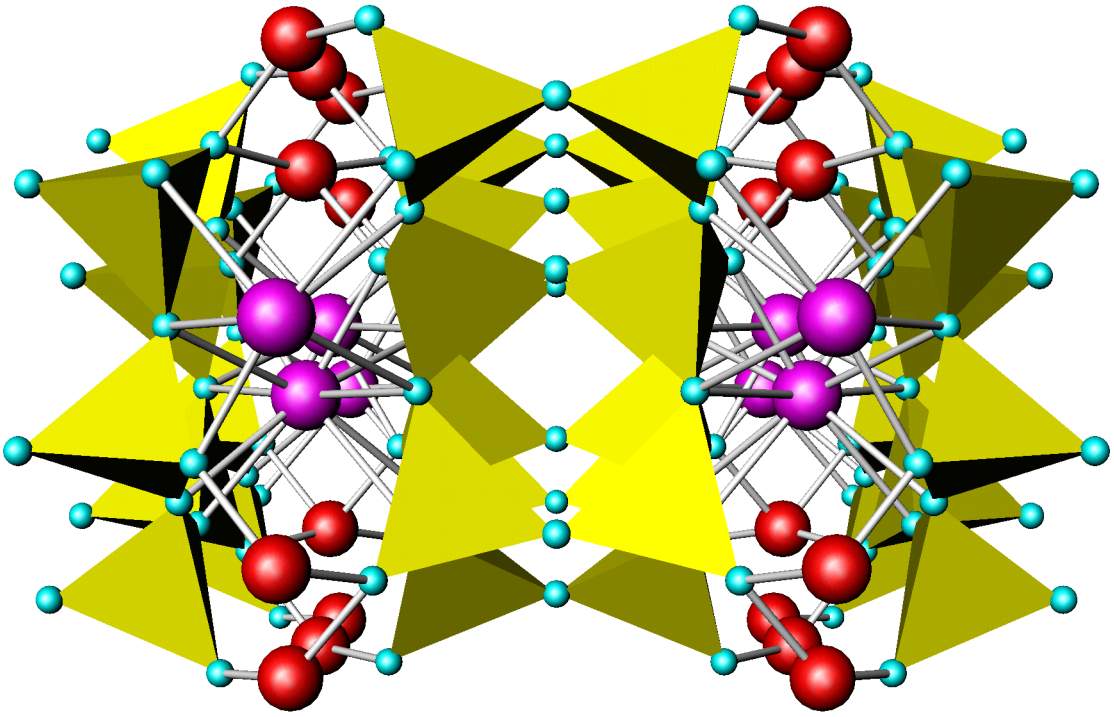


ATOMS

ATOMS
Version 6.2

Shape Software
521 Hidden Valley Road
Kingsport, TN 37663 USA

Telephone:
(423) 239-4771

Fax:
(423) 239-6360
or
(423) 239-3003

E-mail:
support@shapesoftware.com
dowty2000@cs.com

WWWeb:
www.shapesoftware.com

Table of Contents

1 Introduction

The topics in this section give information about the capabilities of ATOMS, what information is needed to draw a structure, general procedure for starting up, and a description of the calculations.

See:

Types of Windows for more information about the windows which are used;

Menus and Dialogs for detailed help on input;

Reference for general topics;

Tutorials for some simple examples of input.

1.1 Capabilities of ATOMS

ATOMS is a program to display atomic structures of all types, including molecules, polymers and crystals, and combinations of any of these.

If symmetry is used, the coordinates of only one atom of each equivalent set need to be entered. The symmetry elements for all 230 space groups and 32 crystallographic point groups are on file and can be called up by number or with their standard symbols. Non-crystallographic symmetry - such as pentagonal or icosahedral - can also be used. An auxiliary program SYMGRP is provided to derive complete symmetry matrices for any point group. ATOMS also supports Shubnikov symmetry for illustration of magnetic or other vectorial aspects of structures.

The boundaries for drawings of crystals and polymers can be specified in several ways. First, the contents of any given number of unit cells can be shown by setting limits to translational repetition. Second, any crystal faces, at any distance from the origin, may form the boundaries. Third, there is an option to show a slice of the structure parallel to a specified face with thickness equal to the *d*-spacing. Different boundary levels may be specified for different atoms if necessary. Fourth, a sphere about any atom or arbitrary point may be shown. Fifth, all molecules or other bonded units may be identified and shown in their entirety.

Molecules, polymers or other bonded groups may be isolated (independently of the fifth boundary option above). The generated atoms may be converted to input atoms, so that individual atoms may be deleted, removed or otherwise modified without affecting symmetry- or lattice-equivalent atoms.

Individual structure fragments may be combined to model twinning, epitaxy and crystalline defects.

There are several ways of displaying atoms and bonds in the Standard display mode: (1) spherical atoms and stick or line bonds; (2) line bonds only; (3) interpenetrating spherical atoms; (4) coordination polyhedra. Any of these types of representation may be intermixed in a single drawing. The same representations are available in the 3D display mode. In addition, there is a thermal ellipsoid mode which draws atoms and bonds in the manner of ORTEP (by Carroll K. Johnson).
Shading, according to angle of illumination, can be automatically applied to atoms, bonds and polyhedra in the Standard display mode. The 3D display mode, which uses OpenGL (Windows) or QuickDraw3D (Macintosh) provides additional options for lighting and material properties. The 3D mode can display thermal ellipsoids in a variety of ways.

The Cavities display mode shows a surface enclosing the possible center locations of a given-size spherical particle within the unit cell.

The drawing may be shown in strict projection, or in perspective at any given perspective distance. Exact scales may be specified in terms of inches or centimeters per Angstrom for the hard-copy output.

Atom labels and bond distances may be automatically added, drawn in proper location for stereopair views.

Hard copy can be made with dot-matrix printers, laser printers, inkjet printers or pen plotters. Also, you can write raster or bit-image files in several formats as well as vector files, for use in other software. Files can also be written in 3D formats (3DMF, VRML).

1.2 Information Needed to Draw a Structure

The first three categories of information listed below are intrinsic to a given structure, and do not change in the course of a calculation. These categories require very specific data from some source, if the structure is not theoretical or imaginary. Some sources of structural information are listed at the end. Categories 4 and 5 are somewhat arbitrary, but are generally fixed by chemical or geometric considerations. Categories 6 and 7 describe not so much intrinsic information about the structure, as attributes which are assigned for display purposes.

1. Reference Axes/Coordinate System/Unit-Cell Parameters.
The natural coordinate system for crystals is the crystal axes, which give the length and direction of the lattice translations. These are specified by as many as three axis lengths and three interaxial angles (a fourth redundant axis which is frequently used in hexagonal and trigonal crystals is ignored in ATOMS). The axis types fall into seven different crystal systems, depending on the constraints of symmetry on the equality in length of the axes and the interaxial angles. The coordinates of atoms and indices of face (if present) in the crystal system are eventually converted to coordinates in a

Cartesian system with a standard orientation ($z = c$, $x = a^*$; see section IV-6), but space-group symmetry operations (reproduction of atoms within the unit cell) are most easily carried out on the original crystal coordinates.

Coordinates of atoms in molecules are usually given in a Cartesian axial system. If the molecule has one 3-fold or 6-fold axis of symmetry, i.e. has trigonal or hexagonal symmetry ATOMS can either use reference axes which also have this symmetry, that is trigonal or hexagonal "crystal" axes (a_1 and a_2 axes at 120 degrees, c axis at 90 degrees to a_1 and a_2), or use unit Cartesian axes. The symmetry matrices for the standard point groups are actually stored in the form appropriate to hexagonal axes, and then converted to the Cartesian form during calculation if the structure axes are unit Cartesian.

2. Atom Coordinates.

Any structure must be specified by the locations of the atoms. In the case of crystals, this is normally done in terms of fractional coordinates on the structure axes. If symmetry is used, only one atom of each equivalent set need be entered. Atoms may be grouped by types (e.g. all Si atoms, all C atoms, etc.) to facilitate location of bonds and polyhedra.

When drawing magnetic or other vector structures, the coordinates or indices of the vector on each input atom is required.

3. Space- or Point-Group Symmetry.

This describes the way the atoms are repeated by the symmetry operators. The combinations of symmetry operators fall into a limited number of groups called space groups for crystals, and point groups for molecules. At a minimum, it is necessary to know which of these groups the crystal or molecule belongs to. The standard reference for space groups is the *International Tables for X-ray Crystallography*, published by Kluwer (4th edition). All of the 230 space groups are listed by number in Volume A, or Volume I in older editions (all references to the *Tables* will assume Volume I or A), and it is only necessary to give this number, or the standard Hermann-Maughin (International) or Hall symbol of the space group.

For molecules, ATOMS can also use the data from the *Tables* to provide the point-group symmetry given the standard symbol for the group (either the International symbol or the Schoenflies symbol), subject to some orientation restrictions, and to the limitation that the point group is crystallographic, that is that it belongs to one of the seven crystal systems.

If a structure is described in a crystallographic space- or point group in which the orientation or choice of origin is non-standard, it is still possible to enter the symmetry by essentially copying the information in the *Tables* or other source, provided the symmetry is described in the standard format.

Point groups containing n-fold axes with n equal to 5 or larger than 6 are theoretically

possible for molecules or one-dimensional polymers but not crystals. For such cases, the symmetry must be entered in the form of Cartesian matrices; these matrices, for any point group, can be prepared with the auxilliary program SYMGRP.

4. Boundaries of the Structure.
For a molecule, it may be presumed that all atoms entered, and usually all those generated by symmetry, are to be shown in the drawing, although selected individual atoms can be hidden or "deleted" after generation of the structure (see Deleting Atoms). Crystals and polymers, however, are ideally infinite structures, in which the unit cell is repeated by translation in as many as three directions, and some limitations must be placed on the extent of this repetition by translation. In some crystals it may be desirable to isolate molecules or other units. There are several different ways that such limitations can be imposed in ATOMS — see Boundary Options**.**

5. Definitions of Bonds and Coordination Polyhedra.
To specify bonds, you only need to give the types of the two atoms involved, and minimum and maximum bond distances between the two atoms; all bonds with these specifications are automatically located. These bond specifications can also be derived automatically from a set of atomic radii. To specify polyhedra, you need to give the type of the central atom, the coordination number, the types of the coordinating atoms or ligands, and the maximum distance between central atom and ligands. Normally, all polyhedra will be identified except incomplete polyhedra, i.e. those in which some of the atoms are not within the specified structure boundaries. If the coordination number and/or bond distances are not known, they can be determined with preliminary runs in which incomplete polyhedra are also accepted.

6. Sizes and Colors of Atoms, Bonds and Polyhedra.
In the Standard display mode, atoms are shown as spheres if they are shown at all; the radius (in Angstroms) must be specified. Bonds can be represented as single lines, or as "sticks" or cylinders with a given radius. If atoms interpenetrate, there is no size parameter, but a bond between the two atoms must be identified (item I-3.5 above) if the junction is to be handled properly in the Standard display mode (this is not necessary for the 3D mode). If a color screen display is used, colors may be assigned to the atoms and bonds according to several schemes. For the dot-matrix plot (including laser printer) and black-and-white screen displays, different shades of gray, normally represented by dot-patterns, may be specified for atom or bond colors. For pen plots, different pen numbers or colors may be specified for different atoms, bond, and polyhedra.

For drawing in the thermal ellipsoid mode, temperature factors are required for each atom, although default isotropic values are used if the temperature factors are not available for a given atom.

7. Orientation, Projection, Scaling.
These things all have defaults, but can be changed after initial input, and it may require some thought and experimentation to find the best settings. See Coordinate Systems. The projection may be orthographic (straight down the x-axis) or perspective. Perspective generally gives the most realistic appearance, while orthographic retains strict geometric relations and scaling. The drawing may be on some fixed scale (in inches or centimeters per Angstrom) or expanded automatically to fill the plotting area.

Sources of Structure Information. The two principal journals for crystal and molecular structure information are *Acta Crystallographica* and *Zeitschrift fur Kristallographie*, although many other chemical, biological and mineralogical journals publish structure determinations. Structure information is periodically summarized in *Structure Reports*. Most of the important structures are described by R.G. Wyckoff, in *Crystal Structures* (7 Volumes).
There are many sources of structure data in the form of computer files. See the Import Files option in the File menu for details on the formats supported by ATOMS.

1.3 Starting Up

When ATOMS is started, you see the Startup Window, which has buttons for the usual ways to input data. The same choices are in the **File** menu. There is a choice of starting a new file (New), opening an old file (Open), or importing a file (Import File). Also, a list of files recently worked on is shown in the **File** menu - single-clicking on one of these will open the file.

When you double-click on an ATOMS data file (.STR file) instead of the program icon the file is read in and you see a message box giving you the choice of calculating the structure or cancelling (see below).

The first time you run ATOMS you may want to check the dialogs in the **Settings** menu, especially the Preferences dialog. If you intend to use a pen plotter [Windows only], you should select the Pen Plotter Settings command, and verify or change the settings as needed. Likewise, you many need to change or verify the PostScript Settings.

Opening a sample file or an old structure file. You can read in one of the sample files (in the SAMPLES sub-directory) or folder, using the Open command or the most-recently-used list in the **File** menu. Alternatively, when ATOMS is not active, you can double click on one of the ATOMS data files (.STR files).

Entering a new structure. You can enter a new structure with the New item in the **File** menu. This will step automatically through all the categories of information necessary. Between each of the main dialogs in this sequence there will come a dialog titled "Enter

New Data Set". This dialog gives you a chance to back up to the last dialog completed, or to abort the **New** data entry. You can cause this dialog to be omitted with Preferences in the Settings menu.

The first part of the input is commands in the **Input1** menu. The first three categories, Title/Axes, Symmetry, and Boundary, are all mandatory. The next three categories, Crystal Forms, Atoms, Polyhedra and Bonds are optional, although all structure drawings must have either atoms or a crystal shape (forms). If the data entry is aborted during this first sequence, the entire file is abandoned.

At this point, you have the option of stepping through the remaining items, which are from the **Input2** menu and mostly control the way the structure is displayed, or of accepting default values. (You can cause the current values and settings in the **Input2** menu to be used as the defaults with the Save Defaults item in the **Settings** menu.) The data entry can be aborted at any point during this sequence and the new data set will be preserved.

Importing a file. This refers to files from other software. New formats are frequently added, so see on-line help for details.

After an old ATOMS data set or an import file has been read in or a new data set entered, you are asked if you want to "..calculate now". If you reply **Yes**, the structure is calculated and should appear in the Graphics window in a short time. If you reply **No**, the Graphics window is blank when it opens; you can then modify the data for the structure or the display parameters using the menus and dialogs, as described in Chapter III. When corrections or additions have been made, use the **Calculate** command in the **File** menu.

While the structure is plotting in other than the 3D display mode, pressing any key will temporarily halt the plot. Pressing **Esc**ape will then abort the plot, while any other key will continue the plot. The plot cannot be halted if double-buffering is in effect (Preferences dialog, **Settings** menu).

The **Calculate** command in the **File** menu and the **Replot** command in the **Display** menu are two of the most important and frequently-used in ATOMS. **Calculate** constructs crystal faces for boundaries (if used), reproduces atoms with symmetry and lattice translations, identifies atoms in bonds and polyhedra, and then plots the structure in the Graphics window. You must use this command if you change anything which determines the number and location of atoms, or the atoms involved in bonds and polyhedra. This includes many parameters in the dialogs of the **Input1** menu, although there are are also some parameters, such as atom, polyhedron and bond colors and atom and bond radii, whose changes do not require recalculation. **Replot** simply redraws the structure without changing the lists of atoms, polyhedra or bonds. Changes in any of the parameters in the dialogs of the **Input2** menu can be put into effect with **Replot**.

The **Calculate** and **Replot** commands are also in the Dialog Bar - Left, which are both controlled in the **Display menu**.

1.4 Description of the Calculations

It is impossible to give a complete description of the calculation methods, but some account of the procedures should be helpful to guide the use of the program.

Locating Atoms, Bonds, Polyhedra and Vectors

If crystallographic symmetry is present, symmetry operations in the form given in the *International Tables for X-ray Crystallography* are converted to matrices. For non-crystallographic symmetry (e.g. pentagonal, icosahedral) the matrices, generated by the auxilliary program SYMGRP, are read in directly. The atom coordinates are multiplied by these matrices, and translations are added if there are screw axes or glide planes in the space group, to find all the atoms in the unit cell or molecule. The coordinates of the atoms are then converted to a Cartesian system if necessary.

If the structure is a molecule, then no further location of atoms is necessary, but for polymers or crystals, the lattice translations must be applied, subject to one of several types of boundary. In some cases, especially for polymers, it may be sufficient to take all atoms in unit cells related to the initial one by specified numbers of lattice translations in each of the three crystal or polymer axis directions — one or two of the translations may be disabled, leading to two- or one-dimensional polymers, respectively.

For crystals a more general and powerful method of determining the structure boundaries is by means of crystal faces. The crystal faces are specified by their standard Miller-Bravais indices (the reciprocals of the intercepts on the three crystal axes), and by a central distance, which is the perpendicular distance from the center of coordinates to the face. If the crystal has symmetry, this can used in specifying faces; i.e. only one face of each symmetry-equivalent set, or form, need be entered. Symmetry equivalents of the faces are derived similar to that used for atoms. However, if desired the symmetry used in the generation of faces can be lower than that used in the generation of atoms.

A special case of boundary faces is a slice, which is a slab of the structure bounded by a given face and its negative, with a thickness determined by the crystallographic interplanar or *d*-spacing — the limits to the extent of the structure in the two dimensions parallel to the given face are arbitrary and may be specified.

To identify the the corners and edges defined by the crystal faces, all possible intersections of triplets of faces are located; those which are further from the center than any face are rejected as crystal corners. Edges are defined by pairs of corners which have two faces in common.

Atoms within the specified face boundaries are simply those which are not at a positive distance from any face. Starting with atoms in the central unit cell (fractional coordinates 0 to 1), lattice translations are added or subtracted until all possible atoms have been tested for inclusion. The algorithm which does this is rather complex, as finding the starting and ending unit-cell limits for the atoms search in the general case of face boundaries is not trivial.

If coordination polyhedra are to be shown, the atoms involved must be located. ATOMS will identify all polyhedra consisting of specified types of ligands within a given distance of a central atom. The ligand atom locations (points) form the corners of opaque polyhedra. Edges and faces of each polyhedron must be identified, which requires some rather complex calculations. Because of possible variation in coordination number, data on corners, edges and faces of polyhedra must be packed into special arrays, and unpacked each time they are used.

In the Thermal Ellipsoids mode, at the start of the calculation the temperature factors for each input atom are converted to the principal axes of a thermal ellipsoid. During generation of the atoms within boundaries, the number of the symmetry matrix used is saved, to be used later in plotting.

If atomic vectors are present, they are represented by pseudo-atoms (at the ends of the vectors) and by pseudo-bonds. This simplifies the geometric relations for plotting in Non-3D modes. These pseudo-atoms and pseudo-bonds are generated in a special loop.

The atom locations, identity of bonds and data on polyhedra if present, constitute a "permanent" set of parameters for each structure. The atom coordinates may be rotated in any of several ways to obtain a suitable view.

Plotting - Non-3D Modes

Whenever a drawing is made for the screen, dot-matrix plotter or pen plotter, the actual elements which appear in the drawing, that is arcs of circles representing spherical atoms and lines representing bonds and polyhedra, must be recalculated, since their interrelations depend on the viewing angle. Each polyhedron must be examined to classify edges as to whether they are front, back or boundary.

For screen or dot-matrix drawings, the procedure is somewhat simplified since it is possible to blank out or draw over elements which lie underneath others. The atoms, polyhedra and bonds are sorted according to their height, or distance from the viewer. The elements are then plotted in sequence from the most distant to the nearest. Atoms are represented in the sorting process by their centers, bonds by their midpoints, and polyhedra by the central atom. This sorting process is a simplification of the true relationships, and conceivably could lead to error, but only if the bonds are unusually long. In fact the drawing method relies on displaying only normal chemical bonds, not

arbitrary connections between atoms. If desired, atom labels are drawn during the process of plotting atoms from back to front.

If crystal edges are also shown, the "back" edges, i.e. those that would be invisible in an opaque crystal, are plotted before the atoms, bonds, etc., and the "front" edges are plotted after. Sorting the crystal edges is not practicable because of their length. There is no attempt to solve for interpenetration relations of edges with atoms, bonds or polyhedra and errors will usually result if the edges are not completely outside the structure.

For pen plots actual blanking or overlaying is impossible, and it is necessary when drawing a given element to consider every other element which lies higher (closer to the observer), find all the possible intersections and remove the segments which are obscured. Insofar as possible, intersections of structure elements (bonds and atoms, polyhedra) are considered as intersections of two-dimensional figures (circles, lines, ellipses), rather than computing the intersections in three dimensions and then finding the projections. One approximation which is made here is to represent ellipses (which only arise as junctions of atoms and stick bonds, and junctions of interpenetrating atoms, and thus cannot overlie other elements) by means of line segments for purposes of locating intersections; they are actually drawn as ellipses, but slight errors in locations of intersections involving ellipses may occasionally result.

For perspective drawings, the atom locations (and crystal corners if present) are projected from a given perspective distance onto a plane passing through the center of the structure. Overlay relationships with other elements (for pen plots) are then determined on the basis of circular projections for spherical atoms, again making calculations in two dimensions as much as possible. This is not true perspective, but the difference is not likely to be noticed unfavorably in the normal case. In fact, when true perspective is used and the drawing is viewed at other than the (scaled) perspective distance specified in making the projection, the distortion of the projected atom shapes from circles can be very disturbing - this can be verified in the 3D display mode.

