supported by all TIF readers, but in fact some do not support it, and this algorithm does not work well for 24-bit (RGB) images.

PICT bitmap files on the Macintosh are compressed by the system software and the algorithm may vary. PNG files are usually smaller.

There are dozens of raster graphics formats and it will never be possible for CRYSCON to support all of them. CRYSCON users who work with raster files should consider investing in a conversion program - there are many such programs which are not expensive. The PNG home page ([www.cdrom.com/pub/pnp](http://www.cdrom.com/pub/pnp)) has links to many shareware and conventional commercial conversion packages.

#### 2.4.1.7 Metafiles

**Dialog Box: Metafiles** [ [File Menu](#) ]

---- Windows Only -----

Windows metafiles are basically vector images (but including fills) that can be rescaled without necessarily losing resolution. They record the drawing commands that are used for the screen or standard printer output, but the result may depend on the software or device for which they are intended. You can write .WMF files or send the image to the clipboard.

To prevent loss of resolution, CRYSCON writes of metafiles with a standard scaling of 2540 dots or pixels per inch (1000/cm). For 16-bit metafiles (.WMF), this means that the size cannot exceed 12.9 inches or 32.7 cm. (that is 32767 dots, the maximum capacity of unsigned 2-byte integers). If you enter larger values for the frame, CRYSCON will automatically halve both values (with your permission).

See [Frames](#) for details of the frame and frame units.

#### 2.4.1.8 PICT/Clipboard

**Dialog Box: Clipboard/PICT** [ [File menu](#) ]

----- Macintosh Only -----

Note that this type of output may be referred to elsewhere as Metafile output. This option can write images either to the Clipboard or to PICT files, in either of two formats: (a) a rescalable 2-dimensional Picture or metafile, or (b) a raster image or bitmap.

Macintosh **Pictures**, as used here, are images containing lines or vectors and fills of

regions defined by lines, that can be rescaled without necessarily losing resolution. They record the drawing commands that are used for the screen or standard printer output, but the result may depend on the software or device in which they are used.

**Bitmaps** or raster images record every pixel, so they are not susceptible to undesirable modification by other software. Although most "painting" software can resize bitmaps, this usually causes a loss of quality, so it is best to save a bitmap in exactly the desired size. Note that you can also save bitmaps in the **PNG** raster format ([File menu](#)), which is superior in some respects to PICT files.

If color output is selected, you can choose either 16- or 32-bit color depth - 8-bit (256-color) files cannot be written.

You can select the nominal dots per inch/centimeter, but note that programs which read the file may ignore this and show the image at 72 dots per inch.

See [Frames](#) for details of the frame and frame units.

## 2.5 Precession Pattern Window

This is a graphics window which appears as the result of the [Precession Pattern](#) dialog (Graph option) in the [Diffraction Menu](#). It may show either the old/original atoms, or the new/transformed atoms.

To return to the [Control Window](#) if it is not visible, use the [Window Menu](#).

[File Menu](#). In addition to the standard Save, this has options for printing and graphics file output.

[Window Menu](#). To set the font (for all diffractogram windows) and switch between windows.

## 3 Reference

Topics of general interest.

[Atom Parameter Files \(Free-Form\)](#)

[ATOMS and VIBRATZ files](#)

[Files used by CRYSCON](#)

[Frames](#)

[Samples](#)

## Standard PostScript Type Faces

### 3.1 Atom Parameter Files (Free-Form or .inp)

This type of ASCII or text file may be used to read in atomic coordinates alone, or to supply complete structure information. Listings of atomic coordinates from almost any source can be used as the basis of a free-form file.

CRYSCON will also export this type of file, which can be read into ATOMS, SHAPE or VIBRATZ (Shape Software).

All or part of the parameters for each input atom, namely label, fractional coordinates, type, radius and display colors and pattern numbers, can be read in. You can also supply default values for some parameters, so that the parameters neither need to be present on every line of the file, nor need to be supplied through the dialog.

Except for the **TITL** line, keywords and actual values to be read in should be separated by spaces or commas, and there should be no spaces within keywords or values. There is no need for alignment by column, except that keywords should start in the first column.

The input file may contain two overall types of lines; *General and crystallographic information* lines; and actual data or *atomic parameter lines*.