For shading of atoms, the given illumination vector and the number of shading zones are used to set up outlines for each zone, consisting of circle and ellipse segments. The angle with the illumination vector gives a shade for each zone. The zones need to be set up only once for a given illumination vector, since all atoms are identical except for scaling by the radius. Zones can also be set up for stick bonds, but since the bonds make various angles with the illumination vector, the shade can only be determined at plot time. For polyhedra, the shade of each face is determined at plot time.

In the Thermal Ellipsoid mode, at plot time, atoms are sorted and plotted from back to front as for ball-and-stick, but as each atom is drawn the principal axes are transformed using the appropriate symmetry matrix, and the ellipsoid is drawn. Bonds are located in the same way as for standard ball-and-stick, but because the algorithm for finding the

intersection of stick bonds with ellipsoids is completely different from that used for spheres, thermal ellipsoids and ball-and-stick cannot be intermixed.
Atomic vectors, which are represented as pseudo-bonds, are in fact drawn much like normal bonds, except that cones (arrowheads) are substituted for the atom on the positive end of the vector (if it is two-ended) for all types of display and output aside from pen plots.

The Anaglyph display mode is a very special case. Because each view is drawn in only one color, it is not necessary to sort objects from back to front, and rotations (for example) may be even faster than the similar skeletal mode.

Plotting - 3D Modes.

In this type of drawing, the surfaces of three dimensional objects such as spheres and cylinders are converted to an assemblage of planar polygons. Then each polygon is drawn essentially independently pixel by pixel. The critical difference with non-3D modes is that a depth buffer is used in 3D imaging. This is an array of integers, one for each pixel in the display or output (or that portion which is currently being drawn, when banding is being used). Each element, representing a pixel, holds the relative x coordinate (in the ATOMS observer coordinate system - this is more often the z-axis and the buffer may be called the z-buffer) of the foremost object or polygon. The color for this object is retained in the color buffer, which is a similar array representing pixels; this array is actually the image itself. Whenever a polygon is drawn, each pixel which it contains is compared against the depth buffer; if the x coordinate of the pixel is greater, or closer to the observer than what is in that element of the depth buffer, the color for this pixel in the new polygon replaces the value in the color buffer. That is, the depth buffer keeps track of the front surface of the drawing, and ensures that only this front surface (not any hidden surfaces) are kept in the color buffer or image itself.

Typically, each corner of each polygon is assigned a vector normal, which is not the same as the normal to the polygon itself. For example for a sphere the normals are simply directed from the center outward through the corners of the polygons (triangles). Color is assigned to each corner according to the light equation (see **3D Lighting** in the **Input2** Menu), and interpolating between the corners at each pixel gives a smooth curved appearance, rather than a collection of flat polyhedra.
When translucency is in effect, it is necessary to blend the color of a new object with what is already in the color buffer. It is normally necessary to plot translucent objects in sequence from back to front, although opaque objects in the same drawing do not have to be sorted. Translucency always requires increased plotting time.

The "double buffer" method is normally used, the "color buffer" being kept in an area of memory and then copied to the screen memory when the drawing is completed. This is usually faster than drawing directly to the screen.

The standard display mode of ATOMS does not use a depth buffer: the atoms, bonds and polyhedra are sorted from back to front and drawn in that order. When necessary, the intersections of objects are solved analytically and only the required portions of each are drawn.

Using a depth buffer has the advantages that it is not necessary to solve analytically for intersections, nor to sort the objects with respect to depth. This may save considerable time, especially for complex drawings, since the time for sorting tends to increase exponentially with the number of objects. Since analytical solution of intersections is not necessary, it is possible to place essentially any objects into the drawing. in any location. This overcomes the problem in ATOMS non-3D drawing modes of sometimes-incorrect drawing of crystal edges or unit-cell edges which intersect with atoms, bonds and polyhedra. The 3D method allows more complex shading and lighting effects, such as specular highlights and multiple light sources. It also allows translucent objects. For a completely 3-dimensional image, on a computer which has sufficient memory, the 3D display mode is superior to the ATOMS Standard display mode.

Without special hardware for 3D drawing, it is about as fast as fully-shaded Standard display mode drawing with about 16 shading zones.

However, there are disadvantages to the 3D method. The depth buffer may result in excessive memory requirements even for the screen (but some 3D accelerator cards may have special memory for the depth buffer). The 3D method is not very suitable for black-and-white drawings, which typically are simplified, showing mutual intersections of atoms with bonds and polyhedra as lines or curves; such intersections simply are not drawn in the 3D method. Both Windows and Macintosh implementations currently have some severe limitations in terms of printing. It is necessary to draw each image into a bitmap and then copy that bitmap to the printer. Because printers have much higher resolution than the screen, this causes even higher memory requirements, and for reasonable sized printed drawings it is usually necessary to do the printing in bands or segments. ATOMS itself uses "Immediate mode" to draw atoms, bonds, etc. - that is, it draws each object and then discards the memory associated with that object. On the other hand, many 3D applications, especially the standard viewers for VRML and 3DMF files, use "Retained mode". In this mode every vertex of every object is read into memory before drawing. This allows simple drawings to be redrawn and rotated rapidly, but it may take a long time to load large drawings initially and uses enormous amounts of memory (typically 16 MB for 300 atoms in a ball-and-stick model).

3D files (VRML, and 3DMF for Macintosh) contain the locations and material properties (especially color) of such common objects as spheres, cylinders, disks and lines, and their orientation where appropriate. Polyhedra are represented as assemblages of polygons. The viewers for these files then use methods similar to those used by ATOMS to draw the objects. As explained in the previous paragraph, beware of viewers using Retained mode - they may crash or take forever to draw a complex crystal or molecular structure.

2 Types of Windows used in ATOMS

ATOMS uses four types of windows besides dialogs and alerts: the Startup window; the main Graphics window; secondary (Powder and Precession) Graphics windows; and Text windows. Each type of window has its own menu bar. The Help system also has its own windows and menus.

Note that under the Windows operating system the ATOMS windows are not confined to reside within a framework window, as in pre-V6.0 ATOMS.

All the current windows are listed in the Windows menu, and this menu can be used to switch between windows if some are not visible.

When starting up ATOMS, the menus displayed in the Startup window include only a File menu, a Settings menu and a Help menu. Use the commands in the File menu to start a new ATOMS data set, read an old one from a file, or import data from a file with an external format.

After you have entered or read in the data for an ATOMS file, the main Graphics window opens and the Startup window disappears; if you have elected not to Calculate, the Graphics window may be blank, otherwise it will show the current ATOMS drawing. Only one data set at a time is allowed in ATOMS, and there is only one main Graphics window. When this window is active, there is a File menu and various other specialized menus such as Input1 for data input and modification and graphics output.

The secondary Graphics windows appear only when you have selected Powder Diffraction (**Graph** Option) or Precession Pattern from the Display menu. These windows have their own menu bars, with only a File menu, a Windows menu and a Help menu. When a secondary window is active, output, such as Print, Raster File, etc. in the File menu, is for the Diffraction results, not the atomic structure in the main Graphics window.

The File menu of the main Graphics window has four commands, List Input, **List Generated Atoms**, **List Generated Faces** and **List Totals**, each of which lists the relevant data to a separate Text 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 INPUT.ATD, GENATOMS.ATD, FACES.ATD and TOTALS.ATD. These files are written over again for each new ATOMS data set, so if they are to be preserved they should be saved with the Save As command in the File menu, using a different name.

A Text window is also generated when Calculation Output is selected in the **Input2** menu. The output is written to the file *infile*.ATD, where *infile* (.STR) is the name of the

ATOMS data file. Similarly, the Coordination button in the Input Atoms dialog of the **Input1** menu writes a file called BONDS.ATD, and the Powder Diffraction (**List** option) dialog writes output to the file LIST.ATD. The **List Coords** button in the Cavity Parameters dialog lists the fractional coordinates of all grid points which can accomodate the sphere of the specified **Particle radius** in the file CAVVAL.ATD.

Secondary Graphics windows and Text windows are "children" of the main Graphics window, since their contents pertain only to the current structure, and they are destroyed if the main Graphics window is closed.

An output Text window or a diffraction Graphic window may sometimes come up behind the main Graphics window. If the new window is invisible, use the Window menu to bring it to the front.

2.1 Startup Window

This window appears when ATOMS is first started, or when a data set (Graphics Window) is closed.

The structure image at the bottom of this window is from a file called default.png. You may save a new version of this file (Raster option, File menu) - the image should be about 300 pixels wide by 200 pixels high.

It has its own menu bar Startup Menu Bar, and the following buttons for getting a data file into ATOMS.

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

Open - Open an old ATOMS 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 ATOMS program.

2.2 Graphics Window

This is the main window which shows the current structure drawing. When it is active, most menus are available, allowing modification of the data and other operations.

Also, the controls or commands in the Dialog Bar - Left and Dialog Bar - Right are active (if selected in the Display menu), and they operate on the drawing or on the main ATOMS data set.

To switch to another window, such as a text window or the Powder or Precession windows (see Types of Windows), click on that window if it is partially visible, or use the Windows menu.

2.3 Powder Diffractogram Window

This graphics window (see Types of Windows) shows the results from the Precession Pattern dialog (Display menu). It has its own menus, which essentially allow only input of a new data set or saving of the current data set, and graphics output of the Powder diffractogram to the printer or files (EPS, raster, metafiles).

Use the File menu for this window for Print, Raster, PICT or Metafile output.

To access the menus which allow modification of the ATOMS data (and even recalculation of the Precession Pattern), click on the main Graphics Window if it is visible, or use the Window menu. The main Graphics Window has the title of the current ATOMS data file (.STR).

2.4 Precession Pattern Window

This graphics window (see Types of Windows) shows the results from the Precession Pattern dialog (Display menu). It has its own menus, which essentially allow only input of a new data set or saving of the current data set, and graphics output of the Precession Pattern to the printer or files (EPS, raster, metafiles).

Use the File menu for this window for Print, Raster, PICT or Metafile output.

To access the menus which allow modification of the ATOMS data (and even

recalculation of the Precession Pattern), click on the main Graphics Window if it is visible, or use the Window menu. The main Graphics Window has the title of the current ATOMS data file (.STR).

2.5 Text Window

Text windows are generated by several commands (below). When a text window is active, there is a special menu bar which allows modification and saving of the particular output file (.ATD) which is being edited - the commands in these menus do not pertain to the current ATOMS data file. To return to the main Graphics Window for modification, saving etc. of the ATOMS data file, click on that window if it is visible, or use the Window menu.

The File menu of the Graphics window has four commands, List Input, **List Generated Atoms**, **List Generated Faces** and **List Totals**, each of which lists the relevant data to a separate Text 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 INPUT.ATD, GENATOMS.ATD, FACES.ATD and TOTALS.ATD. These files are written over again for each new ATOMS data set, so if they are to be preserved they should be saved with the Save As command in the File menu, using a different name.

A Text window is also generated when Calculation Output is selected in the **Input2** menu. The output is written to the file *infile*.ATD, where *infile* (.STR) is the name of the ATOMS data file. Similarly, the Coordination button in the Input Atoms dialog of the **Input1** menu writes a file called BONDS.ATD, and the Powder Diffraction (**List** option) dialog writes output to the file LIST.ATD.

3 ATOMS Menus and Dialogs

ATOMS Menu Bars

Startup Menu Bar - This menu bar appears when starting ATOMS, or when all windows (Graphics or Text) have been closed.

Graphics Window Menu Bar - This is the main menu bar for entry, alteration and display of atomic structure data sets.

Text WindowMenu Bar - This menu bar is used for text windows produced by the **Listings** group in the File menu of the Graphics window, and by the Calculation Output command in the Input2 Menu, or by the Powder Diffraction listing option. The Text window is a more-or-less standard edit window.

3.1 Startup Menu Bar

File menu - Use the commands in this menu to start a new ATOMS data set, open a file for an old data set, or import a data set from a data base.

Settings menu - This contains settings for hardware, palettes and preferences for modes of operation.

Help menu - On-line help

3.1.1 File Menu (Startup Window)

To start up ATOMS, you must select either **New** to enter an all-new data set; **Open** to open a previously-saved ATOMS data file; or **Import File** to open a data file written by other software.

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

Open - Open an old ATOMS data file.

Recent File List (Windows only) - The last four ATOMS data (.str) files can be opened by selecting here.

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.

Page Setup - Set the page size and select the printer.

Exit/Quit - Quit the ATOMS program.

---------Windows Only ----------

Note that you can also start ATOMS for Windows from the DOS command line, reading in an ATOMS data file or an import file.

3.1.1.1 New Command

New Command [File menu (Startup) or File menu (Graphics)]

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

When you use this command to start a new data set, ATOMS first steps through most of the dialogs in the Input1 menu, which involve parameters which are considered to be intrinsic to the structure in question. After you click OK in each dialog, a dialog appears (Entering New Data) giving you the choice of continuing or aborting the data entry. You can eliminate this dialog with the **Confirmatory alerts** checkbox in the Preferences dialog in the Settings Menu. At the end of the dialogs in the Input1 menu another dialog appears (End of Mandatory Input) giving you three choices: 1) you can continue with the non-mandatory part of the input, which consists of the dialogs in the Input2**menu**, involving mostly display aspects of the structure; 2) you can stop here and accept the display parameters currently in memory; or 3) you can read in the default display parameters from a disk file (the current display parameters can be saved as the defaults with the Save Defaults command in the **Settings** menu. If there is no data set in memory, option 2) will give the default values.

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

3.1.1.1.1 Entering New Data Set

Dialog Box: Entering New Data Set [During New input]

This dialog comes up in between the main categories of data during input of a **New** data file. Usually you can just click on **Continue** (or hit **Enter**), but you can **Abort** the input, or **Revise** the category you have just finished.

The appearance or non-appearance of this dialog is controlled by the **Confirmatory alert...** checkbox in the Preferences dialog in the Settings menu.

3.1.1.1.2 End of Mandatory Input

Dialog Box: End of Mandatory Input [During New input]

The mandatory input for a **New** data file consists of the commands in the **Input1** menu, through the **Bonds** item, although you do not necessarily have to specify all of them. The non-mandatory input consists of the display parameters, or most commands in the **Input2** menu (3D parameters are omitted). If you elect not to continue with these display items, the display parameters will be taken from a) a set of default parameters, if you click on **Default** or if this is the first file in your current ATOMS session; or b) from the display parameters of the current file if you click on **Quit**. You can save the current display parameters (including mostly parameters in the dialogs of the **Input2** menu but also some from the **Display** menu) as the default parameters with the **Save Defaults** command in the **Settings** menu.

3.1.1.2 Import Files Submenu

Sub-Menu: Import File [File menu (Startup) or File menu (Graphics)]

This offers a selection of file types to import, including CCDC FDAT, SHELX-93, CIF, DBWS/LHPM Rietveld, ICSD, ORTEP, XTLVIEW, VIBRAT,PDB, RIETAN, GSAS, AM MINERAL, FULLPROF and Free-Form.

The boundary option in most cases can either be Default Unit Cell, suboption as selected with the **Default** radio button, or Locate Molecules in Crystal.

Multiple occupancies are not permitted in ATOMS, and when more than one atom is found to be in the same position (same fractional x, y and z coordinates) the second and subsequent occurences will be deleted.

There is a limit of 500 input atoms in most cases.

Depending on the format, there may be many sources of error in importing files. Open the file with a word processor and check the symmetry and atom list in ATOMS against the file contents.

3.1.1.2.1 Import File

Dialog Box: Import File [File menu (Startup) or File menu (Graphics)**]**

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

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 ATOMS data file will be taken from the name of the file, and the title (Title/Axes dialog in the Input1 Menu) will be taken from the data set or phase. The extension.STR will be appended to the structure file.

If the **Generate bonds** box is checked, the Generate Bonds from Atomic Radii dialog will come up as soon as the file is read in.

Read default display parameters. If this box is checked, the display parameters last saved (**Settings** menu) will be read for the new data set.

Read temperature factors. This option may not be available for all types of import file. In some file formats, such as ICSD RETRIEVE, the temperature factors are in a separate list from the atomic coordinates. In order to assign the temperature factors to the atoms, the atom labels in these two lists must match exactly. For this reason, "OH" and "OH2" in the atom lists in RETRIEVE files are changed to "O", since the labels in the temperature factor lists use only "O". If you get the message "Temperature factor atom label not identified", you may need to edit the atom labels in the original file so that the two lists agree.

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

Atomic Radii. You can choose standard ionic or covalent radii, which will be multiplied by the factor in the edit box. For a ball-and-stick drawing, a factor of 0.5 or less is appropriate. For interpenetrating atoms (space-filling), a factor of greater than 1.0 is usually necessary. All radii can later be multiplied by a given factor in the Atoms-Global command in the Input1 menu. The radii, as well as default colors, are obtained from the selected version of the ELEMENTS file (either ELEMENTS.ION or ELEMENTS.COV) supplied with ATOMS (these files can be modified by the user).

Boundary Option. The boundary option can either be Default Unit Cell, using the default suboption selected in that dialog, or Locate Molecules in Crystal. If the Locate Molecules in Crystal option is used, the **Generate bonds** box will be considered to be checked, as bonds (or polymers) must be defined.

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 (Input1 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-Maughin 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 may be required for the Slice boundary option. 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). ATOMS 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 it is your choice whether this or the atom label (if either) will identify the element.

Note that in the case of multiple occupancies for a site, ATOMS ignores all but the first atom.

For more information about the specific file types, see one of the following
CCDC FDAT
SHELX-93
CIF
DBWS/LHPM Rietveld
ICSD
ORTEP
XTLVIEW
VIBRAT
PDB
RIETAN
GSAS
AM MINERAL
FULLPROF
Free-Form (.inp)

---- Macintosh only ----

You can show all text files, or only those with the specified extension (.xxx) in the File Open dialog - make this choice, which applies to most types of files, in the Preferences dialog in the **Settings** menu.

3.1.1.2.2 Data Sets... in Import File

Data Sets...in Import File [Import File **Command -** File menu (Startup) or File menu (Graphics)**]**

When you open a CIF, DBWS/LHPM or other type of import file, ATOMS will search through it to find all the data sets or phases within it, up to a limit. If there is more than one, this dialog will present you with a list. The name of the ATOMS data file will be taken from the name of the file, and the title (Title/Axes dialog in the **Input** Menu) will be taken from the data set, phase or crystal selected. The extension.STR will be appended to the structure file.

3.1.1.2.3 Free-Form (.inp) File

Import Free-Form (.inp) File [File menu (Startup) or File menu (Graphics)]

See the Import File dialog for general aspects of importing atomic-structure data files.

This imports files in the free-form format described elsewhere (Atom Parameter Files). Note that this format has been expanded since earlier (pre-V4.1) version of ATOMS, so that essentially all relevant data for a crystal may be entered.

3.1.1.2.4 CCDC FDAT File

Import CCDC FDAT File [File menu (Startup) or File menu (Graphics)**]**

See the Import File dialog for general aspects of importing atomic-structure data files.

Most of the FDAT files have a "connection table" which specifies the bonds defining a single molecule, while the unit-cell may contain several molecules. Thus the radio buttons give you a choice of importing the file as a molecule or as a crystal.

When imported as a molecule, the structure will use the No Boundaries (Molecule) boundary option, and no symmetry. The files normally contain a unique set of input atoms, which are the same as those required for input of a crystal in ATOMS, plus in many cases some extra symmetry-derived atoms necessary to complete the molecule; all these atoms are used as input atoms when importing as a molecule. With the **Atomic radii** radio buttons, you can choose to use either the radius values in the CCDC files, or

those in the ELEMENTS file; in any case, the type number (atomic number), colors and patterns will be obtained from the ELEMENTS file using the elemental symbol which is in the first one or two characters of the FDAT atom. The radius values in the CCDC files typically are covalent radii, slightly smaller than those required for contact of bonded atoms. For a space-filling or interpenetrating atoms model, they may need to be increased, and for a ball-and-stick model they may need to be decreased. The radii of all atoms can be changed by a factor with the Atoms - Global dialog in the **Input1** menu. All bonds between atoms will be the same; the radius, colors and patterns can be defined with the **Define Bonds for Molecule** button; this will call up a dialog which is similar to that which comes up for individual bonds (Bond Data in the **Input1** menu); however, atom types and distance limits are not used and are omitted from this dialog. After calculation, the radius, colors and patterns can be changed with the **Bonds** command in the Input1 menu. There will be only one bond type in the list.

Note that importing a CCDC FDAT file as a molecule uses a different procedure from the Locate Molecules in Crystal boundary option, which is used in most other cases when importing a crystal structure as molecules. The Locate Molecules in Crystal boundary option uses the bond and polymer specifications entered in ATOMS to isolate the molecules, whereas the FDAT files usually already contain the linkage information which defines molecules. If you wish to use the Locate Molecules in Crystal option, you must import the FDAT file as a crystal, then change the boundary option.

When imported as a crystal, the structure will use only the unique set of atoms, omitting the extra ones. The boundary option will be Default Unit Cell, current default suboption.

3.1.1.2.5 SHELX .INS File

Import SHELX.INS-93 File [File menu (Startup) or File menu (Graphics)**]**

See the Import File dialog for general aspects of importing atomic-structure data files.

ATOMS is programmed only for SHELX-93 files, although it may also be possible to read SHELX-76 files.

Atom type numbers from. The **Type labels** radio button will use the SHELX SFAC (scattering factor) number which is the number which follows the atomic label and preceeds the atomic coordinates in the SHELX file. The numbers correlate with elements through the SFAC instruction, which must be in the SHELX file. These elements will be used to determine the atomic radii and colors using the ELEMENTS files supplied with ATOMS (which can be modified by the user). The SHELX atomic radii are not used; if an element is not in the current ELEMENTS file, the correct radius will not be supplied.

Symmetry. The Custom point or space group option will be used. Typically the true symbol can be recovered from the title. ATOMS 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 with the Symmetry command in the **Input1** menu.

Multiple occupancy of sites. If there is an EXYZ instruction, ATOMS will use only the first atom - all others will be *deleted*.

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 ATOMS. Frequently, the positions of the hydrogen atoms are not in the.INS file, and must be taken from the output. There are several ways to do this. First, 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. Second, the hydrogen lines can be put into a file of their own and read in with the input-file provision of the Input Atoms dialog in the **Input1** menu, after the SHELX.INS file has been imported. Since the label and coordinates are in the default order, no modification is necessary, and a FIELDS line is not needed - only the lines with the labels and coordinates (any other fields following on the same line will be ignored). If you do this, do not check the **Generate bonds** box. You can generate bonds after the SHELX and the hydrogen input files have been read in, with the Bonds dialog in the **Input1** menu.

Most of the instructions in a SHELX file will be ignored. However, ATOMS 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 SCRPTR setup file, separated by spaces and preceeded by the number of instructions. You can edit this list if necessary.

You should scan the atom list (Input Atoms dialog in the **Input1** menu) to be sure nothing has been included by mistake.

3.1.1.2.6 CIF File

Import CIF File [File menu (Startup) or File menu (Graphics)]

See the Import File dialog for general aspects of importing atomic-structure data files.

ATOMS 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 CPATOMS.EXE file).

Cell setting. If a cell setting (crystal class) is not present or is undecipherable, ATOMS will try to recover the crystal class from the unit-cell parameters.

Errors in CIF files. Many CIF files which are written by databases and other software violate one or more of the CIF syntax rules (Acta Cryst. 1991, A47, 655) and are therefore unreadable without modification. Some common errors:

1) Line length greater than 80 characters.
2) Failure to enclose character fields in single quotes
3) Fields ("data names") too long - for example "data_" field longer than 32 characters.

The "data_" line should be truncated to 36 characters. Many of the lines in a typical file are not used by ATOMS and may simply be deleted.

Extensions to CIF files and special versions. Some database operators have taken to producing special versions of CIF files, with extensions which may or may not have been approved and which may not readable without special knowledge or assumptions.

The Cambridge Crystallographic Data Centre generates CIF files which may contain all the atoms in an asymmetric unit, plus other atoms related by symmetry to complete all molecules in the structure. The choice of **Boundary Option** in the Import File dialog determines how the structure is handled, as in the CCDC import option. If **Default Unit Cell** is chosen the "extra" atoms are deleted and the structure is handled as a crystal; if **Locate Molecules in Crystal** is chosen, all the given atoms are accepted and no symmetry is applied. For the **Default Unit Cell** option, the list of valid atoms is cut off when an atom label is encountered with a non-numeric last character. If this results in an incorrect atom list, choose **Locate Molecules in Crystal,** delete any unwanted atoms and reset the Symmetry and Boundary options.

The Protein Data Bank (PDB) can also export files as CIF, which in this case are actually "macromolecular" CIF or mmCIF file, and extension of the CIF standard. Like the PDB files themselves, these can only be imported as molecules with Cartesian coordinates.

If possible, CCDC and PDB files should be downloaded and imported in the "native" formats, rather than as CIF - in these format, information can only be lost in the process of translation to CIF. In other cases where there may be a choice of formats, such as ICSD, a CIF file may be more successfully imported than the native version.

3.1.1.2.7 DBWS/LHPM Rietveld File

Import DBWS/LHPM Rietveld file [File menu]

See the Import File dialog for general aspects of importing atomic-structure data files.

The DBWS or 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.

ATOMS can read three revisions of the DBWS format - 1990, 1994, and 1998 - but there is no version number or other direct indication of the revision in the file itself, so some trial and error may be involved. 1990 files will probably fail on the first attempt at reading, and you are then given a chance to try again.

3.1.1.2.8 ICSD File

Import ICSD File [File menu (Startup) or File menu (Graphics)**]**

See the Import File dialog for general aspects of importing atomic-structure data files.

Five types of ICSD file are supported, classified according to source:

1) Files from the CD-ROM database, accessed by the program **RETRIEVE** (see below for the CD-ROM program FINDIT). 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 CD-ROM database, accessed by the newer program **FINDIT** (see above for the CD-ROM program RETRIEVE). As for RETRIEVE, the exported file must be a copy of what is in the results window. FINDIT can also write CIF files.

3) Files from the Canadian Scientific Numeric Database System (**CAN/SND**). This service may no longer be available. The files are referred to as CRYSTIN, but are different from original 4) CRYSTIN files.

4) Original **CRYSTIN** files, available from the Netherlands CAOS information system, from ETH (Switzerland) and perhaps other sources.

5) Files from the the ICSD World Wide Web site (barns.ill.fr/dif/icsd/). The "raw" (ICSD) data format for this source is unreliable and is not shown in the menus. The data should be exported in one of the formats which is supported by ATOMS. Unfortunately again, these exported files may be incorrect - certainly the exported CIF files often violate

many of the CIF rules and may be unreadable without modification (see CIF files).

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

ATOMS actually distinguishes among the four different readable file types by reading part of the main title or "Collection" line, which gives the ICSD index number:

1) RETRIEVE - " COL Collection Code " or " COL ICSD Collection Code"

2) FINDIT - "*data for ICSD #"

3) CANSND - "ID: "

4) ORIGINAL - " **** COLLECTION CODE COL= "

5) WWW - " COL ICSD Collection Code " with "DATE=" in the same line

In each case the index number follows the above excerpt. Note that in all file types except CANSND and FINDIT there is always a blank character in the first column.

The different ICSD entries in the various import options exist only to allow different file extensions for the Open File dialog - when ATOMS opens and tries to read any ICSD file it will determine the file type itself according to the "Collection" line.

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.

3.1.1.2.9 ORTEP File

Import ORTEP File [File menu (Startup) or File menu (Graphics)]

See the Import File dialog for general aspects of importing atomic-structure data files.

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 - one of the two ATOMS boundary options Default Unit Cell or Locate Molecules in Crystal is used.

Most of the ORTEP ellipsoid and bond plotting parameters are read from the file, and can be accessed in the Ellipsoid Parameters dialog in the Input2 Menu. See Thermal Ellipsoids for more details on display modes, etc.

3.1.1.2.10 XTLVIEW File

Import XTLVIEW File [File menu (Startup) or File menu (Graphics)]

See the Import File dialog for general aspects of importing atomic-structure data files.

ATOMS may need to shift the fractional coordinates to insure that the origin is placed on a center of inversion.

3.1.1.2.11 PDB File

Import Protein Data Bank (PDB) Files

See the Import File dialog for general aspects of importing atomic-structure data files.

These files can be imported and displayed in all the methods available in ATOMS, i.e. as ball-and-stick, interpenetrating (space-filling), skeletal, anaglyph and even polyhedra. ATOMS supports one protein-specific display mode, the Protein mode, which displays the bonds between the backbone atoms of the amino acids as skeletal cylinders, omitting other atoms in the amino acids (although individual amino acids or residues can be selected for complete plotting in the Protein Display Attributes dialog in the Input2 menu).

Other specialized programs such as RASMOL can display protein structures faster and with more protein-specific options. However, ATOMS may have an advantage over some of these programs in the quality and flexibility of the printed output, for example in using the full resolution of the printer, either directly or as EPS files, Metafiles or PICT files

In order to isolate the protein itself, there is an option in the Protein Display Attributes dialog in the Input2 menu which allows omission of all hetatoms, or just water hetatoms. This dialog also sets the parameters for the Protein Display Mode.

Symmetry specified in the PDB file itself is not supported directly, as the specifications in use prior to V2.0 are not adequate for computer input (often being simply verbal descriptions). MODEL statements, greater than 99,999 atoms and temperature factors are not supported. In most cases you will be able to display only the atoms in the file, although it is certainly possible to use point-group symmetry if applicable.

ATOMS is able to use the information on residues which is present in the file, as well as CONECT records, to greatly decrease the time required to locate bonds, compared to standard ATOMS methods for crystals. However, if some bonds are missing from the drawing it may be necessary to uncheck the **PDB quick bonds** box in the Bonds dialog (**Input1** menu), and generate a complete set of standard ATOMS bonds.

Connectivity tables. The PDB connectivity or bonding tables, as derived from the CONECT records in the file, are somewhat problematic as there may be conflict with the bond-locating algorithms in ATOMS, and consequent duplication. Currently, on importing a PBD file ATOMS will query if you want to ignore the connectivity tables - unless there is a special reason for keeping the table(s), it is usually best to do so. If you choose to keep the table(s), or in old ATOMS files which always kept the table(s), the properties of bonds in the connectivity table(s) are given as the first item(s) in the Bonds dialog in the Input1 menu. Deleting one of these items deletes the connectivity table.

Doing the Generated to Input conversion (Transform menu), or adding hydrogens (Atoms dialog in the Input1 menu) will automatically delete any connectivity tables.

3.1.1.2.12 GSAS (.EXP) File

Import GSAS (.EXP) File **[** File menu (Startup) or File menu (Graphics)**]**

See the Import File dialog for general aspects of importing atomic-structure data files.

The General Structure Analysis System can give magnetic moment vectors, and the results for magnetic structures can be given in terms of Shubnikov black/white symmetry. Unfortunately the information on magnetic reversals by symmetry is not given in an intelligible form in the.EXP file, and if the magnetic space group differs from the conventional space group it will be necessary to determine the Shubnikov space group and enter it in the Space Group Symmetry option.

3.1.1.2.13 American Mineralogist File

Import American Mineralogist Structure Database File [File menu]

See the Import File dialog for general aspects of importing atomic-structure data files.

The American Mineralogist structure database is currently available on the Internet at www.geo.arizona.edu/xtal-cgi.test. This may change, but the database should be locatable by searching for American Mineralogist.

3.1.1.2.14 FULLPROF File

Import FULLPROF file **[** File menu (Startup) or File menu (Graphics)**]**

See the Import File dialog for general aspects of importing atomic-structure data files.

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. It may be necessary to

select the Shubnikov symmetry, if the magnetic symmetry is different from the conventional symmetry. Non-commensurate magnetic models are not currently supported (they may be supported if there is interest).

3.1.1.2.15 VIBRATZ Files

Import.MOT or .VBR (VIBRATZ) Files [File menu (Startup) or File menu (Graphics)**]**

Both the.VBR main data files and the.MOT vibrational displacement files from VIBRATZ can be imported. The.VBR files simply contain standard crystallographic information. The remainder of this topic pertains to the .MOT files. See the topic Coordinating ATOMS and VIBRATZ in the Reference section for more information.

When importing either type of VIBRATZ file, ATOMS will read the type numbers modulo 100 - that is, atom types number 6, 106, 206 etc. will all be converted to 6 (carbon).

The.MOT vibrational displacement files are written by the VIBRAT program (Dowty, Phys Chem Minerals, 1987, 14:67) or the Windows version VIBRATZ (available from Shape Software). ATOMS converts the infomation in the.MOT file into a standard.STR ATOMS data file, and also a special.MDT file which contains the atomic displacements and other information for each vibrational mode. When the.MOT file is imported, the first vibrational mode in the list is selected and displayed (after calculation). When you re-read the.STR file, it will contain the information for the vibrational mode in the list which was selected when the file was saved. To see other modes, you must select the Vibrational Modes option in the **Input1** menu. You must recalculate after changing the mode, since new pseudo-atoms and bonds representing vectors need to be generated.

To see on the screen or output which vibrational mode is being displayed, select the **Print title on plot** option in the Title/Axes dialog in the **Input1** menu.

The atoms will be given the default colors specified in the ELEMENTS file, as for other types of import file. However, you have the choice of using radii in the ELEMENTS file (or some fraction thereof - see the Preferences dialog in the Settings menu), or of using constant radii.

Bonds. When importing a .MOT file, bond specifications are taken directly from the VIBRATZ data. If there is a structure in memory, and if there are bonds (Bonds dialog in the Input1 menu), the radius and colors of all the new bonds are taken from the first old bond - if there are no bonds, radius and colors of the bonds derived from the .MOT file will be standard (radius 0.0, black rim, white fill), or from the values of the first bond the last time defaults were saved (Save Defaults in Settings menu).

Crystal import mode. VIBRATZ.MOT data for a crystal can be displayed in either of two ways; showing the atoms in the *primitive* unit cell as a molecule; or using the normal

ATOMS boundary options for crystals. If the choice is a "molecule", there will usually be both primary and secondary atoms (next paragraph). Lattice translation will be disabled. If the choice is to show as a crystal, there will be no secondary atoms, and every translationally equivalent atom will be the same - they will all have the same motion vector. The boundary option will be Unit Cell, current default, but this can later be changed. The atom list (Atoms in the Input1 menu) will include all atoms in the *Bravais* (not primitive) unit cell. With either option, there will be no non-translational symmetry, that is all atoms in the unit cell will be in the atom list.

Secondary atoms (applicable only to crystals imported in molecule mode). VIBRAT uses two types of atoms for crystals or infinite polymers: *primary* atoms, which are just those in the primitive unit cell; and *secondary* atoms, which are those required to complete the bonds and angles of the complete set of internal coordinates (force constants). Often there are more secondary than primary atoms. If you choose to show the structure as a molecule (last paragraph), you have the option to show the secondary atoms in just the same way as the primary atoms; to mark the secondary atoms with a triangle; or to omit the secondary atoms altogether. If you omit the secondary atoms, the bonds to them will also be omitted. Molecules do not require secondary atoms.

The **Vector** button calls up the Atomic Vectors dialog (**Input1** menu), for specification of the details of the vectors which represent the atomic displacements, including the scale factor.

3.1.1.3 Page Setup

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

---Macintosh only ------

Use the Page Margins dialog to set margins.

3.1.2 Settings Menu (Startup Window)

Preferences - Sets parameters for modes of operation.

PostScript Settings - Hardware settings for direct PostScript output.

Pen Plotter Settings - Hardware settings for the pen plotter.

Palette - Modify, save or read the RGB values for the main 16-color palette.

Read Defaults - This reads structure display parameters, mostly those in the **Input2**

menu, from a setup file. These will replace those currently in memory.

Save Defaults - This saves structure display parameters, mostly those in the **Input2** menu, for use when inputting a new structure with the New command in the File menu, or when a standard set of parameters is desired.

3.1.2.1 Preferences, Operation Tab

Dialog Box: Preferences - Operation Tab [Settings Menu**]**

See also Preferences - Constants Tab.

Sounds. This turns on or off the sounds emitted by ATOMS, for example at the beginning and end of calculation and/or plotting (some system sounds are unaffected).

Draw into buffer. If this box is checked, the image is drawn into an off-screen memory buffer, and then copied to the screen. If not, the drawing is made directly to the screen, and then copied afterwards into the buffer. Drawing into a buffer is usually faster, but the difference may be small. No memory is saved by not checking the box, since the buffer is always used anyway for refreshing the window after another window is draw over it.

Confirmatory alerts in New input. If this box is checked, during input of a New structure file (**File** menu), after every input dialog there is an alert or dialog box (Entering New Data Set) giving the choice of proceeding to the next dialog, aborting data input, or revising the last dialog. Without these dialogs, there is no escape from the sequence of Input1 dialogs, and no escape from the sequence of **Input2** dialogs.

Calculate query on file open. If this box is checked, you are asked if you want to calculate the structure - if not, the structure is calculated as soon as it is read in.

Scale lettering to screen. If this box is checked, in printed output or output to a file, the labels in that output will be scaled to approximately the same relation to the drawing itself as on the screen. This is a very approximate process, and trial-and-error adjustment will still be necessary to get the desired label sizes in output. This option should be thought of as adjusting the labels on the screen to look similar to those in the output, rather than the other way around.

Screen start-up. This sets the color/black-and-white state of the screen at start of ATOMS. It can be changed with the Color command in the **Display** menu.

Mark selected atoms. This refers to selecting atoms in the screen plot with the mouse. If **Show last** is selected, the last atom selected is outlined in a contrasting color, but this marking disappears when another atom is selected, or an empty area is clicked. If **Show all** is selected, all markings remain until a Replot.

Skeletal mode during interactive rotation. When rotating using the mouse cursor, ATOMS can switch to a Skeletal mode so as not to slow down the motion. When starting in 3D mode, the 3DSkeletal mode is used. This is not usually necessary when the number of atoms is small as the redraw is usually fast enough, so the best choice may be "**If more atoms than**". The number of atoms may be 100 or so, but this will depend on the speed of your system.

Skeletal mode choice. Starting with V5.1 of ATOMS there are two possible methods of drawing in Skeletal mode. In the **Bond colors** or "old (pre V5.1)" mode, all atoms are shown as small dots, except those in polyhedra; all bonds are shown as lines using bond colors (either fill or edge colors as selected in the next item), and polyhedra are shown by lines joining the corners (outlining the faces). The lines indicating polyhedron edges use the polyhedron fill colors. In the **Atom colors** or "new" mode the bonds are shown in the colors of the two atoms (fill color), half-and-half. Polyhedron edges are not shown; instead the central-ligand bonds are shown.

Color for line bonds. When in the Skeletal drawing modes (**Bond colors** option above), and when bond radii are 0.0 in the Standard drawing mode, the colors for lines representing bonds may be either the rim or fill colors given in the Bond Data dialog.

3.1.2.2 PostScript Settings

Dialog Box: PostScript Settings [Direct Postscript Output Dialog**] [** Settings Menu**]**

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.

The Transfer Function is analogous to the PostScript function of the same name. The linear option is standard; modify the function to get lighter or darker shading in PostScript print-out.

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.

Background color. If this option is on, the color selected in the Background Color dialog of the Input2 Menu will be applied in color output only. Background in b/w output is always white.

Atom algorithm. ATOMS shows shading for atoms by computing concentric zones around the point of emergence of the illumination vector. This can be done in two ways:

1) For non-PostScript display and output, points are calculated on lines radiating outward from the point of emergence. This means that the curves defining atoms and atom shade zones are defined by a large number of short line segments - this is called the "lengthy" algorithm. 2) The default algorithm for Postscript, called the "compact" algorithm, simply sends the parameters for the circle and ellipse segments which make up these curves (this cannot be done for normal drawing because the system drawing routines do not deal with general ellipses). The lengthy algorithm typically requires twice the disk space as the compact algorithm for shaded atoms. The compact algorithm is also more precise in its drawing of curves, and it allows all illumination vectors (for the lengthy algorithm, the point of emergence of the illumination vector must be within the atom outline, which may be truncated by interpenetrating atoms or large stick bonds). The only case in which the lengthy algorithm might be necessary is when three or more atoms interpenetrate, so that the segments removed from the outline of an atom overlap. This condition in principle could also arise if two stick bonds to an atom overlap.

---- 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 ATOMS).

3.1.2.3 Preferences, Constants Tab

Dialog Box: Preferences - Constants Tab [Settings Menu**]**

See also Preferences - Operation Tab.

Increment for drawing circles (degrees). Arcs of circles are drawn with line segments at specified angular increments (full circles are drawn with system routines). Ellipses are also drawn with proportionate line segments, although the increments are variable. The default circle increment of 12.0 degrees has been found to give satisfactory results for laser and pen-plotting, provided atoms are not too large. Making the increment smaller may improve the appearance, at a penalty in plotting time, especially if your computer has no math coprocessor or you are using lines of finite width.

On-screen rotation increment (degrees). This is the amount by which the image is rotated in the Dialog Bar - Left. This is the value which exists when ATOMS is started; this value and not the latest value in the dialog bar itself is saved on quitting ATOMS.

On-screen displacement increment (Angstroms). This is the default amount by which a structure fragment is translated in the Dialog Bar - Fragments (**Display** menu). This is the value which is in the dialog when it is first called; this value and not the latest value in the dialog itself is saved on quitting ATOMS.

On-screen rescaling factor (%). This is the default amount by which the drawing is rescaled with the **Scale** button in the Dialog Bar - Right (**Display** menu). This is the value which is in the dialog when it is first called; this value and not the latest value in the dialog itself is saved on quitting ATOMS.

Default radius for atom location (Angstroms). When identifying atoms with the cursor, the given atomic radius is used for deciding when the mouse is clicked "on" an atom. However, if the input radius is zero or negative (denoting either polyhedral atoms or wire-frame atoms), this default radius is used instead.

Factor for scaling to screen or frame. In either the Maximize or Universal scaling modes (Scaling dialog, Input2 menu), the image is scaled to almost fill the screen or frame. This factor specifies how close the image comes to the edges. This scaling is not precise when Perspective projection is used, so a relatively smaller factor may be necessary if the perspective distance is small.

Dash length and dash ratio. The dashes are used for back edges of crystals (Crystal Edges and Faces) and in display of Crystal Axes and Unit Cell. Length or repeat distance is in inches/centimeters, and the length factor is the actual length of the solid part divided by the repeat distance. Note that when using Frames in output the dash length remains the same - it may be desirable to decrease the length for very small plots.

Atomic radii. One or the other of the two files, ELEMENTS.ION,ionic radii, or ELEMENTS.COV, covalent radii, is used during input of Import files and input of atomic parameters through the Input Atoms dialog (see ELEMENTS files). The **Factor** multiplies the full radius values during this input. Values of around 0.5 are appropriate for ball-and-stick display, while values well over 1.0 may be required for interpenetration (space-filling).

Scaling units. This sets either inches or centimeters as the units for overall use in ATOMS. This choice may be locally overridden for printing or other output by the **Units** setting in some of the dialogs involved.