*General and crystallographic information lines.* These lines should all precede the atomic parameter lines. Each line consists of a keyword followed by one or more values or character constants. The keyword should start in the first column and be followed by at least one space before the actual values. Where more than one value is called for, they are separated by spaces. All of these lines are optional - when a free-form file is used for import (**File** menu), if any lines are absent, default values will be supplied.

**TITL** line. Up to 76 characters (may contain spaces).

**CELL** line. The unit-cell lengths in Angstroms and the interaxial angles in degrees (6 floating-point values). If the atomic coordinates are Cartesian, the axes should be 1.0 and the angles 90.0.

**SPGP** line. The Hermann-Mauguin or standard International symbol for the space group. There should be no spaces in the symbol, although there may be underscores (which are ignored when the symbol is interpreted).

**HALL** line. The Hall symbol for the space group. There should be no spaces in the symbol, although there may be underscores (which are ignored when the symbol is interpreted). If this line comes after the **SPGP** line (or that line is absent), the Hall symbol will be used in the [Space Group Symmetry](#) option.

**SYMM** lines. These give symmetry operators in "xyz" form, that is in the form in which the

coordinates of the general position are listed in the *International Tables for X-Ray Crystallography*. Fractions must be given as integers separated by a slash ("1/2", "2/3"), rather than decimals("0.5", "0.333"). The x, y and z positions must be separated by commas and there should be no spaces in the operator. There should be one line for each operator. If the space group is centrosymmetric, only half the operators need be given, if the origin is on a center of inversion. If the origin is not on a center, all operators must be given and the space group should be denoted non-centric in the **LATT** line. If these lines come after the SPGP and HALL lines (if the latter are present), the [Custom Symmetry](#) option will be used.

**LATT** line. This gives the Bravais lattice type (single capital character), followed by a space and 0 if the space group is centrosymmetric or 1 if it is non-centric.

**FACTOR** line. A single (floating-point) factor which multiplies all the fractional or atomic coordinates.

*Atomic parameter lines :*

The file should have all the information for each atom, except for temperature factors, on a single line with a maximum of 80 characters per line, and the values must be in *fields*, which are set off or delineated with either spaces or commas. There can be no spaces or commas within fields. The names of fields are given in the following in capitals, but in the actual input they may be lower case; all letters are converted to upper case when the line is read in.

**DEFAULT** lines supply values to the parameters, such as colors, which are not read in for each atom. If default values are not entered in this way, default values are obtained from the separate ELEMENTS file, using the chemical symbol of the atom which is assumed to be in the first two characters of the atom label. See the further description of **DEFAULT** lines and the ELEMENTS file below.

**FIELDS** lines. These lines set up the CRYSCON input parameters which are to be read from the file, and the order in which they are to be read. This is followed by the keywords giving the order of the fields. The allowed keywords are as follows (INTEGER fields may not contain a decimal point):

- 1) **LAB** - (6 characters maximum). Any label for the input atom may be used, but the label normally begins with the chemical symbol for the element. The first two characters may be used to determine default values for some of the parameters, as described below. The characters may be upper or lower case. This is a required field.
- 2) **COO** - This actually denotes three floating-point fields giving the fractional atomic coordinates. After input, the coordinates are multiplied by the number in the FACTOR line, if this line is present. These are required fields.
- 3) **TYP** - This is the type which is used in locating bonds and polyhedra. INTEGER

Fields 4-9 are for use in ATOMS and are not used by CRYSCON, but if the data was originally imported from ATOMS (.STR), they will be written in an [Export](#) file for re-introduction into ATOMS.

- 4) **RAD** - This is the radius used when the atom is plotted as a sphere. FLOATING-POINT
- 5) **RMC** - This is the color number for the atom rim or edge. INTEGER
- 6) **FLC** - This is the color number for the atom fill. INTEGER
- 7) **RMP** - This is the pattern number or gray shade used in black-and-white display or output. INTEGER
- 8) **FLP** - This is the b/w pattern number for fills. INTEGER
- 9) **PEN** - This is the pen number used for atom outlines in pen plots. INTEGER

The following fields may be used by CRYSCON.

10) **TFB** - Temperature factors in B or bij (beta) form, types 0 (anisotropic) or 6 (isotropic) in ORTEP. If this keyword is present, the temperature factor(s) are present on a second line for each atom, in up to six fields. The order is 11, 22, 33, 12, 13, 23. If the second value is absent or zero, the temperature factor will be read as isotropic. Note that CRYSCON will save temperature factors only if at least one atom has non-zero for the first value or b11.

11) **TFU** - Temperature factors in U or uij form, for anisotropic type 8 in ORTEP. Similar to TFB. Isotropic U values will be given number 10, although this is not standard ORTEP.

12) **VEC** - Atomic vectors, e.g. for magnetic spins or vibrational displacements. If this keyword is present, the vector coefficients are present on a second line, in four fields. The first three are the relative components in the structure axes, and the fourth is the length. Vectors and temperature factors may not both be present.

13) **DUM** - This designates a field (character, integer or floating-point) that exists in the input data line, but should be ignored by CRYSCON.

Note that the actual atom data lines do not contain any keywords. The keywords in the FIELDS lines set up the sequence of parameters in each data line.

An example FIELDS line:

```
FIELDS DUM LAB COO TYP RAD
```

Some corresponding data lines:

```
1 C1 0.1234 0.2345 0.3456 6 1.2
```

```
2 H2 0.4321 0.5432 0.6543 1 0.1
```

Here the first field, which is simply a sequence number, must be ignored by CRYSCON, and is designated with a DUM.



Here is an example of some lines copied from an (old) ATOMS .STR file (spinel):

```
FIELDS DUM LAB TYP COO RAD
```

```
1 MG1 12 .12500 .12500 .12500 .000
```

```
2 AL2 13 .50000 .50000 .50000 .000
```

```
3 O3 8 .26200 .26200 .26200 .000
```

There should normally be a FIELDS line at the beginning of the atomic parameter lines, but additional FIELDS lines can be inserted at any point to redefine the fields. If there is no FIELDS line, the fields are by default; LAB and COO.

In the actual data lines, fields denoted INTEGER above should not be more than 6 characters; the COO and RAD fields (floating-point) should not be more than 20 characters.

**DEFAULT line.** This is used to set particular default values for fields other than LAB or COO. DEFAULT must be the first 7 characters. Then the default values are indicated with the name of the field connected with an equals sign (with no intervening spaces) to an appropriate value. Example default line:

```
DEFAULT TYP=1 RAD=0.95 FLC=15
```

There are twelve possible input fields for each input atom, or each line in the file, plus the placeholder DUM field. The LAB and COO fields are required for each atom and must be read in from the file; the other fields are optional. If the latest FIELDS line does not define a field for a particular parameter, then the value of the missing parameter is determined by reading the first two characters of the label (LAB field) and trying to identify the element. You can turn off defaults, thereby accepting the values on the input atom line, with a line containing the word DEFAULT and no other keywords.

## 3.2 ATOMS and VIBRATZ files

CRYSCON users may want to use or transform the data in the Shape Software programs ATOMS, for drawing crystal structures, and VIBRATZ, for normal-coordinate calculations. The data files for both these contain far more data than CRYSCON requires, and while Crycon will [Import](#) either type of data file, it will not export either type. The procedure for taking data from these programs, using it or transforming it, and returning it to these programs is as follows.

- 1) In CRYSCON, directly [Import](#) the ATOMS (.STR) or VIBRATZ (.VBR) files. All data required by CRYSCON should be in these files. Of course both of these programs handle molecules or polymers as well as crystals, and CRYSCON deals only with crystals.
- 2) If the objective is to simulate [Powder](#) or [Precession](#) patterns or diffraction listings, no transformation is required - just select the desired option from the [Diffraction Menu](#).

- 3) To transform the data, follow the procedure outlined in [General Procedure](#)
- 4) To return the transformed data to ATOMS or VIBRATZ, select [Export](#) in the File menu, and write a Free-form (.INP) file.
- 5) ATOMS or VIBRATZ can now import the .INP file through the **Import** options in their **File** menus. In the case of ATOMS, it is also possible to read the data into an existing file (for example the original data file) through the **Input Atoms** dialog (Input menu). This has the advantage that all pre-existing specifications, including bonds and polyhedra, are preserved.

When an ATOMS file is read into CRYSCON, the data on color and atomic radius are preserved, although they are not used by CRYSCON. They are written out in the .INP export file and will be read back into ATOMS (see [Atom Parameter Files](#)).

The program SHAPE will also read .INP files, so can use transformed data from CRYSCON.  
Transformed {linkN

### 3.3 Files Used by CRYSCON

CRYSCON recognizes two file folders or directories; the *home* directory and the *data* directory.