3.1.2.4 PostScript Transfer Function

Dialog Box: PostScript Transfer Function [Postscript Settings dialog**]**

The **Transfer Function** is analogous to the PostScript function of the same name. It changes the nominal gray values (0.0-1.0 for black-white) calculated by ATOMS as true illumination to values actually output. (Note that the PostScript gray scale, 0.0-1.0 for black to white, is in the opposite direction to the ATOMS gray scale, 0-15 for white-black; the transfer function applies to the Postscript gray scale.) If your printer gives gray shadings that are too dark (this is common, especially for lighter shades), you can increase the output values. Values in between the listed values are linearly interpolated.

The actual gray values output to the printer or EPS file are changed; the transfer function itself is not part of the EPS file. Note that the gray-scale conversion also applies to lines of greater than single-dot width (single-dot lines are always black).

3.1.2.5 Pen Plotter Settings

Dialog Box: Pen Plotter Settings [Pen Plot dialog**] [** Settings Menu**]**

Current plotter radio buttons. There are several pre-programmed plotters; clicking on the Get Data button reads the pen-plotter data file (PPLOT) and obtains the commands and parameters. Even if your plotter is not listed here, you may be able to input the commands through the **Other** option. In this case, click on the Commands button to set or revise the commands and parameters.

Pen-change mode radio buttons. If you have a multiple-pen plotter, you can elect to run in the **Use single pen** mode with the pen number entered in the edit field, and conversely if you have a single-pen plotter you can draw with multiple colors, but you will have to change the pens manually. If you choose the **Change pens manually** mode, the plotter returns to the zero position after drawing all lines of each color, and a message box appears, prompting you to change pens.

Blank border. A blank border can be added to atoms, bonds and polyhedra in the pen plot in order to increase the illusion of depth. Lines which are part of atoms, etc., "behind" the atom in question are cut off when they get within the specified distance of the atom, etc. which is in "front". This option may add considerably to the plotting time, since it involves much recalculation. If the width of the border is set to 0.0, there is no recalculation.

Speed number. This is the parameter (see Commands) which controls velocity of the pen - for example for the Comrex, speed number 1 is slowest and 15 is fastest. Although some plotters, like the HP7475A, allow decimal speeds, you must use an integer here.

---- Windows only ----

Port. This should be either a serial or parallel port: "COMn" or "LPTn". Even if this box shows the correct port, if it is a serial port you should verify the baud, parity, stop bits and data bits in the **Ports** item in the Windows **Control Panel**. These parameters should be set to match the settings on your pen plotter (which are usually controlled by DIP switches).

3.1.2.6 Pen-Plotter Commands and Parameters

Dialog Box: Pen-Plotter Commands and Parameters [Pen Plotter Settings dialog**]**

This allows you to enter or revise the pen-plotter commands and parameters, for non-standard pen-plotter types.

It is assumed that the plotter accepts ASCII commands that follow a simple syntax of "command, parameters, terminator". For example, the Hewlett-Packard command for moving the pen, raised, to the coordinates x,y is "PUx,y;". "PU" is the command, which should be entered (without parentheses) in the text box **Move - pen up**: x and y are the parameters, which are always supplied internally by ATOMS; and the semicolon is the terminator required in the **Terminator** text box. Commas between parameters are also supplied by ATOMS. **Move - pen up** means move to the new coordinates with the pen up (not marking).

You must enter or edit the commands in the text boxes on the left of the dialog. If more than one command is required to perform the operation requested, give all the commands with any intermediate parameters and terminators required, but omit the last terminator. If your plotter does not use a command, just leave that field blank.

Following are comments on the plotter inputs. The type of variable required, and the maximum number of characters in case of a character variable, are given in parentheses. View samples by clicking on the selections in the **Current Plotter** group in the Pen Plotter Settings dialog.

Commands

Move - pen up. (6 chrs) Move to the new coordinates with the pen up.

Move - pen down. (6 chrs) Move to the new coordinates with the pen down.

Raise pen. (6 chrs) Raise the pen without movement.

Pen speed. (6 chrs) This is the command which causes pen speed to be set or changed; the parameter is entered as a separate item in the Pen Plotter dialog menu.

Change pen. (6 chrs) This is required only for multi-pen plotters.

Start plot. (12 chrs) Initialize the plotter. May require no commands, or several.

End plot. (12 chrs) Terminate plotting. Like (12).

Terminator. (2 chrs) The character which signals the end of a command. In most cases the semicolon.

Parameters

Maximum x/y. (Decimal) Maximum x and y coordinates. These values establish the centering of the plot. Increments on the x and y axes are assumed to be equal.

x/y at finish. (Decimal) The "base" coordinates, in plotter units, to which the paper or pen will be returned at the end of the plot, or when pens are to be changed manually.

Units/inch(or centimeter). (Decimal) This establishes the resolution of the plotter and is used in scaling. If your plotter instructions do not give this number, divide the maximum x or y coordinate (item 1 above) by its length in inches.

3.1.2.7 Palette

Dialog Box: Palette [Settings Menu**]**

The Palette is used to set up a 256-color palette for 8-bit screen display or raster output, and also to set the primary choices for color in all cases (you can always select other colors using different RGB values). See Colors, Palettes and Dot Patterns for more detail. The default **Main** palette has the same RGB values as the "alternate" palette used in DOS versions of ATOMS, but rearranged to a more logical order.

You can read and write values to palette (.PAL) files. Two palettes are provided on file: STANDARD.PAL and ALTERNATE.PAL, which are respectively the standard IBM palette and the default alternate palette used in DOS versions of ATOMS. It is easy to write or modify the.PAL files directly; they simply contain the RGB values, from 0 to 255, separated by spaces (or commas).

The **Default** button will reset the palette to the current default values.

3.1.2.8 Read/Save Defaults

Read and Save Defaults Commands [Settings Menu]

When inputting data for a drawing with the New command in the File menu (Startup) or File menu (Graphics), you can elect to use default values for display parameters, rather than set these in the dialogs of the Input2**menu** . If no data set is in memory, the default display parameters are always read from disk; and if there is a data set in memory, you can use the current values or read the defaults from disk.

Also, when importing a file (File menu (Startup) or File menu (Graphics)), you have the choice of reading in the saved parameters or using the current ones.

Also, if you desire to convert the current parameters, which may have been read in from a.STR data file, to the standard set, you can use the **Read Defaults** command at any time.

The **Save Defaults** option saves the current display parameters, i.e. most values in the dialogs of the Input2 Menu and some in the Display Menu.

3.2 Graphics Window Menu Bar

File menu - In addition to the usual **New**, **Open**, **Print** etc., this menu has commands for listing input and generated data, and for for PostScript, pen plotter, raster or bit-map and Metafile or PICT output.

Modes menu - This allows setting the Display mode, and the Cursor mode.

Input1 menu - This contains dialogs involving mostly the basic data for the structure, such as axes (unit cell), atom coordinates, etc.

Input2 menu - This contains dialogs setting display parameters specific to each structure.

Display menu - This contains commands and dialogs which set the overall display attributes of ATOMS, and modeless dialogs for rapid rotation and displacement of the structure.

Rotation menu - This contains several options for rotating and aligning the structure.

Transform menu - This contains specialized options for converting generated to input atoms, locating groups and dealing with multiple structure fragments.

Settings menu - This contains settings for hardware, palettes and preferences for modes of operation.

Window menu - This contains commands relating to the display or activation of the different kinds of windows - the main Graphics window, diffraction Graphics windows and Text windows.

Help menu - On-line help.

3.2.1 File Menu (Graphics Window)

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

Open - Open an old ATOMS data file.

Close - Close the current graphics window.Startup Menu Bar

Save - Save an ATOMS data file.

Save as - Save an ATOMS data file with a new name

Open Recent File Select from most-recently-used files.

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 etc. from almost any source.

Export File - This will write a file in one of several molecular formats, containing labels and Cartesian coordinates of the *generated* (not input) atoms. Some files may also have bond tables and other information
Calculate - Reproduce atoms within specified boundaries and locate bonds and polyhedra.
Print - Print out the graphics image; see **List...** commands below for listing data and calculation results, and Calculation Output in the **Input2** menu for listing results of the calculation.
Page Setup - Set the page size and select the printer.
Listings group - the following four commands are in a secondary pop-up menu
List Input - List all input data parameters to the file INPUT.ATD and to a Text window.
List Generated Atoms - List all generated atoms to the file GENATOMS.ATD and to a Text window.
List Faces - List all generated faces to the file FACES.ATD and to a Text window.
List Totals - List various totals, such as generated atoms, bonds, etc., to the file TOTALS.ATD and to a Text window.
Output group
PostScript -

Direct output to a PostScript printer (Windows only) or to an EPS file.
Pen Plot - Output to a pen plotter or HPGL file.

Raster Files - Writes raster or bit-map files in.BMP,.PCX,.TIF or.PNG (Windows) or.PNG (Macintosh) format.
Metafiles (Windows) or PICT (Macintosh) - Writes metafiles or PICTs to the clipboard or disk files.
Save Graphics Window - Dumps the exacts contents of the Graphics window to the clipboard or a file (.BMP format for Windows or PICT for Mac).
VRML Files - Writes output in the Virtual Reality Modeling Language 3D format.
POV-Ray Files - Writes output for the ray-tracing program POV-Ray.
Exit - Quit ATOMS.

3.2.1.1 New command

The New command in the File Menu of the Graphics Window is identical to the New command in the File menu of the Startup Menu.

3.2.1.2 Open command (Graphics)

Open command (File menu (Startup) or File menu (Graphics)**)**

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

Use this command to open an existing ATOMS data file. After the file has been read in, you are asked if you want to calculate immediately (this query can be eliminated with a checkbox in the Preferences dialog, **Settings** menu). If you reply OK, the structure will be plotted in the Graphics window. If you decline to calculate immediately, you can modify the structure or display parameters. When finished, use the Calculate command in the File menu.

You can create a new ATOMS data set with the New command, or import various kinds of files from

other software with the Import command.

3.2.1.3 Save command (Graphics)

Save command (File menu**, Graphics window)**

When called from the Graphics window, this saves the active data set to its current name and directory. If you have changed the orientation from that specified in the Initial Orientation dialog in the **Input2** menu, you are asked if you want to save the current orientation. If you choose to do this, the current orientation will be converted to initial orientations on the observer x, y and z axes

When you save a data set for the first time, ATOMS displays the **Save As** dialog box so you can name your data set. If you want to change the name and directory of an existing data set before you save it, choose the Save As command.

3.2.1.4 Save As command (Graphics)

Save As command (File menu**, Graphics window)**

When called from the Graphics window, this saves the active data set. ATOMS displays the **Save As** dialog box so you can name your data set.

If you have changed the orientation from that specified in the Initial Orientation dialog in the **File2** menu, you are asked if you want to save the current orientation. If you choose to do this, the current orientation will be converted to initial orientations on the observer x, y and z axes

To save a data set with its existing name and directory, use the Save command.

3.2.1.5 Close Command (Graphics)

Close Command [File menu (Startup) or File menu (Graphics)**]**

When exiting ATOMS, closing the graphics window, reading another file or starting a new file, ATOMS tries to determine if you have made any changes in the structure currently in memory; if so, you are asked if you want to save the file.

First, it checks whether the orientation has changed from the Initial Orientation established during calculation. If so, you can save the current orientation as initial rotations. It also checks whether any dialog in the **Input1** and **Input2** menus have been opened, or whether there has been any change in the status of atoms marked for non-plotting (see Deleting Atoms).

3.2.1.6 Import Files Submenu

The **Import Files** submenu in the **File Menu** of the Graphics Window is identical to the Import Files submenu in the Startup Menu.

3.2.1.7 Export Atom Data File

Dialog Box: Export Atom Data File [File menu**]**

This exports the current *generated* atom data, with Cartesian coordinates, to a choice of molecular file formats.

ATOMS does not necessarily write a complete file for any particular format since it may not have all the information required - manual editing may be necessary. If an elemental symbol is written it assumes that the type number (modulo 100) is the atomic number.

Export: As drawn/All generated atoms. If you choose **As drawn**, the atoms in the file will be just those shown on the screen, excluding atoms in incomplete polyhedra, atoms

marked for non-plotting, etc. **All generated atoms** will export all atoms within the current boundary.

Strip non-alphabetic characters from label. This will end the label string at the first non-alphabetic character. Some programs are not able to identify the element from labels like "C1", "O12", which are common in crystallographic files.

Convert polyhedra to bonds. This will export bonds between the central atom and the ligands of any polyhedra. Not all export formats have bond specifications.

PDB files. The space-group symbol in the CRYST1 record is not necessarily in the form required by PDB and may need to be edited. The standard crystal-Cartesian orientation in PDB files is a = x and c* = z, whereas in ATOMS it is a* = x and c = z. If the crystallographic orientation is important it may be wise to reorient the crystal in ATOMS to the standard PDB orientation. This can be done in the Align Face or Vector option in the Rotation menu. Orient on vector [100], with alignment face (001).

ATOMS does not directly export crystallographic file formats. However, the shareware program **Cryscon**
(Shape Software - www.shapesoftware.com) can convert among several crystallographic formats, and write files such as CIF from ATOMS data.

3.2.1.8 Calculate Command

Calculate Command [File menu**]**

This may need to be used whenever an "intrinsic" or "input" parameter of the structure, including most items in the **Input1** menu, is changed. For parameters which affect display only, such as atom, polyhedron or bond colors and items in the **Input2** menu, use the Replot command in the **Display** menu or the **Replot** button in the Dialog Bar - Left. Changing atomic radii does not require recalculation as long as stick bonds are not changed to interpenetration or vice-versa.

With Version 6.1, there is a change in orientation behavior on the use of this command. In previous versions, Calculate always completely reoriented the structure, returning to the Initial orientation. Now, the current orientation is retained. If you wish to return to the Original or Initial orientation, use the buttons in the Dialog Bar-Right, or the command Save-Recover Orientation in the Rotation menu.

3.2.1.9 Print Graphics Image

Dialog Box: Print Graphics Image [File menu**]**

------ Linux only ---------

PostScript printing is standard in Linux, so for non-3D output, including diffraction diagrams, printing is handled by the Direct PostScript option, not by the dialog below. However, for 3D output (including Cavity mode) printing is controlled by this dialog.

------- Windows only----------

This command is for normal printer output through the printer driver (see below). If you have a PostScript printer, you should probably use the PostScript command in the **File** menu rather than this one for non-3D images; that command sends PostScript language commands directly to the printer, bypassing the printer driver. The PostScript language has a few capabilities which are missing from the system routines. Using Direct PostScript output may give somewhat different, and usually more correct colors, than using the Print option (although color inaccuracies may possibly be fixed by changing the settings of the printer driver in the Page Setup command).

In the case of 3D images (that is printing while in the 3D Display mode), ATOMS does not send drawing commands to the printer - rather the entire drawing (or sections thereof) must be imaged in memory, and this raster or bitmap image is sent to the printer.

------ Macintosh only ----------

Three different **Print Modes** may be used, depending on the settings in this dialog and the ATOMS display mode - 1) Standard or QuickDraw, 2) Direct PostScript or 3) Bitmap.

Option 1) sends standard QuickDraw graphics commands (the same as those used for the screen) to a printer driver, which may be supplied by Apple or the printer manufacturer. The printer then makes the image in its own memory. You select the printer or printer driver in the **Chooser** option in the **Apple** menu (OS 8/9) or in the **Print Center** (OS X). This option sometimes results in poor quality output, with too-thick or irregular lines, patterns at a scale of 72 dpi instead of the true printer resolution, or incorrect colors. If this happens try one of the other options.

If you have a PostScript printer, for non-3D output you should probably select the **Direct PostScript** option - this causes ATOMS to send PostScript language commands to the printer instead of the QuickDraw drawing commands, although these commands are transmitted through the currently-selected printer driver. Some printer drivers, especially the standard LaserWriter drivers, may not print at the maximum resolution of the printer without this option. Note that direct PostScript printer output is only supported through this option, not through the PostScript item in the **File** menu. The **Pattern Series** selection is ignored - patterns are determined by the Printer.

Option 3) forms the image in memory, then sends it as a bitmap to the printer. This option is always used for 3D Display modes. This method may be very slow, but often

gives higher quality than option 1).

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

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 or in some cases the resolution. The orientation (portrait or landscape) can also be set in the Page Setup dialog in the **File** menu.

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 Page Setup option in the File menu. Background applies only to color printing; for black-and-white printing the background is always white (although you could print on black paper).

See Frames for details of the frame and frame units.

In this print option, for non-3D images, ATOMS sends standard graphics commands to the operating system, which passes them on to the *printer driver*, a piece of software which is normally written by the printer manufacturer (but sometimes by Microsoft in the case of Windows). For color printing, it is standard to send RGB values to specify colors for lines and files, and for black-and-white printing, it is standard to send gray-scale values (actually, RGB values with all three components equal). The printer driver interprets these values in terms solid areas and/or dot patterns of ink on the paper. No color printer can print all colors as solid areas; traditional printing uses as few as three or four colors, most commonly cyan, magenta, yellow and black, intermixed or dithered in dot-patterns to produce a full range of colors. Microcomputer printers may use more colors, but the principle is the same, and dot density is typically lower than in traditional printing, so it may be important to select colors which are as simple as possible in terms of red, green and blue or cyan, magenta and yellow (see Colors, Palettes and DotPatterns).

Use ATOMS b/w patterns - Pattern Series. Black-and-white printer drivers must interpret the gray values for fills as dot patterns of varying density. The patterns supplied by the printer driver may or may not be satisfactory for the ATOMS user. Rather than send gray-scale values for fills, ATOMS can also send its own dot patterns, which have been carefully designed for its purposes. The **Fine** series is appropriate for small drawings which will not be reproduced photographically. The **Coarse** series simulates halftone screening and is appropriate for photographic reproduction. To be precise, at a printer resolution of 300 dots per inch, most of the patterns have a screen density of 53 lines per inch, at 45 degrees; this is about half the density of typical standard printing, so a reduction of about a factor of two is generallly satisfactory. Of course, different printer resolution would dictate different reduction factors. Note that this coarse/fine setting is

the same as that in the Raster and Metafile or PICT files dialogs in the **File** menu.

------ Macintosh only ----------

ATOMS patterns are always used for b/w printing, but they may be rescaled or otherwise changed by the printer driver.

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

Actually, different printer drivers may interpret the standard gray-scale commands in terms of patterns which are similar either to the fine or coarse series supplied by ATOMS. Some may convert the ATOMS patterns to their own patterns, and some may not accept the ATOMS patterns at all. Some may offer their own choice of pattern types or densities (typically in the printer dialog above or the Page Setup dialog in the **File** menu). Thus some experimentation may be necessary to find the best choice for patterns (i.e. printer-driver patterns, fine ATOMS patterns; or coarse ATOMS patterns). Gray lines of greater than one-dot width are always drawn by filling an outline with one of the ATOMS patterns - gray-scale values are not used because many printers will not print gray lines. Thus the coarse/fine setting is always used for wide b/w lines.

Maximum memory. This is used only when printing in bitmap mode, which is always used for the 3D display mode. Operating system support for printing in 3D mode is incomplete, and ATOMS itself must therefore draw raster or bitmap images and send these to the printer, rather than relying on the printer driver. Memory considerations similar to those involved in Raster Files therefore come into play.

Both Macintosh and Windows operating systems use *virtual memory*, which means that they pretend that a hard disk can be used in place of actual hardware memory chips. For some purposes this is useful, but when writing raster files it usually results in "disk thrashing", or constant reading and writing of data to the hard disk.

ATOMS 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 the operating systems do not provide this information in a useful way. Thus the user may need to determine this by trial and error using the **Maximum memory** parameter. This is the same parameter which is set in the Raster Files dialog.

When the **Maximum memory** parameter is set to zero, ATOMS will simply ask the system for a block of memory large enough to image the entire drawing at once. If this amount of memory is greater than the amount of chip memory which is made available by the system (and this may be considerably less than the actual amount of chip memory in the computer), the operating system will use virtual memory, which is typically

manifested by disk thrashing. If you change the **Maximum memory** to some amount less than that require for the image (say half), ATOMS 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, ATOMS 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.

3.2.1.10 Page Setup

The **Page Setup** dialog box in the **File Menu** of the Graphics Window is identical to the Page Setup dialog in the File Menu of the Startup Window

3.2.1.11 Listings Group

This submenu allows listing, in Text Windows, of Input Data (below), Generated Atoms, Generated Faces and Totals with memory usage.

Dialog Box: List Input Data [File menu]

This lists out the input data to a Text Window (see Types of Windows). The categories selected by the check boxes correspond to the various dialogs in the Input1 and **Input2** menus.

The Generated Atoms list gives a symmetry number (Symm.) which can be correlated with the list of symmetry operations, or equivalent positions of the general equipoint, in the Input/Symmetry listing. This number, in roman numerals, can be shown as a superscript on the Atoms Label (Display menu).

3.2.1.12 Direct Postscript Output

Dialog Box: Direct Postscript Output [File menu]

------ Linux only ---------

PostScript printing is standard in Linux, so for non-3D output, including diffraction diagrams, printing is routed to this dialog, not the Print Graphics command in the File menu. Output can be directly to the printer or to an EPS file, as for Windows (below).

---- 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 Linux/Windows/Macintosh only ----

In 3D Display modes, ATOMS always writes data (or sends it to the printer) in the form of a bitmap (or "image" in PostScript terminology). Because of the facts that PostScript files must be ASCII (text), and that efficient data-compression schemes (other than the copyrighted LZW) are not supported in PostScript level 2, PostScript files for 3D drawings tend to be much larger than the best Raster formats, especially PNG. Thus the PNG Raster format is generally preferable for all 3D Display mode drawings.

The **Maximum memory** setting limits the amount of memory used for bitmap buffers when in the 3D mode - see the Raster section for further details. The number of pixels on each raster line must be divisible by four - the image width will be increased if necessary to achieve this.

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 Title/Axes, Atom Labels, Bond Labels, Axes/Unit-Cell or Magnetic Labels 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.

3.2.1.13 Pen Plot

Dialog Box: Pen Plot [File menu]

---- Windows only ----

This option can be used to send commands directly to a pen plotter, provided the plotter is connected to one of the standard parallel or serial ports, or to write files such as **HPGL** which may be read by other software.

---- Macintosh only ----

This option writes pen-plotter-language files such as **HPGL** which may be read by other software.

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

On first using this command, be sure to click on the Settings button to set or verify the characteristics of the plotter.

To write **HPGL** files, click on the Settings button and make sure that the plotter selected is "HPGL plotters".

See Frames for details of the frame and frame units.

3.2.1.14 Raster (Bitmap) 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 Clipboard/PICT 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.

Using colors other than white, black or gray for background may result in increased size of raster files or PostScript files in 3D modes. In some cases a simple run-length-encoding method is used for compression of these files (see below), and this fails for 24-bit RGB (true color) files when the three components are not identical. That is, for a row of white pixels the sequence of bytes is 255, 255, 255, 255... whereas for a row of red pixels it is 255, 0, 0, 255, 0, 0...

The images will look much the same as a screen image, except that for black-and-white files gray shades are always rendered as dot patterns, and there is a choice of coarse or fine patterns, as for printing (see the Print dialog in the File menu). Fine patterns are appropriate for small images which will not be reproduced photographically, or for images which will be shown on the screen only; coarse patterns mimic halftone screens used in printing, and generally reproduce better photographically, especially when the image is reduced in size. Note that this coarse/fine setting is the same as that in the Print and Metafiles or PICT files dialogs in the File menu.

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 pretends 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.

ATOMS 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 or NT) 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, ATOMS 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), ATOMS 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, ATOMS 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 ATOMS 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 ATOMS (although 3D images do not compress as well as standard-mode images). 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 ATOMS does not use this type of compression because of the copyright problem. The run-length-encoding which ATOMS 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 ATOMS to support all of them. ATOMS 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) has links to many shareware and conventional commercial conversion packages.

3.2.1.15 Clipboard/PICT (Mac)

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. For the 3D Drawing mode, this option writes a two-dimensional image and only bitmaps are available, but see the VRML Files and POV-Ray options for files which actually contain three-dimensional data

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 file** format (File menu), which is superior is 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.

Background color. If this option, which applies only to PICT output, is on, the color selected in the Background Color dialog of the **Input2** menu will be applied in color output only. Background in b/w output is always white.

In the 3D drawing mode PICT (bitmap) output always has 32-bit pixel depth.

See Frames for details of the frame and frame units.

3.2.1.16 Metafiles (Windows)

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. A metafile image may either be saved in the Clipboard, to be Pasted into another application, or written to a file.

ATOMS can write three types of metafiles. The original or **Standard** metafile format has proven inadequate for transmitting scaling information, and many applications do not even accept Standard metafiles. **Placeable** metafiles, a format which was originated by Aldus Corporation, contain scaling information in an additional header. The standard and placeable metafiles have the .WMF extension. WMF or standard files are 16-bit format, i.e. use 2-byte integers. **Enhanced** metafiles are 32-bit format files which also contain scaling information. They are the preferred type of metafile for use in 32-bit Windows systems (Windows NT or Windows 95), but cannot be used in standard 16-bit Windows 3.1or Win32s.

Original (16-bit or .WMF) metafiles can be written with either of two Scaling Modes; Isotropic or Anisotropic. Isotropic supposedly keeps the same proportions. Generally, Isotropic is the best as it allows rescaling while preserving proportions. However, some applications only accept Anisotropic files, and some ignore the scaling mode completely.

The type of image written by this option is strictly two-dimensional. It is also possible to write files containing three-dimensional images with the VRML Files and POV-Ray options.

When writing to a file, to prevent loss of resolution, ATOMS uses a standard scaling of 2540 dots or pixels per inch (1000/cm). However, some drawing applications may not

read the scaling correctly (assuming 72 dpi) and it may be necessary to rescale the drawing after importation.

When writing to the clipboard, ATOMS uses the current screen resolution, which usually is about 92 dpi. This is because most drawing applications assume screen resolution or 72 dpi. The clipboard image can be either 16-bit (.wmf) or 32-bit (.emf) according to the setting of the **Type** option.

See Frames for details of the frame and frame units.

Limitations of Metafiles. As designed and implemented by Microsoft, the metafile allows recording of all Windows drawing commands, so that a file image can be a copy of what is shown on the screen but rescalable. Unfortunately non-Microsoft drawing applications (e.g. Corel Draw, Adobe Illustrator) sometimes implement metafiles incompletely or incorrectly so that there are some limitations in metafiles written by ATOMS, in order to allow them to work in as many applications as possible. It many be necessary to try many combinations of settings (Destination, Scaling mode, Type of file) to get satisfactory results in an importing program.

1) Resolution for the clipboard is now that of the screen, typically 72-96 dots-per-inch (dpi) - earlier versions of ATOMS used 2540 dpi. The lower resolution should not cause problems except for very complex drawings - if a drawing looks good on the screen, it should look good in a document. If the clipboard is unsatisfactory use a file.

2) ATOMS bitmap patterns for black-and-white images cannot be used. Fills are transmitted as gray shades which are interpreted by the importing application and/or printer.

3) A background is always present, to insure correct scaling. With some care, this drawing element may be removed in importing applications.

4) There is no clipping of the image, although some importing applications may use the drawing frame for clipping. For ATOMS structure drawings this will usually only cause problems if the fixed scaling mode is used, and parts of the drawing extend beyond the frame. For Powder and Precession graphs, the title lettering may extend beyond the frame. In some importing applications (e.g. Corel Draw) it may be necessary to reset the size and/or proportions.

5) Transmission of the image in Corel Draw with the Clipboard may require use of Edit/Paste Special rather than a simple Paste.

6) Adobe Illustrator generally does not do well with labels - is may be necessary to use an EPS file for Adobe Illustrator. Label backgrounds may not be transmitted in other applications.

7) Some drawing applications may alter atom outlines and other curves in ATOMS, apparently attempting to "smooth" them. This is especially likely if a clipboard image is expanded (made larger) - in this case try a file instead.

If a metafile is not satisfactory, a raster file can be used. PNG raster files are often smaller than metafiles, especially for complex drawings. Also, many drawing programs now support import of EPS (Direct PostScript) files. EPS is usually the preferred type of file for Adobe Illustrator.

3.2.1.17 Save Graphics Window

Dialog Box: Save Graphics Window [File menu**]**

This command writes a bitmap giving *exactly* what is shown *inside* the current graphics window.

This option is appropriate for applications which will use the image on the screen. For applications which will use a printed or other high-resolution image, either the Raster Files or Metafiles (Windows) or PICT (Macintosh) options will usually give better results.

---Windows Only ---------

This will save a Device-Independent-Bitmap (DIB) either to the clipboard or to a.BMP file.

You can also copy the current window to the clipboard with the **Print Screen** key (this is a standard Windows function). However, this includes the window title bar and border and parts of overlapping windows, whereas the **Screen to Bitmap** command only copies the graphics part or the client area.

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

This will save a PICT file as raster, or put the image in the clipboard.

---End Windows/Macintosh Only --------

3.2.1.18 VRML Files

Dialog Box: VRML Files [File menu**]**

Virtual Reality Modeling Language files were intended for exchange of virtual reality data on the Internet. However, they have become a *de facto* standard for interchange of 3D data of all types.

ATOMS currently supports V1.0 ascii files.

VRML files can be viewed with Internet browsers for either Windows or Macintosh, using plug-ins such Cosmoplayer (www.cosmosoftware.com). Since the files are text, they can also be viewed on SGI and other UNIX systems. 3D Exploration (www.righthemisphere.com) is a stand-alone viewer for Windows which is independent of Internet browsers.

Most of the settings for 3D display mode (3D Parameters dialogs, Input2 menu) apply to VRML files, although there is little control of lighting (the viewer application or plug-in usually controls this, although most viewers offer few choices). Thermal ellipsoids may be drawn in VRML files, as selected in the 3D - General dialog or the Ellipsoid Parameters dialog, Input2 menu. Thermal ellipsoids are always solid, without the cut-out octant which is possible in direct screen or print drawing, and bonds are always cylindrical, not tapered.

If the buttons in this dialog are used to change 3D settings, these changes will also apply 3D Display mode on screen and in output.

For the latest information on crystallographic and molecular-modeling applications of VRML see http://193.49.43/dif/3D_crystals.html or http://fluo.univ-lemans.fr:8001/vrml/intvrml.html.

3.2.1.19 POV-Ray File Output

Dialog Box: POV-Ray File Output [File menu**]**

POV-Ray is a program which draws a 3D image pixel-by-pixel, calculating all possible light-ray paths. It allows for much more elaborate lighting effects than the OpenGL software used in the 3D mode in ATOMS. Some obvious effects are shadows and refraction but there are many possibilities. Backgrounds and other objects may be added as well. The files are text (ASCII) and may be edited.

Since the calculation is much more elaborate than that done by OpenGL, this is not a method that can be used for real-time display on the screen - POV-Ray images may take many minutes to complete.

The POV-Ray package, with instructions, samples, etc., may be obtained from www.povray.org.

While adding shadows to ball-and-stick or space-filling structure drawings may make them more "realistic", it also may tend to complicate things. Shadows are usually most beneficial to Cavities mode drawings of crystals. The default output from ATOMS has shadows, but this can be changed by adding the keyword "shadowless" after the color definition in the "light_source" definition near the beginning of the file.

Cavities - use spheres. Povray can show Cavities in its own way, using "constructive

solid geometry". For this, it only needs the unit cell and the atoms. This makes for a smaller file and usually gives a much smoother appearance than the standard method used for cavities in ATOMS. If this box is not checked, the POV-ray rendering is exactly the same as that shown on screen.

Currently only one unit cell is shown, and crystal axes cannot be shown.

3.2.1.20 Exit/Quit command

Exit [Windows] or Quit [Macintosh] command [File menu (Startup) or File menu (Graphics) **]**

Use this command to end your ATOMS session.

If you have changed the orientation from that specified in the Initial Orientation dialog in the **File2** menu, you are asked if you want to save the current orientation. If you choose to do this, the current orientation will be converted to initial orientations on the observer x, y and z axes. If clinographic viewing is in effect at the time of saving, the initial clinographic viewing flag will be turned on. The initial rotations can be changed or deleted in the Initial Orientation dialog in the **Input2** menu. See also Coordinate Systems.

ATOMS also checks whether any dialog in the Input1 and Input2 menus have been opened, or whether there has been any change in the status of atoms marked for non-plotting (see Deleting Atoms).

3.2.2 Input1 Menu (Graphics Window)

Note: if the screen is narrow, this may be a submenu in the **Input** menu.

Title/Structure Axes - Title and axial system (unit cell for crystals).

Symmetry - Symmetry of the structure.

Boundary - Boundaries for limiting the reproduction of atoms by lattice vectors.

Display Faces - The optional crystal faces for display surround the structure - they can be the same as boundary faces, or different.

Atoms - The coordinates and other attributes of input atoms.

Polyhedra - Specifications for locating polyhedra, and display attributes.

Bonds - Specifications for locating bonds, and display attributes.

Atoms - Global - This allows changing the radius, colors etc., of all input atoms, or specified subsets, at once.

Atomic Vectors - This specifies general attributes of vectors for magnetic spins or vibrational displacements or other purposes.

Vibrational Modes - For data sets originating from the VIBRAT program, this allows selection of individual vibrational modes..

Cavity Parameters - This sets the parameters for showing "open spaces" in the Cavities display mode.

3.2.2.1 Title/Axes

Dialog Box: Title/Axes [Input1 Menu**]**

The title may have up to 80 characters of identifying information. This may now use non-ANSI character sets, selected with the **Font** button. The size of the text in the edit box is fixed, and will not reflect the size selected with the **Font** button.

The axial system determines the type of coordinate axes for crystal faces (if present) as well as atoms. If you are drawing a molecule you will probably want to choose **Unit Cartesian** axes unless the symmetry is trigonal or hexagonal - see Coordinate Systems.

If you choose a crystal system you must 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). If you are entering a new structure, the unique angle for the monoclinic system is always called beta at this point. However, in the Symmetry options the selection of space or point group may change this, and if you return to the Title/Axes dialog the correct angle should be shown. If the angles are still incorrect you can use triclinic axes.

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

If the **Print title on plot** box is checked, the title will be shown in the lower left on all display and output (of the structure, not the Powder or Precession patterns). If the **Scale** box is checked, the lettering on print and file output will be scaled to approximately the same relative size compared to the drawing as it is on the screen.

Use PostScript font. This allows you to enter a character string for PostScript fonts supported by a PostScript printer if such fonts do not appear in the standard system font dialog called up by the **Font** button. This character string usually specifies the weight

(normal, bold) and slant (italic, oblique) of the font, but not the size, which is specified in the **Font** dialog. Certain PostScript typefaces are standard, and should be present on most PostScript printers.

3.2.2.2 Symmetry

Dialog Box: Symmetry [Input1 Menu**]**

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

Space group from table - Choose a space group by symbol or number.

Point group from table - Choose a crystallographic point group.

Cartesian matrices - Use non-standard or non-crystallographic point symmetry.

Custom point or space group - Enter all the individual operators.

Use no symmetry - Use no symmetry at all. Check **Crystal** to enable lattice translations - the space group will be P1.

Except for the last option, **Use no symmetry**, each choice calls up a sub-dialog.

3.2.2.2.1 Space-Group Symmetry, Basic Tab

Dialog Box: Symmetry - Space Group from Table: Basic Tab [Symmetry dialog**]**

Starting with V4.0 of ATOMS, space-group symmetry is obtained using licensed excerpts from the SGInfo program of Ralf Grosse-Kunstleve. This allows more complete selection of alternate orientations and origins than in previous versions of ATOMS, and also Shubnikov black-and-white symmetry.

You can specify the space group in any of three ways: 1) the Hermann-Maughin (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 symbol can be typed into the 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. This is a change from versions of ATOMS previous to V4.0, in which the orientation of the space group was automatically determined from the Title/Axes dialog. 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.

Shubnikov Symmetry. You can use Shubnikov black-and-white symmetry to show magnetic or other properties of crystals. If you choose this option you must enter at least some of the relevant parameters in the Shubnikov Tab. You enter the Shubnikov space-group symmetry using modified versions of either the H-M or Hall symbols. After entering the Shubnikov symmetry in the Basic Tab, you can check the Shubnikov lattice type and basis operations in the Shubnikov Tab after clicking **OK** or **Apply**. The H-M symbol is modified in the standard way, by a) adding a subscript (actually a postscript) to the lattice symbol; or b) adding a prime or apostrophe to the individual "positions" or basis operations in the symbol. To enter a Shubnikov symbol you must separate the lattice symbol and the individual positions by at least one space or underscore. The entries in the list box already have these separations, so it is advisable to select one of these and then edit it. The Hall symbol is modified in a similar way, but instead of using a prime you must use the "^" character. An initial minus sign on the Hall symbol signifies a center of inversion - if you want to assign Shubnikov inversion to this center, add "^" to the lattice symbol, not to the minus sign.

Standard H-M Shubnikov lattice symbols use both lower- and upper-case subscripts A, B, C for "color" face centering, and a, b, c for edge centering. In ATOMS a capital letter will always indicate face centering, and either lower-case a, b, c or x, y, z (or X, Y, Z) will indicate edge centering. Note that there is little checking for self-consistency, either for input through the symbol or explicit operators in the Shubnikov Tab. The user is responsible for entering a valid Shubnikov space group.

Shubnikov inversion is considered to apply to the spin of a magnetic atom, rather than directly to the vector which shows the magnetic direction. This means that improper operations, including a center of inversion, planes of symmetry and improper (bar) axes, result in inversion or reversal of the magnetic spin vector when the operation is not primed or Shubnikov, and no inversion when the operation is primed or Shubnikov. Of course, the resulting spin-vector orientation depends also on the orientation of the spin with respect to the symmetry operator - when the vector is parallel to an axis or plane the result is completely different from when it is perpendicular. ATOMS can apply Shubnikov symmetry in this way, or in certain other ways - see the Shubnikov Tab.

Magnetic or other Shubnikov symmetry normally involves entries in three different places:

1) The **Space Group from Table** symmetry option (this dialog), including the Shubnikov Tab;
2) The Atomic Vectors dialog (**Input1** menu), to set the display parameters of the vectors; and
3) the **Revise Atom** dialog, Vector Tab for individual input atoms, to set the orientation of the vectors on the atoms.

Molecules. It may sometimes be desirable to use the **Space Group** symmetry option for a molecule rather than the Point Group option because in some point groups you can select different orientations of the symmetry operators with respect to the coordinate axes by choosing the operations from different space groups. Space-group operations are applicable to point groups, provided there are no translations - that is, you cannot use space groups with screw axes, glide planes, or non-primitive lattices. For example, in number 111, P42m - D2d1 the mirror planes are 45 degrees from the structure axes, whereas in no. 115, P4m2 - D2d5, the mirror planes are parallel to the axes. If you choose the Point Group symmetry option and enter the point group 4m2 - D2d, the first of these orientations, as in number 111, will always be used. These two space groups actually differ in other ways than the 45 degree rotation, but this is irrelevant if the operations are used without lattice translations. The choice between the two space groups depends on the relative orientation of coordinate axes and symmetry elements. In this case, if an atom lies on a 2-fold axis it will belong to a set of four (rather than eight if it does not lie on any symmetry elements). For no. 111, such atoms will have coordinates like x,0,0, whereas for no. 115 they will be like x,x,0.

In the trigonal, hexagonal and tetragonal systems several space groups have alternate orientations at 30 or 45 degrees from each other as in the case of D2d. If the symmetry for a molecule is specified with the Point Group option, the "standard" orientation is generated. One may access the alternate orientation by the **Space Group** option and giving the alternate space group as follows (a B before a number indicates a "bar" or inversion axis:

	Standard Orientation	Alternate Orientation
42m - D2d	PB42M (no. 111)	PB4M2 (no. 115)
32 - D3	P321 (no. 150)	P312 (no. 149)
3m - C3v	P3M1 (no. 156)	P31M (no. 157)
32/m - D3d	PB3M1 (no. 164)	PB31M (no. 162)
6m2 - D3h	PB6M2 (no. 187)	PB62M (no. 189)

You can also use this symmetry option to select a non-standard setting for monoclinic or orthorhombic point groups as
discussed in the previous section. For example, you can cause the unique axis of groups 2 - C2, m - Cs or 2/m - C2h to be either a, b or c (the standard setting for ATOMS is unique axis b). You can also cause the 2-fold axis of mm2 - C2v to be parallel to any of the three structure axes. If you do choose this option, using space-group operations for a molecule, be sure that the space group has no screw axes or glide planes, and has a primitive Bravais lattice.

3.2.2.2.2 Space-Group Symmetry, Shubnikov Tab

Dialog Box: Space-Group Symmetry: Shubnikov Tab [Symmetry Dialog**]**

ATOMS uses several tools for description and depiction of magnetic structures, loosely gathered in the "Shubnikov" tab.
These tools include 1) constant vector orientation for all atoms in a site; 2) full Shubnikov symmetry in that the vectors themselves obey the full specified symmetry; 3) Shubnikov symmetry with vector orientations remaining constant except for inversion; and 3) lattice inversion or magnetic supercells independent of Shubnikov symmetry.

Magnetic or other Shubnikov symmetry may involve entries in three different places: 1) The **Space Group from Table** symmetry option, including the Shubnikov Tab (this dialog); 2) The Atomic Vectors dialog (**Input1** menu), to set the display parameters of the vectors; and 3) the **Revise Atom** dialog, Vector Tab for individual input atoms, to set the orientation of the vectors on the atoms.

In the upper part of this dialog, the methods of **Display** and **Application** of the Shubnikov symmetry are selected.

Display:

1) Labels +/-. In this mode, only the two "colors", signified by the +/- symbols, are shown. Select the size and other properties of the symbols with the dialog called up by the **Labels** button. *Caution* : this option may not be suitable for showing Shubnikov magnetic symmetry. Whether or not an atomic vector is reversed or inverted by the combination of ordinary and Shubnikov symmetry depends on the orientation of that vector with respect to the symmetry operator. Most published diagrams of magnetic structure using black and white or + and - atoms are not actually showing the Shubnikov inversions, they are showing symbolically the reversals of spin vectors which are typically in special orientations. If you want to show arbitrary black/white inversion which does not conform to Shubnikov symmetry, you can simple draw up a normal structure, convert Generated to Input (Transform menu) and recolor individual atoms as desired.

2) Vectors - reversal only. In this mode, each input atom has a vector, but the orientation is constant except that the direction may be reversed by the Shubnikov operators. This is not what most workers seem to understand by Shubnikov symmetry applied to atomic spin vectors, but it can be useful in illustrating many magnetic structures or in non-magnetic applications. Especially, it can be used to align all atoms in a particular site in the same direction, regardless of space-group symmetry. To do this, you should also uncheck the Shubnikov box in the Space-Group Symmetry: Basic Tab. Virtually any commensurate magnetic structure can then be illustrated by converting Generated to Input (Transform menu) and reversing or otherwise reorienting the vectors manually. When in the Input=generated mode, clicking on a magnetic atom brings up a dialog which has a button for vector reversal or inversion.

3) Vectors - full symmetry. In this mode, the orientation of the vector on each generated atom is subject to all symmetry operations, both standard and Shubnikov reversal.