The *home* directory is the one containing the CRYSCON program file or application. This directory must also contain the following data and setup files:

**SCRPTR** This is the setup or preferences file for CRYSCON. If it is damaged or lost another will be created, with default values.

**HALL.DAT** This is the file containing space-group data.

**CIFDIC.SHT** This is a required dictionary file for importing CIF files.

**SCATFAC.DAT** This file contains the X-ray scattering factor data for neutral atoms in the exponential form as given in the *International Tables*, Vol. 4. This file may be modified to use other scattering factors (e.g. for ionized atoms). The scattering factors are keyed by sequence number as read from this file to the atom type. There is a maximum of 100 scattering factors. Type numbers are taken modulo 100, that is 6, 106, 206 etc. all indicate carbon. By default number 99 is deuterium (symbol D) and 98 is tritium (symbol T). For neutron diffraction involving isotopes it is a simple matter to copy the line for the element in question into a position which is unlikely to be used, such as numbers 93 to 97, and change the neutron scattering length, which is the last coefficient (the first 9 coefficients give the X-ray form factor).

The following files are always written to the home directory.

**BONDS1.CCD, BONDS2.CCD** These files contain the results of the **Bond Lengths and Angles** command (Control Window).

**POWDER1.CCD, POWDER2.CCD** These files contain the listing of d-spacings, etc. from the

**Powder Diffraction** command (**File** Menu), **Listing** option.

The BONDSn.CCD and POWDERn.CCD files are rewritten every time you use the **Bond Lengths and Angles** or **Powder Diffraction (Listing)** commands. Thus to save these results permanently, use **Save As (File Menu)** to save them with a different name.

The *data* directory is the one containing the current data file. This directory is saved in the SCRPTR file, and thus the **Open** command returns to it when you start up CRYSCON.

*infile*.CCD This is the output file from the **Transform** command (button) in the [Transformation Parameters](#) dialog - here *infile* is the name of the CRYSCON data file (*infile*.CCO). It contains a listing of the atoms in the original unit cell and the transformed unit cell, and the transformed symmetry-unique(input) atoms. It is displayed in a Text window (see [Types of Windows](#)).

*infile*.XXX [Export](#) files are given the appropriate default extension (.XXX), and are written by default in the data directory, although you can write them with any extension. Changing the directory in which the file is written resets the data directory.

### 3.4 Frames

**Frames** [ [Print Graphics](#), [Metafiles](#) ]

With printed output, you have a choice of using the full page, or confining the output to a *frame*. For [Metafiles](#) (**File** menu) output always goes to a frame.

If you are using the **Fixed** scale mode for a [Precession](#) or [Powder](#) pattern, the image is clipped to the frame. Otherwise, the image is scaled to fit the frame.

In printed output, the frame can be positioned on the page; the offset gives the displacement of the upper left corner of the frame from the upper left corner of the page.

You can choose the units for the size and offset of the window; either inches or centimeters.

### 3.5 Samples

All the examples are real minerals, and the transformations are between non-equivalent but similar structures, not just changes of axes. There are files transforming each structure in the set to the other structure(s).

The transformations type is **Full unit cells**.

**Marcasite(mc)-arsenopyrite(as)** In addition to the substitution of As for one of the sulfurs in S2 groups, the cell and symmetry are different.

**Columbite(co)-huebnerite(hb)-wodginite(wa)** These oxides have the same basic structure, differing in the pattern of cation substitution.

**Cubic boracite(boc)-orthorhombicboracite(boo).** This is a high-low temperature transition. The low-temperature orthorhombic form is ferroelectric and can take several orientations with respect to the cubic high-temperature form. Some atomic displacements are quite large.

### 3.6 Standard PostScript TypeFaces

#### Standard PostScript Typefaces (Font Families)

The names of the fonts should be entered exactly as given, with no embedded spaces. If your printer does not recognize a font string, it will probably default to Courier.

#### Times Roman Family

Standard: Times-Roman  
Slanted: Times-Italic  
Bold: Times-Bold  
Bold Slanted: Times-BoldItalic

#### Helvetica (Swiss) Family

Standard: Helvetica  
Slanted: Helvetica-Oblique  
Bold: Helvetica-Bold  
Bold Slanted: Helvetica-BoldOblique

#### Courier Family (fixed pitch)

Standard: Courier  
Slanted: Courier-Oblique  
Bold: Courier-Bold  
Bold Slanted: Courier-BoldOblique

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