Application :

1) Magnetic. Shubnikov inversion is considered to apply to the spin or electric current loop of a magnetic atom, rather than directly to the vector which shows the magnetic direction. This means that improper operations, including a center of inversion, planes of symmetry and improper (bar) axes, result in inversion or reversal of the magnetic spin vector when the operation is not primed or Shubnikov, and no inversion when the operation is primed or Shubnikov. Of course, the resulting spin-vector orientation depends also on the orientation of the spin with respect to the symmetry operator - when the vector is parallel to an axis or plane the result is completely different from when it is perpendicular.

2) Dipole or Black/White. In this case the inversions are applied directly to the vectors, not to the spin or electric current loops. Thus improper operations result in no inversion or reversal of the vector when the operation is not primed, and inversion when the operation is primed. This type of symmetry could be applied to atomic dipoles, or to displacements, for example.

See the table below for the various combinations of Display and Application.

Set the overall properties of atomic vectors with the Vectors dialog called up by the **Vectors** button; set the orientation of the vector for each input atom in the Revise Atom: Vector Tab. Whether each input atom has a Shubnikov reversal at all is also set in the Revise Atom: Basic Tab. In general, not every input atom is Shubnikov or even can be Shubnikov in display modes 1) and 3). The orientation of vectors in special positions may be restricted. Black-white reversal itself may be forbidden in some special positions. Such positions should be identified during the calculation and marked as non-Shubnikov.

Shubnikov Operators. This section of the dialog summarizes the information obtained from the Shubnikov symbol in the Basic Tab. The possibilities for the Shubnikov lattice type or **Lattice centering** are lower-case a, b, or c, indicating translation reversal in the respective axis direction, or S, indicating reversal on all three directions; or upper-case A, B, or C indicating a Shubnikov centering of the respective faces, or I, indicating Shubnikov body centering.

For non-translational Shubnikov symmetry, the possibilities are **Inversion**, and either **Rotation** parallel to, or **Reflection** perpendicular to any of the three axis directions. If present, rotation and reflection are indicated by capital letters A, B and/or C. The face diagonal [110] direction, indicated by AB, is also possible in high-symmetry crystals. The body diagonal [111] direction is not a possible Shubnikov operator orientation as it can only have a three-fold axis.

Note that there is little checking for self-consistency of Shubnikov operators. The user is responsible for entering a valid Shubnikov space group.

Table showing possibilities for Display and Application of Shubnikov symmetry

	+/-	Reversal Only	Full Symmetry
Magnetic	bc	bc	abc
Dipole	bd	bd	abd

a) Operate on vector with ordinary space-group symmetry

b) Proper operators (lattice and non-bar axes) - reverse if primed, do not reverse if unprimed

c) Improper operators (inversion, reflection, bar axes) - reverse if unprimed, do not reverse if primed

d) Improper operators (inversion, reflection, bar axes) - do not reverse if unprimed, reverse if primed

Reverse means to change vector direction by 180 degrees, or to change + to - or vice-versa. The ordinary space-group symmetry operations are always applied to the positions of the atoms.

Lattice Inversions or Magnetic Supercell. This option is not actually part of Shubnikov symmetry, but it offers a simple means of describing many magnetic structures, either by itself or in combination with Shubnikov operators, often without changing the unit cell and overall symmetry from what describes the non-magnetic structure.

Checking one of the boxes causes all magnetic vectors to reverse with each translation on that axis. This normally results in a doubled magnetic axis or cell edge in that direction. When more than one lattice inversion is selected, the operations are applied successively. For example if there is inversion on a and b axes, the 100 and 010 unit cells have inversion, but the 110 unit cell does not.

If the unit cell is non-primitive you can use inversion on either the Bravais axes or the primitive axes, but not both.

Note that the Default Unit Cell boundary option uses the non-magnetic Bravais axes, not the doubled magnetic axes. To show the reversals adequately it may be necessary to select the **-1 to 1 inclusive** option in the Default Unit Cell boundary option, or to use the Translation Limits boundary option.

This option is definitely not the same as using non-primitive Shubnikov lattices, and is apparently equivalent to specifying a magnetic "wave vector". Compare the samples FCCMAG, FCCMAGR, and FCCFULL_II for different ways of showing Type II FCC (MnO) magnetic structure - the most concise is FCCFULL_II which uses inversions on all three primitive (face-centering) lattice translations, with the full Fm3m X-ray symmetry of MnO.

See also the CRCL2MAGD sample, which uses magnetic lattice inversions on two axes in combination with a Shubnikov space group Pnnm' which is simply related to the non-magnetic group Pnnm.

Irreducible Representations. ATOMS could in principle be programmed to use the method of description of magnetic structures by means of the irreducible representations of space groups, as pioneered by Bertaut and others and described in the book by Izyumov, Naish and Ozerov (Neutron Diffraction of Magnetic Materials). This has obvious theoretical advantages over the ad hoc methods now used in ATOMS, but there are practical difficulties in that the representations are numbered in an arbitrary way and and must refer to an essentially arbitrary order of symmetry operators. A description of this type can be concise but it may convey little without reference to a standard compilation such as that of Kovalev.

If there is sufficient interest, using irreducible representations might be attempted in ATOMS.

3.2.2.2.3 Magnetic Labels

Dialog Box: Magnetic (Shubnikov) Labels [Space-Group Symmetry Dialog**]**

The only characters which will be shown are the symbols + and -. The choice between showing these symbols and atomic vectors is made in the **Space-Group Symmetry** dialog, Shubnikov tab.

If the **Background** is opaque, each symbol will lie on a small block of the designated color; this usually makes the labels easier to read. Some other programs may not be able to reproduce these opaque blocks in Metafiles or PICT file output.
Sequence. The labels may be plotted immediately after each atom, or all at once after all atoms have been plotted. The first usually looks better, but some labels will usually be partly or completely obscured.
Use PostScript font. This allows you to enter a character string for PostScript fonts supported by a PostScript printer if such fonts do not appear in the standard system font dialog called up by the **Font** button. This character string usually specifies the weight (normal, bold) and slant (italic, oblique) of the font, but not the size, which is specified in the **Font** dialog. Certain PostScript typefaces are standard, and should be present on most PostScript printers.

The label positions are correct for stereopairs, and labels for central atoms of polyhedra will appear suspended in the interior of the polyhedra.

Use the color options in this dialog, not the color options in the Font dialog to set the color of the letters. Letters are always solid black in black-and-white display or output. See Input Colors/Patterns/Pens for general aspects of color input.

Labels are not supported for Pen Plot output.

3.2.2.2.4 Point-Group Symmetry

Dialog Box: Symmetry - Point Group from Table [Symmetry Dialog]

This is the simplest symmetry option for a molecule, provided the symmetry is crystallographic and atomic coordinates conform to standard orientations. It is not applicable if the symmetry is icosahedral, pentagonal or other non-crystallographic type; choose the Cartesian matrices symmetry option in any of these cases. If the symmetry is crystallographic, but the orientation is non-standard, it may be possible to use the Space group option.

To use this option, click on the point group symbol; symmetry operations will then be taken from a space group belonging to the given point group in the *International Tables* ; the space group chosen will have a primitive lattice, no screw axes or glide planes, and the standard orientation of axes. Usually, but not always, this is the one with superscript 1 on the Schoenflies symbol. In the case of monoclinic groups (2 - C2, m - Cs or 2/m - C2h), the first setting (unique axis parallel to c) is standard: this is different from the standard for settings of monoclinic crystals in the Title/Axes dialog in the **Input1** menu, but when you select the point group the unique angle will be applied to the proper axes. For group mm2 - C2v the 2-fold axis is parallel to c. For groups with 3-, 4- or 6-fold axes, the unique axis is c, but there may be alternate orientations at 30 or 45 degrees from one another: see the Space group option for the standards and how to access the alternate orientations using space-group operations.

Coordinates of atoms in molecules are usually given in a Cartesian axial system. If the molecule has one 3-fold or 6-fold axis of symmetry, i.e. has trigonal or hexagonal symmetry ATOMS can either use reference axes which also have this symmetry, that is trigonal or hexagonal "crystal" axes (a_1 and a_2 axes at 120 degrees, c axis at 90 degrees to a_1 and a_2), or use unit Cartesian axes. The symmetry matrices for the standard point groups are actually stored in the form appropriate to hexagonal axes, and then converted to the Cartesian form during calculation if the structure axes are unit Cartesian.

3.2.2.2.5 Cartesian Symmetry

Dialog Box: Symmetry - Cartesian Matrices [Symmetry Dialog]

This symmetry option, for point symmetry only, assumes that Cartesian axes are in use, although it will work in any structure with axes at right angles. It is the only option applicable to non-crystallographic symmetry, and it can be used if desired in any other case. However, it is usually easier to use one of the other options for crystallographic symmetry.

This option requires a file containing the Cartesian symmetry matrices. The auxiliary program SYMGRP writes files which are normally given the suffix.SYM. If you type the

name into the edit box, give the full name of the symmetry file, including the.SYM suffix. Some such files, namely those for pentagonal (C5, S10, D5, C5v, C5h, D5h and D5d) and icosahedral (I and Ih) point groups, have already been provided. For other point groups, it will be necessary to run the auxilliary program SYMGRP to generate the file before running ATOMS.

The **Get Symmetry** button reads the file and fills out the symbol, number of matrices and centric/non-centric state, which are printed out below the file name.

The file name as entered in the edit box is saved in the data file for the structure. If the complete path is not given, the Cartesian symmetry file should be in the same directory as the data file. If the file cannot be found when the structure is calculated, you will get an error message and a chance to locate the file with a standard file dialog. The complete path name, as determined in this way or with the **Browse** button, will then be saved in the data file.

Obtaining SYMGRP. To get SYMGRP, download the demo for SHAPE from www.shapesoftware.com - SYMGRP is in a sub-folder.

3.2.2.2.6 Symmetry - Custom

Dialog Box: Symmetry - Custom [Symmetry Dialog**]**

ATOMS 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: ATOMS needs all the operations for the general position.

The **Symbol** is for your reference only - it is not used by ATOMS, unless you click the **Get Symbol** button (below).

Get 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, they should be identified and can be removed at your option.

If you specify **centric**, rather than **acentric**, you must enter only half of the symmetry operations, 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 **Bravais lattice type** is in most cases the capital letter which begins the space-group symbol. However, ATOMS 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". Enter "P" for a molecule.

If the group is monoclinic, you should specify which is the **Unique axis**. This is normally c for a molecule and b for a crystal. The angle specified in the Title/Axes dialog will then be applied correctly, the other two interaxial angles being set to 90 degrees.

In the **Operations** group, you must enter all the "symmetry operations" for the most general position in the structure. Click on the **Add Operation** button to add an operator, or **Delete** to remove an operator. The operation which is selected in the **Operations** list box is available for editing in the box to the right. Note that earlier versions of ATOMS allowed several operations per line; currently, there should be only one operation per line. Semicolons at the end of each operation (line) are optional.

It is assumed in the following that you will be using data listed in the *International Tables*, but this is only for purposes of illustration; if you find it necessary to enter the operations through this dialog, you will very likely be using data from another source. Reports on crystal structures, especially older ones, often list the relevant operations in the same format as the *Tables*.

In the *Tables*, the "Co-ordinates of equivalent positions" can be regarded as operations (or at least the operations can be easily derived from them). These coordinates occupy the middle of the page in each space-group entry in the *Tables*, and the general position is the uppermost group. The general position has the point symmetry 1, and the list of operations for this position always begins with "x,y,z;". The individual operations are separated in the *Tables* by semicolons.

Copy these operations, including the commas (semicolons optional), one per line. They are entered just as given in the *Tables*, except that a negative sign, indicated by a small bar over the letter in the *Tables*, must be indicated with a minus sign in front of the letter. The first operation, "x,y,z;" is present in all symmetry groups and must always be entered. Ignore the translations for non-primitive lattices (e.g. 0,0,0; 1/2,1/2,1/2) which may be listed in the *Tables* above the operations; these are taken care of if you enter the proper Bravais lattice symbol. Some older structure reports may include lattice-centering in the equivalent positions.

Important: if you have specified a centric space group with origin on the center of inversion, you should omit half the operations, which are related to the other half by the center (opposite signs for x, y and z coordinates). If you have difficulty making this separation, you can specify non-centric and enter all the operations. The **Get Symbol** button should detect a center of inversion on the origin, and remove it if desired.

3.2.2.3 Boundary Option

Dialog Box: Boundary Option [Input1 Menu**]**

For crystals and polymers, some limitations must be applied to the repetition of atoms by means of the lattice translations. Ten choices are available, as listed below. Note that the first three are not usually applicable to molecules, while the fourth, **No Boundaries**, is not applicable to crystals. There is an additional boundary option and operating mode, **Input atoms = generated atoms**, which is only accessible by choosing Generated to Input in the **Transform** menu.

Options applied to individual atoms :

Default Unit Cell - Offers five sub-options to outline a volume with the same faces as the unit cell.

Enter Forms - Use specified crystal faces for the boundaries.

Slice - Isolate a slab of the structure parallel to a given face, with thickness equal to the d-spacing (or multiple thereof).

No Boundaries (molecule) - Use no boundaries at all. This option is primarily for a single molecule not in a crystal structure, not isolation of molecules in a crystal structure (see below).

Translation Limits (polymer) - Use integral numbers of unit cells.

Sphere - Include all atoms within a given distance of a given point (or atom).

The **Unit Cell** and **Slice** options always use lattice translations in all three axis directions, and the **No Boundaries** option never uses lattice translations. The **Translation Limits** option, primarily intended for polymers, allows you to specify which axis directions use lattice translations. The **Enter Forms** option also allows disabling of any of the lattice translations.

Options applied to groups of atoms (molecules) in crystals.

In all these options, molecules or other bonded groups within the unit cell are located, and the center point of each group is found by taking a non-weighted average of the atomic positions. Then the selected boundary method is applied to these molecular centers.

Atoms within molecules or groups must be connected by Bonds or Polyhedra, and there must be no standard bonds or polyhedra connecting atoms of different molecules. However, bonds can be specified as inter-molecular, so that they will not be used in the molecule-locating algorithm but will be displayed.

Note that these options are not applicable to 1- and 2-dimensionally continuous groups (polymers) - bonding must be discontinuous in all three lattice directions. In order to isolate polymers, it is necessary to first use one of the six options above, then click on an atom in the polymer and use the **Find** button in the Generated Atom Data dialog, or use the Locate Groups option in the Transform menu. See Dealing with Molecules, Groups and Fragments for more information about handling groups of atoms.

Unit Cells - Molecules - This will find any and all symmetry-unique bonded groups, and can also show groups in additional unit cells. This option starts with a seed atom inside the unit cell and finds all atoms bonded to it including those outside the central unit cell - thus the bulk of a molecule may be outside the unit cell.

The other options below are actually identical to the options of the same name above, except that they are applied to the centers of molecules instead of individual atoms. The center, which is the average of all atoms in the molecule, is always within the given boundaries (this is not guaranteed in the Unit Cells - Molecules option).

Enter Forms - Molecules - Use specified crystal faces for the boundaries.

Slice - Molecules - Isolate a slab of the structure parallel to a given face, with thickness equal to the d-spacing (or multiple thereof).

Sphere - Molecules - Include all molecules within a given distance of a given point (or atom).

3.2.2.3.1 Boundary - Unit Cell

Dialog Box: Boundary - Unit Cell [Boundary Dialog**]**

This option (not intended for molecules) locates the faces of the unit cell, at various choices of central distance.

Each of the sub-options may be chosen as the **Default,** which is the boundary option used when importing a file (Import File command in the **File** menu).

You can choose either the primitive or Bravais cell if the lattice is non-primitive. If the Bravais lattice is primitive, or if you elect not to use the primitive cell, the faces will be (100), (010) and (001) and their negatives. If you choose to show the primitive unit cell for non-primitive lattices, the faces will be {110} and {001} for a C-cell, etc.

The central distances for the faces depend on which **Sub option** is chosen. The central distance is the perpendicular distance from the face to the center of the crystal.

If you choose the **-0.5 to 0.5 cell contents** sub-option, the faces are at central distances of 0.5009 of the dimensions of the unit cell if the h index is positive, or 0.499 if negative; if h is zero, k is used; and if k is zero, l is used. Thus the volume enclosed is essentially that of the unit cell, with the origin at the center. This is the only option which gives the correct number of atoms for one unit cell.

The **0.0 to 1.0 inclusive** sub-option gives you faces at the full d-spacing for positive indices, and zero for negative indices, plus a small increment in both cases. Thus the "unit cell" in this case includes atoms with fractional coordinates 0.0 to 1.0 inclusive.

The **0.0 to 1.0 plus bonds** sub-option adds to the central distances of the preceeding sub-option the largest bond distance or coordination distance entered in bond and/or polyhedron input. This allows for completion of the coordination of all atoms in the unit cell. Note that atoms may be included which are not considered to be coordinated to the atoms in the cell, and that the distances used are the limits entered in the bond and polyhedron dialogs, not the actual bond distances.

The **-1 to 1** inclusive sub-option gives faces at the full d-spacing, plus a small increment, for both positive and negative indices. While all the previous options give one unit cell or somewhat more, this option gives *eight* unit cells and somewhat more. Using this option insures that at least one complete molecule, or any other non-polymerized unit, will be included.

The **Central Distance** sub-option sets all the faces of the unit cell at the given central distance. Atoms "on" the faces are included.

The **Get Faces** button will calculate d-spacings and list the faces.

A single unit cell will not necessarily include a complete molecule or polymer; see the Locate Groups command in the **Transform menu** for information on isolating groups.

If you select this boundary option, you can later switch to the Enter Forms option; this preserves the forms and the symmetry (i.e. no symmetry for the faces).

Note that the Translation Limits option, with all limits set to zero, will include atoms with fractional coordinates 0.0 to 0.99999, or in other words the same volume as sub-option **-0.5 to 0.5 cell contents**, but displaced by half a unit cell on all axes.

3.2.2.3.2 Boundary - Enter Forms

Dialog Box: Boundary - Enter Forms [Boundary Dialog**]**

This dialog may apply either to individual atoms, or to molecules (in which case the dialog title will be **Enter Forms - Molecules**). In the latter case, bonded groups in the unit cell will be identified and the center of each taken as the non-weighted average of atomic positions. Then the boundaries will be determined with respect to the molecular centers.

With this option, the most powerful of the boundary options, you can set the boundaries of a crystal structure to be any rational faces consistent with the axial system defined in the Title/Axes dialog. You do not need to enter every individual face; you can enter any one of the faces of a form (symmetry-equivalent set), and the remainder will be supplied by symmetry. You can use the full symmetry of the crystal class (point group), but you may also elect to use a lower symmetry (center of inversion only, or no symmetry at all) to have more flexibility in the volume defined.

The **Revise** or **Add Forms** buttons call up the Add/Revise Form dialog for actual entry of indices and central distance.

The **Use individual atom distances** option allows the boundary surfaces to be non-planar with respect to the centers of the atoms. If you use this option, the actual central distances for each boundary form are then entered (actually revised) during input for each atom (Revise Atom: Central Distance Tab). However, the distance entered for each form in this dialog is still necessary - it will be used: 1) As the default distance for the boundary faces for each atom. You will need to revise the actual boundary face distances for each form during atom input. 2) As the default for display of the crystal edges. The display forms can be given new distances or changed completely with the Crystal Forms for Display dialog in the Input1 menu. 3) For the initial boundary search limits while locating atoms. The distance entered here in the boundary option should therefore not be too different from the distances for individual atoms to be entered in the Revise Atom: Central Distance Tab in the **Input1** dialog.

Individual atom distances are not used in the Enter Forms - Molecules option.

There is a maximum of six forms (not faces) if you choose individual atom boundary distances.

You can disable lattice translation on any of the structure axes, if you wish to use this option to draw a molecule or polymer. Although it is generally simpler to use the Translation Limits option for polymers, you can use the **Enter Forms** option to show more diverse shapes for a two-dimensional polymer. For example with appropriate choice of faces you can give the sheet a hexagonal shape, while the Translation Limits

option will always give a parallelogram shape.

You can use this option for molecules to isolate a section, slab, or any convex polyhedral volume. To prevent the repetition of the structure by translation, you must disable all the lattice translations. It is not necessary to specify enough faces to define a closed polyhedron, although you will get warning messages during calculation if you do not. For example, to effectively slice through the middle of a molecule and just view the back half, give only the "face" (100) at central distance 0.0 (set the face symmetry to **No symmetry**).

Hint : specifying a center of symmetry for boundary faces, and the simple forms (100), (010) and (001) at central distances of about 10 Angstroms will usually give 500-700 atoms for typical inorganic crystal structures. Central distances of about 7 Angstroms usually gives about 300 atoms. Numbers are usually smaller for organic crystals.

3.2.2.3.3 Add/Revise Form

Dialog Box: Add/Revise Form [Crystal Forms for Display Dialog**] [** Boundary - Enter Forms Dialog**]**

The central distance is the perpendicular distance, in Angstroms, from the center of the structure to the faces of the form in question: the greater the distance, the greater the number of atoms which will be included. Also, if there are many forms, the greater the distance the less prominent the form (the smaller the area of the faces). Decimal values may be used for the central distance, but not for the indices. Use the **Next Form** button to add a form.

Keep in mind that there may be alterate orientations of symmetry elements with respect to structure axes, and the indices of faces in a standard morphological setting may be different from those in the setting of a particular space group. See section IV-5 for further details of variant orientations.

You can use negative central distances to define a region which does not include the origin. For example, if you want to display the part of the structure from y = 0.25 to y = 0.75 in an orthorhombic crystal with b = 10.0, enter the face (010) at distance 7.5 Angstroms and the face (0-10) at distance -2.5 Angstroms. If the crystal axes are not orthogonal, you should use fractions of the d-spacing for central distances, not axis lengths. The Enter Forms and Default Unit Cell boundary options list d-spacings of the forms, uncorrected for systematic absences; the Slice boundary option will give a d-spacing corrected for systematic absences.

For hexagonal and trigonal crystals with hexagonal axes, four indices, (hkil), are commmonly used, but one of the first three is redundant. In ATOMS, you must omit the third, or i index.

3.2.2.3.4 Boundary - Slice

Dialog Box: Boundary - Slice [Boundary Dialog**]**

This dialog may apply either to individual atoms, or to molecules (in which case the dialog title will be **Slice - Molecules**). In the latter case, bonded groups in the unit cell will be identified and the center of each taken as the non-weighted average of atomic positions. Then the boundaries will be determined with respect to the molecular centers.

This gives a section of a crystal structure parallel to a given face, with the thickness of the X-ray d-spacing, or a multiple thereof. Such a "slice" is intended primarily to represent a growth layer, but is often useful for illustrating special structural features.

In addition to the indices of the face, you need to specify several other things. An **Alignment vector** is also necessary - when the calculation is complete, the slice will be lying in the plane of the screen or paper and this vector will be vertical (parallel to z). The vector must lie in the slice: a vector [uvw] lying in a face (hkl) satisfies the condition hu+ kv + lw = 0. If the default alignment vector is chosen, the alignment vector will be taken as the intersection of the face (hkl) with the face (100), whose indices are given by the vector cross product (hkl)x(100). If the slice face (hkl) is (100), the alignment vector will be taken as its intersection with (010), which is the vector [001].

You must also specify the **Height** and **Width** of the slice, parallel and perpendicular to the alignment vector.

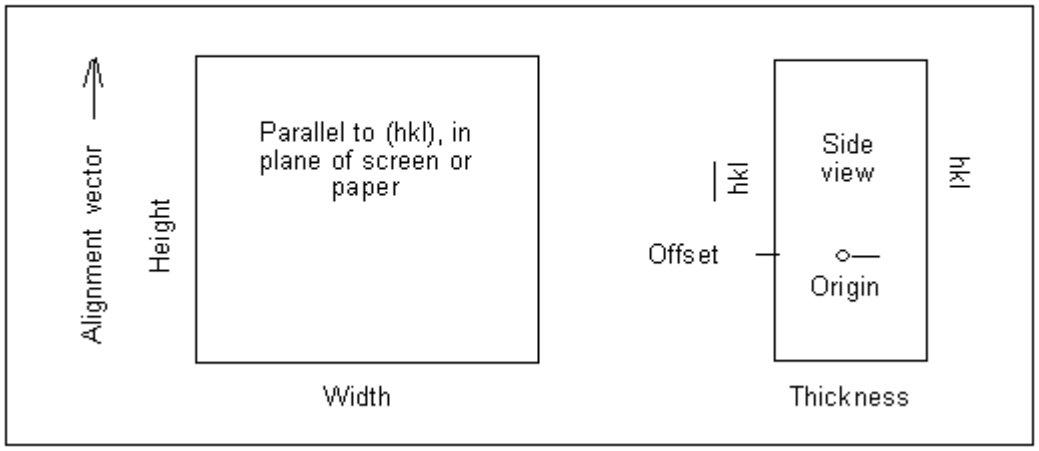
The location of the slice within the crystal structure must also be specified in terms of the **Offset** from the origin. One can specify different offsets, or boundary locations, for each atom (set of symmetry equivalent atoms) in case the slice is not considered to be strictly planar (see below). The **Thickness** of the slice is a fraction of the d-spacing: in most cases it should be 1.0.

Atoms lying exactly on the "upper" boundary - (the face to which the slice is defined to be parallel) are excluded from the slice, whereas atoms lying exactly on the "lower" boundary (the face with indices negative to the "upper" face) are included.

The **Use individual atom offsets** checkbox allows the boundary surface to be non-planar with respect to the centers of the atoms. If you use this option, you should revise the offsets for the forms during atom input - the overall offset entered in this section sets the default values. It is also used as the default for display of edges of the slice (the display forms can be changed in the Crystal Forms for Display dialog), and to determine preliminary unit-cell search limits for atoms during the calculation; thus this overall offset and the offsets for individual atoms should not differ too much.
Systematic absences can be used to take account of d-spacings which are a submultiple of those obtained solely from the cell parameters because of non-primitive lattices, screw

axes or glide planes. The subdivision of the central distance for each form is done when the d-spacing is calculated, after **OK** is clicked; to see the d-spacing values you must re-select the dialog. You cannot manually edit or add absences as in pre-V4.0 ATOMS. The Custom symmetry option does not contain information on systematic absences - if you want to use systematic absences, you should switch to the Space Group symmetry option.

Slice Dimensions



3.2.2.3.5 Boundary - None

Dialog Box: Boundary - None [Boundary Dialog**]**

No boundaries whatever are used if this option is chosen, nor are any translations applied. That is, the atoms in the molecule are just those, and all of those, generated by the point-group symmetry specified (or the input atoms only, if there is no symmetry).

This boundary option is primarily for the case in which you already have absolute coordinates of a single molecule. To draw a single molecule which is in a crystal, using fractional coordinates and other data for the crystal, use one of the Molecules in Crystal options in the Boundary dialog, or use the Default Unit Cell, Enter Forms or Translation Limits boundary option to generate a volume large enough to include the molecule or other group, then use the **Find** button in the Generated Atom Data dialog (which appears when you click on an atom) or the Locate Groups dialog in the **File** menu to isolate the molecule or group. Also, you can use the Enter Forms boundary option to use pseudo-crystal faces to isolate part of a molecule - see the last paragraph of that section.

3.2.2.3.6 Boundary - Translation Limits

Dialog Box: Boundary - Translation Limits [Boundary Dialog**]**

In this option, the contents of the central unit cell plus others within specified limits are accepted. The central or "zero" unit cell contains atoms with fractional coordinates 0.00000 to 0.99999. The lower limit to unit-cell translations is normally zero or negative and the upper limit is normally zero or positive. Disabling the translation entirely for an axis is equivalent to setting the limits at zero. The translations belong to the Bravais lattice, not the primitive lattice.

As an example of application to a crystal, putting the lower limit at -1 and the upper limit at 0 for all axes results in a box with the shape of the Bravais unit cell, centered on the origin and containing eight unit cells. Note that the "zero" unit cell, containing atoms with fractional coordinates 0.0 to 0.99999, extends in the positive directions of the axes.

This is the primary option for one-dimensional polymers. It is also the simplest option for two-dimensional polymers, but the shape of the resulting sheet is limited to the shape of the unit cell, always a parallelepiped. You can use the Enter Forms option to give a different shape to sheets.

3.2.2.3.7 Boundary - Sphere

Dialog Box: Boundary - Sphere [Boundary Dialog**]**

This dialog may apply either to individual atoms, or to molecules (in which case the dialog title will be **Slice - Molecules**). In the latter case, bonded groups in the unit cell will be identified and the center of each taken as the non-weighted average of atomic positions. Then the boundary will be determined with respect to the molecular centers.

This option is primarily designed to isolate a coordination sphere around a given atom, although the center of the sphere can be at an arbitrary location in structure coordinates.

If you check the **Specify structure coordinates** radio button, you must enter the coordinates in the x, y, z edit boxes below. If you check **Input atom number**, enter only the input atom number in the edit box to the right. Then clicking the **Get Coords.** button will fill out the coordinates (as will clicking OK).

If the structure is a molecule or polymer you should uncheck the appropriate lattice tranlation(s), i.e. for a molecule uncheck all three.

3.2.2.3.8 Boundary - Locate Molecules in Crystal

Dialog Box: Boundary - Unit Cells - Molecules (Locate Molecules in Crystal) [Boundary Dialog**]**

This option will locate all symmetry-unique bonded groups, or all bonded groups, within an integral number of unit cells. The central-ligand bonds in Polyhedra are used as well as the standard Bonds. Like the Locate Groups option (Transform menu), this boundary option starts with a seed atom, in this case the first input atom, which is within the zero or central unit cell (fractional coordinates 0.0 to 0.9999) and then finds all others involved. If the first molecule found in this way does not include all input atoms, the excluded input atoms are in turn used as seed atoms, until all are located. An alert informs you if there is more than one molecule or group. While the seed atoms are always in the central unit cell, any other atoms may be in adjacent unit cells.

If the number of atoms located exceeds the number in the unit cell the procedure is aborted. In such a case there is presumably continuous bonding.

You can locate all molecules in the unit cell, or only symmetry-unique ones. You can also show the molecules in multiple unit cells. In this option, the boundaries of unit cells are always the planes at fractional coordinates 0.0, 1.0, etc. To have more control over boundaries you can use the Enter Forms - Molecules boundary option. Note that that option finds the center of each molecule (unweighted average of atom locations), and then places molecules within boundary faces according to that center location, whereas this option does not find the center of each molecule, and molecules may be placed "inside" the unit cell even if only one atom (the seed atom) is actually inside the cell.

After initial isolation of the molecules, it may be desirable to use the Generated to Input conversion (Transform menu). This will simply make a list of the atoms located, which is saved in the data file, and will in the future avoid the molecule-locating algorithm, which can be time-consuming.

Do not use this option to isolate two- and three-dimensional polymer units. Instead, use some other boundary option to generate a volume which you know includes a sufficiently large number of polymer units. Then use the Locate Groups option in the Transform menu - this option allows the specification of particular seed atoms. The Locate Groups option is also appropriate if there are isolated molecules as well as a continuously bonded framework, or polymers. See also Dealing with Molecules, Groups and Fragments.

This is a possible default boundary option for importing crystal-data files, with certain exceptions (PDB, CCDC-FDAT, VIBRAT). If it is allowed, the initial dialog for that import file type will give a choice between Locate Molecules in Crystal and Default Unit Cell. Of course the boundary option can be changed after the import file is read in.

In the case of CCDC FDAT files, the "molecule" option does not use this boundary option, rather it uses data on molecules which is already present in the file.

3.2.2.4 Crystal Forms for Display

Dialog Box: Crystal Forms for Display [Input1 Menu**]**

With this option you can display an external crystal shape which is not the same as the boundary faces for locating atoms. You can even show a crystal shape for structures in which the boundary option is No Boundaries or Translation Limits.

This dialog controls the generation of the faces, corners and edges which make up the display shape; the Crystal Edges dialog in the **Input2** menu controls colors and other display aspects of the crystal edges - of course it is only the edges which are actually shown.

By default, the display shape is the same as the boundary shape for boundary options Default Unit Cell, Enter Forms and Slice, and there is no display shape for options No Boundaries, Translation Limits and Sphere**.** If you choose to change the display shape, or to show one where no crystal forms are used as boundaries, the input and revision thereof are similar to those for input of boundary crystal forms in the Enter Forms boundary option, through the Add/Revise Form dialog

For the non-3D display modes of ATOMS, the edges demarking the external crystal shape should be outside the atomic structure. As discussed in Drawing Crystal and Unit-cell Edges, an external crystal shape which lies inside or interpenetrates with the atomic structure will in many cases be drawn incorrectly. In the 3D mode, interpentration relations are drawn correctly.

Although this option is primarily intended for the Default Unit Cell and Enter Forms boundary options, it can also be used for molecules and polymers.

Note that you may have to change the **Display** radio buttons in the Crystal Edges dialog in the **Input2** menu, to allow the crystal shape to be displayed.

Using display faces with Cartesian symmetry input. The symmetry option Cartesian matrices is intended primarily for molecules with non-crystallographic symmetry. However, it can be used with "crystal" faces with certain restrictions. You must use Cartesian face coefficients or inverse intercepts, and if some of these "indices" or the symmetry equivalents thereof are irrational they must be converted to large integers. For example, the face (100) in a trigonal or hexagonal crystal would also have coefficients 1,0,0 in a Cartesian system with y=b (or a2), but some of the symmetry equivalents of this face, such as (-110) and (0-10) would have irrational coefficients. If you enter 20000,0,0 as the "indices" of the form, then when the indices are multiplied by the Cartesian symmetry matrices the result will be large integral indices for the symmetry equivalents. If you enter 1,0,0, the results would be fractions, which would be incorrectly truncated or rounded off either to 0 or 1. As another example, an icosahedron may be

drawn in either of the icosahedral groups I or Ih by giving the form indices 0,0,20000; the indices 0,0,1 would not work because many of the 19 faces equivalent to this one have irrational indices.

Using integers with up to four or five digits (99,999) gives adequate precision for the calculations involved in determining the external crystal shape.

3.2.2.5 Atoms (Input)

Dialog Box: Atoms [Input1 Menu**]**

You can choose to enter each atom interactively, or ATOMS can read some or all of the atom parameters from a text file, supplying defaults for the atom types, radii and display colors if desired. You can type in the name of this input file, or browse to open the file. The file must contain certain lines specifying the which parameters are to be read in and which set to default values (see Atom Parameter Files for specifications).

If you do not use a file, use the **Revise** or **Add Atoms** buttons to access the Revise Atom dialog. You can also double click on any line to revise that atom.

The list of input atoms in this dialog may not show non-ANSI characters in the atom label correctly because this list must be written in a fixed-width font (Courier or Monaco). In the Revise Atom dialog characters for non-ANSI typefaces should be displayed correctly, but at a fixed font size.

To calculate bond distances and angles, for use in the bond and polyhedra input or just for general information, use the Coordination button. It is not necessary to have calculated the structure to use this option, or even to have selected the boundary option, but you must have entered the correct structure axes or unit cell and symmetry.

The Vectors dialog called up by the **Vectors** button is for specification of general properties of atomic vectors, for use in displaying magnetic symmetry or vibrational modes. The vectors for the individual input atoms are specified in the Revise Atom dialog.

The **T. Factors** button is for adding temperature factors to all atoms, or deleting them all. To view or modify temperature factors for individual atoms, select that atom to call up the Revise Atom dialog, and select the Temperature Factor tab in that dialog.

Z-Matrix. This allows construction of a molecule from a z-matrix or table of bond lengths and angles instead of using Cartesian coordinates.

Hex->Cart and **Cart-Hex** buttons. These are for converting coordinates of atoms, and vectors if present, between the *current hexagonal* axes and unit Cartesian axes. Thus if your current axes (Title/Axes dialog in the Input1 menu) are unit Cartesian, change them

to the desired hexagonal/trigonal axes (a = b, alpha = beta = 90, gamma = 120) before converting. You will be warned if the current axes are not hexagonal. Only the lengths of the axes are used in the conversion, so if your intention is to convert from unit Cartesian to unit hexagonal you do not need to reset the axes before conversion. The axes themselves are not automatically reset after the hexagonal to Cartesian tranformation - do this manually in the Title/Axes dialog .

Note that starting with V6.2 of ATOMS, it is not necessary for crystals with trigonal or hexagonal symmetry to use hexagonal axes - in the calculation, the type of axes is detected and the symmetry matrices are converted to unit-Cartesian form. Types of axes other than hexagonal/trigonal or Cartesian should not be used for hexagonal or trigonal crystals.

Translate all atoms. This will add the given quantities to the coordinates of all atoms. This is typically used for centering a molecule on a given atom (enter the negatives of the coordinates of that atom). It is not normally appropriate for crystals.

Solid Solutions. There is no provision in ATOMS for directly showing solid solutions as fractional atoms. However, it is possible to use the **Randomize** option in the Atoms - Global dialog in the Input1 Menu to change the colors or other properties of selected groups of atoms on a random basis. Of course, it is also possible to modify individual generated atoms manually, after execising the Generated to Input option in the Transform Menu.

3.2.2.5.1 Revise Atom, Temperature Factor Tab

Dialog Box: Revise Atom: Temperature Factors Tab [Input Atoms Dialog**]**

See the Basic Tab for most normal aspect of individual input atoms, the Central Distance and Slice Offset tabs for adjusting boundaries for individual atoms, and the Vector Tab for atomic vectors for magnetic moments or vibrational displacements.

The temperature factor type, according to ORTEP, must be selected with the radio buttons. The most common types are 0 for anisotropic beta; 6 for isotropic B; 7 for a sphere of constant radius, 8 for anisotropic u, and 10 for isotropic U (not a standard ORTEP type).

The instructions and help for some releases of pre-V5.0 ATOMS may be incorrect in stating that type 7 indicates isotropic U. Actually, type 7 should be a sphere of arbitrary radius. Importing files with isotropic U may in some cases have incorrectly assigned type 7 to these atoms (although in most cases these should have been converted to isotropic B). Thus when ATOMS reads a pre-V5.0.STR file with type 7 temperature factors, you will be asked if you want to change these to type 10.

Isotropic values are entered in the first box; if the second or b22/U22 value is zero, the

atom will be considered to be isotropic.

3.2.2.5.2 Revise Atom, Slice Offset Tab

Dialog Box: Revise Atom: Slice Offset Tab [Input Atoms Dialog]

See the Basic Tab for most normal aspect of individual input atoms, the Temperature Factor Tab for modification or entry of temperature factors, the Central Distance tab for adjusting boundaries for individual atoms in the Enter Forms boundary option, and the Vector Tab for atomic vectors for magnetic moments or vibrational displacements.

This applies only to the Slice boundary option.

The default value is the offset entered in the Slice boundary option.

3.2.2.5.3 Revise Atom, Vector Tab

Dialog Box: Revise Atom: Vector Tab [Input Atoms Dialog]

See the Basic Tab for most normal aspect of individual input atoms, the Temperature Factor Tab for modification or entry of temperature factors, and the Central Distance and Slice Offset tabs for adjusting boundaries for individual atoms.

Atom vectors, for magnetic spin direction or atomic displacements in vibrational modes, are specified in the crystal or structure coordinate system. The length is specified independently from the vector giving the orientation.

Vectors are drawn by adding pseudo-atoms to the list of generated atoms, and adding pseudo-bonds between these pseudo-atoms and the real atom to which the vector is attached. Thus if the length or orientation are changed the structure must be recalculated, rather than just replotted. Also, since the length is computed as the visible cylindrical part of the vector, if you change atomic radii the vector lengths will change unless the structure is recalculated.

3.2.2.5.4 Revise Atom, Central Distances Tab

Dialog Box: Revise Atom: Central Distance Tab [Input Atoms Dialog]

See the Basic Tab for most normal aspect of individual input atoms, the Temperature Factor Tab for modification or entry of temperature factors, the Slice Offset tab for adjusting boundaries for individual atoms in the Slice boundary option, and the Vector Tab for atomic vectors for magnetic moments or vibrational displacements.

This tab specifies central distances for an individual atom in the Enter Forms boundary

option.

Only six forms are allowed. The default values are the central distances entered in the option Enter Forms boundary option.

3.2.2.5.5 Revise Atom, Basic Tab

Dialog Box: Revise Atom: Basic Tab [Input Atoms Dialog]

See the Temperature Factor Tab for modification or entry of temperature factors, the Central Distance and Slice Offset tabs for adjusting boundaries for individual atoms, and the Vector Tab for atomic vectors for magnetic moments or vibrational displacements.

Label. Each atom may be assigned a label of up to 6 characters. Labels in ATOMS may not contain any embedded blanks. Any embedded blanks or leading blanks in labels will be converted to underscores. Trailing blanks will be stripped. These labels may now contain non-ANSI characters - see Character Sets. A superscript in roman numerals giving the symmetry operation which generates each atom may optionally be appended to the label on the drawing - this is selected in the Atom Labels dialog (Display menu).

Fractional coordinates. For crystals, the *x*, *y* and *z* coordinates should be in fractions of the unit cell. However, if you are drawing a molecule and have chosen unit Cartesian reference axes, the coordinates should be in Angstroms.

Irrational coordinates. In some hexagonal and trigonal space groups there are special positions with coordinates like 2/3, 1/3, 1/6 etc. Such irrational coordinates should be entered to at least the fifth decimal place - for example 0.66667 instead of 0.67 or 0.667. ATOMS must apply finite tolerance in the generation of all atomic positions, and the second form is not precise enough - multiple atoms will be generated instead of one atom on the special position.

Type. The atom type is used when locating bonds and polyhedra; 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 (see Polyhedra). For diffraction calculations (Powder, Precession) the type number *must* be the atomic number, or a number which gives an entry to the scattering factor table, modulo 100. That is, type numbers 6, 106, 206, 306 etc. will be read as atomic number 6 (carbon). Thus it is recommended that whenever possible type numbers be the atomic number, with added 100's if necessary to differentiate bonds and polyhedra.

Radius. Each atom will be represented by a sphere of this radius, unless it is involved in a polyhedron defined in the polyhedra input. If an atom is given radius 0.0, it will never be

plotted as a sphere and will only appear (as a corner) if it is involved as ligand in a complete coordination polyhedron. Bonds to such atoms will not be plotted unless the atoms are ligands in polyhedra. Thus if you want to show only polyhedra and *never* the individual atoms, give radii of 0.0 to all the atoms which may be involved, either as central atoms or as ligands. Even if you use positive radii for the atoms, you can switch off display of the atoms in incomplete polyhedra with a checkbox in the Polyhedra dialog (**Input1** menu). However, using a radius of 0.0 omits calculation of bonds to atoms in incomplete polyhedra, which can improve computation time and conserve memory.

If you do not want to show an atom at all, but want to show the bonds to the atom, that is draw a wire-frame model, enter a negative number for the radius. The absolute value of the radius can still be used in the Generate Bonds from Atomic Radii option. If atoms with negative radii are involved in polyhedra, they will be treated in the same way as atoms with positive radii.

For ball-and-stick drawings of typical structures, radii of about half the ionic or covalent radii usually work well. For space-filling or interpenetration the covalent radii can be multiplied by a number larger than one. All radii can be changed simultaneously by a given factor with the Atoms - Global dialog in the **Input1** menu.

Colors and patterns/shades. Each atom always has a rim and a fill, the colors for which are specified independently. Rims are turned on and off, and their widths are set, in the Line Widths dialog in the **Input2** menu. Shading applies only to fills. See Input Colors/Patterns/Pens for general aspects of input.

If you have checked the **Use individual atom distances** box in the boundary option Enter Forms, or the **Use individual atom offsets** box in the boundary option Slice, you should use the **Set Boundary Forms** button (Central Distances for Individual Atom or Slice Offsets for Individual Atom dialogs) to correct the central distance or offset for each form, up to six forms for distances. These distances or offsets are the ones which are actually used for the boundaries, but the central distances or offsets entered for each form in the boundary option are used for display of crystal shape and to set up the initial search intervals, so the individual distances or offsets should not be too different.

Shubnikov. This checkbox determines whether the equivalents of this particular input atom show vectors or other Shubnikov indicators (+ or -). Set the orientation of atomic vectors in the Vector Tab, and set the overall properties of vectors in the Vector dialog, called from the **Input1** menu or the Input Atoms dialog.

Protein. This only applies to structure input from Protein Data Bank files. It calls up a dialog (Protein) which gives protein specific information about the atom.

Line Width. If the **Use individual** box for atoms in the Line Widths dialog (**Input2** menu) is checked, the width specified here will be used, rather than the overall value in

the Line Widths dialog.

Hachure patterns are macroscopic patterns of lines which may be drawn within the outlines of atoms. These are useful for black-and-white output in situations where shading patterns are not reproduced very well, or a more definite pattern differentiation is desirable. The patterns are simply drawn in 2 dimensions and do not vary with attitude of the surface like the hachure patterns for Polyhedra.

Hachure patterns are not used in the 3D mode, and this entire section is not applicable to 3D display/output.

The **Spacing** is the distance between lines, in Angstroms. The colors/shades of the patterns are same as those selected for the outlines or edges (above), and the widths are also as selected (above) for each individual atom type, or as selected overall in the Line Widths dialog (Input2 menu).

If the **Use shade** box is checked, the gray shade selected in this dialog will also be applied as fill, in addition to the pattern, in black-and-white non-shaded output. This choice overrides the **Use initial patterns** box in the Shading dialog (Input2 menu). Shading, as selected in the Shading dialog (Input2 menu) is applied independently of hachure patterns, and it is possible to have both, either in color or black and white. In color display and output, the fill color (above) is always used.

3.2.2.5.6 Coordination of Atoms

Dialog Box: Coordination of Atoms [Atoms Dialog**]**

This controls computation of the list of bond or interatomic distances and angles centered on one or all of the input atoms. The radio buttons determine whether distances and angles are computed for all input atoms or only the one currently selected in the Input Atoms dialog.

Only 32 atoms in addition to the central atom are allowed in each coordination sphere, 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 then 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 BONDS.ATD, in the home directory (see File Types), and then shown in a Text window (see Types of Windows). In order for this Text window to operate properly, ATOMS exits from the Input Atoms dialog from which the **Coordination** dialog was originally called.

From this Text window, return to the Graphics window and the ordinary operating mode of ATOMS with the Window menu.

3.2.2.5.7 Construct Molecule from Z-Matrix

Dialog Box: Construct Molecule from Z-Matrix [Atoms Dialog**]**

With this dialog you can construct a molecule or structure fragment from a table of bond length and angles. The table, called a z-matrix, is widely used in molecular science, and you can read files in this form from other sources or write files for use in other software.

Action button section

The buttons at the top of the dialog indicate actions to be taken after the z-matrix at the bottom is filled out

Add will add the new generated atoms to the atoms already in the Atoms (Input) list. If the structure axes are not already Cartesian they are changed to Cartesian.

Replace will remove all the old atoms from the Atoms (Input) list and insert the new generated atoms.

Add and Replace will change the structure axes to Cartesian, since all calculations with z-matrices assume Cartesian coordinates, but most other settings, such as symmetry, boundary option and others in the Input1 menu, will not be changed

Read will read a file containing a z-matrix and insert the contents into this dialog. There should be no title or other extraneous lines, and each line, one line per atom, should contain the fields Label, Bond Connect, Bond Distance, Angle Connect, Bond Angle, Dihedral Connect and Dihedral Angle. Note that atom Type is not in this sequence, but the atom type or atomic number may be on the end of the line. The fields should be separated by spaces, commas, colons or semicolons.

Write will write a file as described in the previous paragraph, with one line for each atom, and with the type number at the end of the line. The Orientation (below) will be added after the atoms.

Show will do a conversion from z-matrix to Cartesian coordinates and display the z-matrix and the results in a Text window.

You can cut-and-paste blocks of atom lines in the z-matrix by using the **Read**, **Write** and **Show** buttons - for example you can save a file from the Text window (**Show**) after suitable editing, then **Read** it back.

Orientation section

The **Orientation** section allows the molecule or fragment to be located and oriented in any desirable way. It always refers to the first three atoms in the z-matrix list. Coordinates are always Cartesian.

The **Position** gives the x, y and z coordinates of the first atom. By default they are 0,0,0.

The **Atoms 1-2 vector** gives the vector from the first to the second atom. By default it is 1,0,0, which puts the second atom on the x-axis at the given bond distance from the first atom.

The **Atoms 1-2-3 plane** gives the normal to the plane containing the first three atoms. The vector from atom 2 to atom 1, the vector from atom 2 to atom 3, and this normal form a right-handed system. By default this normal is 0,0,-1 which puts the third atom in the x-y plane with a positive angle giving a positive y-coordinate for atom 3 (assuming standard placement and orientation for atoms 1 and 2).

The vectors need not be normalized; they will be normalized during the transformation.

Z-Matrix section

Each line in the matrix below refers to an atom. You can select each atom by clicking on the number to the left, and the entries are acted upon by the **Move Up**, **Move Down** (move the line within the list), **Insert** and **Delete** buttons. The up and down arrows to the right scroll the entire list up or down if there are more atoms than the list can hold at once.

The atoms are positioned with respect to other atoms in the list. The first three atoms are oriented and positioned as described above in Orientation, and all other atoms are placed with respect to these three.

Each line describes the positioning of a new atom (1) with respect to up to 3 atoms already in the list (2, 3, and 4).

The **Label** and **Type** give the ATOMS label and type; the type is normally the atomic number. If the type is 0, ATOMS will attempt to determine the atomic number (or other type number) from the first two characters of the label.

Bond Connect: the number in this list of the atom (2) to which the new atom (1) is directly bonded.

Bond Distance: distance in Angstroms from 1 to 2.

Angle Connect: the number in this list of an atom forming an ordinary angle 1-2-3.

Bond Angle: the value of the angle 1-2-3 in degrees.

Dihedral Connect: the number in this list of an atom forming a dihedral angle 1-2-3-4. The dihedral angle is the angle between the normals to the plane 1-2-3 and the plane 2-3-4. This angle (sometimes referred to as tau) is conventionally given values from 0 to 180 and 0 to -180 degrees, and the sign is positive if, viewing the angle along the bond 2-3, with 2 nearer the observer than 3, the angle from the projection of 2-1 to the projection of 3-4 is traced in the clockwise sense (definition from Wilson, Decius and Cross, Molecular Vibrations, 1955, p 60).

Dihedral Angle: the value of the angle between the normals to the plane 1-2-3 and the plane 2-3-4 in degrees.

3.2.2.5.8 Add Hydrogens

Dialog Box: Add Hydrogens [Atoms Dialog**]**

This option currently will attempt to identify carbon, nitrogen and oxygen atoms which should have hydrogen attached. These atoms must have atom types 6, 7 and 8 respectively.

The first option will actually add hydrogen atoms to the list of input atoms - the new H atoms will immediately follow the atom to which they are added.

The second option, "Change types..." will not actually add atoms, it will simply change the atom type of the H-deficient atom to indicate the deficiency. The type number of carbon atoms will be changed from 6 to 106, 206 or 306 respectively if the atom lacks 1, 2 or 3 hydrogens and similarly for N and O. This option is intended specifically for files which will be imported into the program VIBRATZ, and for vibrational models in which the weights of the C, N or O atoms are "corrected" for the attached hydrogens, rather than dealing with the H atoms explicitly.

Orientation. When adding two hydrogens to a double-bonded carbon or to a nitrogen the orientation is quasi-random with respect to rotation about the other bond vector, and likewise when adding three hydrogens to a singly-bonded carbon atom. When adding one H to an oxygen atom the orientation of the plane of the X-O-H angle is also quasi-random. "Quasi-random" means that the hydrogens are added in a fixed orientation with the C-X vector (if the atom in question is a carbon) rotated to [001], then the group is in effect rotated back to its actual orientation in the structure. H2O groups (water) are fully random in that two random rotations are applied.

Symmetry. The generated hydrogen atoms may not be consistent with symmetry, which will be indicated by an excess number of H atoms in the complete structure.

At this time the algorithms for locating hydrogens are very simple, based only on the number of atoms and bond lengths in the first coordination sphere. The procedure was developed specifically for protein structures where there are only a limited number of configurations of nitrogen in particular. The algorithms may be corrected and expanded as necessary. If the hydrogen location in a structure is incorrect or ambiguous, please send the structure file (.str file) to support@shapesoftware.com, with a list of the input atoms, by number if necessary, which are believed to be incorrect.

3.2.2.6 Polyhedra

Dialog Box: Polyhedra [Input1 Menu**]**

This lists the current polyhedra. Click on individual items in the list, then on the buttons

to add, modify or delete polyhedra. The **Revise** and **Add Polyhedra** buttons call up the Polyhedron Data dialog.

To calculate bond distances and angles, for use in bond and polyhedra input, use the Coordination button in the Input Atoms dialog.

If the **Show back edges dashed** box is checked, the invisible back edges of polyhedra will be drawn as dashed lines - the dash parameters are set in the Crystal Edges dialog. Polyhedra are still opaque. This applies to unshaded polyhedra only.

The possibilities for showing polyhedra are diverse, depending on the display mode. It may be necessary to select settings in the 3D Polyhedra dialog and also the Ellipsoid Parameters dialog as well as this dialog. These two other dialogs are accessible directly from this one with buttons.

The **3D parameters** button calls up a dialog (3D Polyhedra) for specification of polyhedron properties unique to the 3D display mode**.** This includes options to draw the polyhedron faces as transparent and to show the central atom and interior bonds. In the 3D Polyhedra dialog, and also the Ellipsoid Parameters dialog, there is an option to show corners and/or central atoms of polyhedra as thermal ellipsoids in the 3D display mode.

The **Ellipsoid Parameters** button calls up the Ellipsoid Parameters dialog. In the Ellipsoid display mode (which mimics ORTEP) polyhedra are never shown with actual flat faces, but there is an option in the Ellipsoid Parameters dialog to draw the ligand-ligand "bonds" or polyhedron edges, and also the central-ligand "bonds" as standard ORTEP bonds.

The **Show ligands as spheres** group has three options. If the **None** button is checked, only the polyhedron faces are shown and ligands are represented as points at the corners. If one of the other boxes is checked, ligands are drawn as spheres. In the Standard display mode, this option is an approximation in that junctions between the atoms and the polyhedra are straight lines. In the 3D display mode, junctions are always correct. For spherical atoms (not thermal ellipsoids) you can use the **Atom radii** entered for each input atom, or you can use a **Single radius** for all ligands, entered in the edit box to the right of this option. The **Single radius** option is not applicable to ellipsoids in the 3D display mode; if either the **Atom radii** or **Single radius** option is selected, ellipsoids will be shown at polyhedron corners. If atoms are not shown at polyhedra corners (**None** option), the bonds to such corners are always cylindrical, not tapered as they could be if they were to ellipsoids. This option does not function as well when **Hachure patterns** (Polyhedron Data dialog) are used - the junctions of the polyhedron corners with the spheres are not correctly drawn.

The **Test for incomplete polyhedra** group determines how atoms in incomplete polyhedra are handled. As detailed in Generated Atom Data, when ATOMS locates

polyhedra, it assigns a certain plot code (5) to atoms which are parts of polyhedra which have fewer than the specified number of ligands. This will always be done, even if the option selected is **No test**, and the atoms thus flagged can either be omitted or plotted as spheres, depending on the setting discussed in the previous paragraph. However, some further screening of possible polyhedral atoms can be made, to eliminate display of potential ligands which are not found to bond to any of the specified central atoms within the given boundaries. While locating polyhedra, ATOMS can make a list of either the **Input atom numbers** or the **Atom types** involved (as ligands) in polyhedra. Then after all polyhedra are located, the generated atom list is searched to find those atoms with the specified numbers, and these atoms are then marked with plot code 5, i.e. as belonging to incomplete polyhedra. The normal option for crystals is **Input atom numbers.** However, this option is of no use when the structure is of type Input=Generated, or for a molecule with no symmetry, since every input atom corresponds to a single generated atom. Thus the default for **Input = Generated** is **No test**. The **Atom types** option works well when each input atom type (normally the atomic number) plays only one structural role, i.e. is either always a polyhedron ligand or not. However when an atom type can be a polyhedral ligand in some cases, and a non-ligand in others (for example when oxygen atoms are ligands in phosphate radicals or other groups and also are present in water molecules or hydroxyls), the atoms which are non-ligands will be incorrectly omitted. When using the **Atom types** option, it may thus be necessary to assign special types to atoms with different structural roles, for example 8 for oxygens which are in phophate (or other) groups; 108 for hydroxyls; and 208 for waters.

3.2.2.6.1 Polyhedron Data

Dialog Box: Polyhedron Data [Polyhedra Dialog**]**

Polyhedra are defined by specifying the **Coordination number**, and the **Types** of the central atom and the coordinating atoms or ligands. Note that atom types are used, not individual atom numbers, so that chemically similar atoms may be grouped. It is usually convenient to use atomic numbers for the types. You must further specify the **Maximum distance** for the bonds from the central atom to the ligands.

If the coordination number is given as 3 or larger, only complete polyhedra are identified and displayed; that is, both the central atom and all the ligands must be within the structure boundaries defined in the Boundary option. Atoms belonging to incomplete polyhedra can be displayed as spheres with the radii assigned in the Revise Atom dialog, unless their atomic radii are zero - then they will be marked as permanently non-plotting. The display of these atoms is controlled by a checkbox in the Polyhedra dialog. If more coordinating atoms are found than specified within the given distance, an error message is shown and the polyhedron is skipped.

If you do not know the coordination number or the bond distances, you may wish to

make one or more runs with the coordination number set to zero. In this case, all polyhedra with three or more ligands within the bond-distance limit will be accepted, and you can examine the Calculation Output to see what the proper coordination number or distance limits should be.

If you want to show polyhedra which do not have central atoms, it will be necessary to enter dummy central atoms. The best way to do this is to take the average of each coordinate for all the atoms in one polyhedron.

In the Standard display mode, polyhedra are always opaque; if you wish to show only the skeletons, you can define bonds among the ligands (next section). Also, you can use the Skeletal display mode, selected in the Display Mode sub-menu of the **Display** menu. Once the ligands are located, central atoms are never shown in non-3D modes.

If a nominally planar coordination is not strictly planar, within tolerances, it will be shown as a polyhedron. In Standard display mode, strictly planar polyhedra will vanish when seen edge-on if display of rims or edges is not turned on with the Rims dialog in the **Input2** menu.

In 3D mode, planar polyhedra have finite thickness. There are also several options for showing polyhedra as opaque, translucent or skeletal (see 3D Polyhedra).

Colors and patterns/shades. Each polyhedron may have a rim and a fill, the colors for which are specified independently. Rims are turned on and off, and their widths are set, in the Line Widths dialog in the File2 menu. Shading applies only to fills. See Input Colors/Patterns/Pens for general aspects of input.

Line Width. If the **Use individual** box for polyhedra in the Line Widths dialog (**Input2** menu) is checked, the width specified here will be used, rather than the overall value in the Line Widths dialog.

Hachure patterns are patterns of lines based on a square grid which may be applied to polyhedra. The patterns are drawn on the surface of each polyhedron face in 3 dimensions (not simply applied in 2 dimensions to the projection of the face), so that they give some illusion of depth or shading. Thus they enhance the 3-dimensional appearance of the drawing while at the same time allowing differentiation of the different types of polyhedra. Differentiation of polyhedra types is almost impossible using gray shades (above) alone.

Hachure patterns are not used in the 3D Display mode, and this entire section is not applicable to 3D display/output.

The **Spacing** is the distance between lines, in Angstroms. The colors/shades of the patterns are same as those selected for the outlines or edges (above), and the widths are

also as selected (above) for each individual polyhedra type, or as selected overall in the Line Widths dialog (Input2 menu).

If the **Use shade** box is checked, the gray shade selected in this dialog will also be applied as fill, in addition to the pattern, in black-and-white non-shaded output. This choice is overridden if the **Use initial patterns** box is checked in the Shading dialog (Input2 menu) - in that case, gray shades or dot patterns will always be applied.

In color display and output, the fill color (above) is always used. Shading, as selected in the Shading dialog (Input2 menu) is applied independently of hachure patterns, and it is possible to have both either in color or black and white. If hachure patterns are used in conjunction with shading for atoms and bonds, the illumination vector (Shading dialog) should probably be 1,0,0, as this is the effective illumination direction for hachures.

Differentiating polyhedra. The size and shape of different polyhedra are not generally sufficient to allow identification of the polyhedron type in a drawing. There are several different display attributes of polyhedra which may be varied alone or in combinations to allow differentiation.

1) *Color*. This is certainly the best option when it is available, especially when using shading, except that a significant fraction of people are at least partially color-blind.

2) *Hachure patterns.* Both the pattern itself and the scale can be varied.

3) *Gray shade of fill (black-and-white)*. This does not usually work well in combination with shading.

4) *Width of edges*.

5) *Gray shade of edges*. Lines of one dot width (width 0.0 in this dialog) are always black.

3.2.2.7 Bonds

Dialog Box: Bonds [Input1 Menu**]**

This lists the current bonds. Click on individual items in the list, then on the buttons to revise, delete or add bonds. The **Revise** and **Add Bonds** buttons call up the Bond Data dialog.

To calculate bond distances and angles, for use in bond and polyhedra input, use the Coordination button in the Input Atoms dialog.

You can also click the Generate from Radii button, to derive bonds automatically.

PDB quick bonds check box. In the case of Protein Data Bank (PDB) structures, ATOMS is able to use the information on residues which is present in the file, as well as CONNECT records, to greatly decrease the time required to locate bonds, compared to standard ATOMS methods for crystals. However, if some bonds are missing or duplicated it may be necessary to uncheck this box.

Color mode. For stick bonds you can use either the color specified in the Bond Data dialog for the entire bond, or the atom colors in a half-and-half arrangement.

3.2.2.7.1 Bond Data

Dialog Box: Bond Data [Bonds Dialog]

Bonds are specified by giving the **Types** of the two atoms involved - in some cases, such as carbon-carbon bonds, these may be the same. The **Minimum**, as well as **Maximum** distance must be specified; this allows differentiating bonds to the same atom. A stick bond has the shape of a cylinder, but if the **Radius** of this cylinder is entered as zero, then the bond is drawn as a single line. The width of this single line, or the width of the lines defining the outline of a stick bond, is normally one dot in screen display or dot-matrix plots, but this can be changed - for all bonds in the Line Widths dialog in the Input2 Menu, or if desired for each input bond (see below).

Bonds to atoms in polyhedra can only be drawn to ligands defined in the Polyhedra input, not to central atoms.

If you wish to show only bonds, not atoms (wire-frame model), you should enter negative radii for the atoms.

If the **Inter-molecule** box is checked, this bond specification will not be used in locating molecules or groups in either the Molecules in Crystal boundary options, or the **Find** button in the Generated Atom Data dialog or Locate Groups dialog. Intermolecule bonds are drawn normally by default, but they can be dimmed, highlighted or hidden (Atom/Bond Plot States dialog in the Input2 Menu, or Dialog Bar - Right)

In Standard display mode, the interpenetration relationships of cylindrical bonds with each other, and with the polyhedra to which they are attached, are not drawn accurately. This affects wire-frame atoms (atomic radius negative), and bonds from polyhedral ligands to other atoms. The affect of this limitation is mimimized if the bond radii are kept relatively small. In Standard display mode, if atoms are interpenetrating (interatomic distance less than the sum of the radii), no sticks or lines will be shown, but it is still necessary to specify a bond between the atom types so that the junctions will be handled properly (if no bond is specified, the atom in front will simply be drawn over the other one). The radius and colors of the bond are immaterial for interpenetrating atoms. In 3D mode, interpenetration relations are always drawn correctly and if atoms are known

to interpenetrate it is not necessary to specify bonds between them.

Colors and patterns/shades. Each bond may have a rim and a fill, the colors for which are specified independently. The color for a single-line bond is the same as the rim color for a cylindrical bond. Rims are turned on and off, and their widths are set, in the Line Widths dialog in the Input2 menu. Shading applies only to fills. See Input Colors/Patterns/Pens for general aspects of input.

Line Width. If the **Use individual** box for bonds in the Line Widths dialog (**Input2** menu) is checked, the width specified here will be used, rather than the overall value in the Line Widths dialog.

Individual input bonds may be **dashed** if they are single-line (radius 0.0). The length of the dashes is specified in the Crystal Edges dialog.

3.2.2.7.2 Generate Bonds

Dialog Box: Generate Bonds from Atomic Radii [Import File**] [** Bond Data dialog**]**

This will derive a set of bond specifications for the atoms currently in memory, which may have just been read in from an import file.

Source of atomic radii. Starting with V4.0, ATOMS can use a constant set of radii in an internal table (read in from the RADII file), rather than the given input atom radii (which is still an option). If you choose to use the table, the element can be identified either using the first two characters of the label, or using the type number which is assumed to be the atomic number. If you choose to use the input atom radii, the atom list is scanned and the radius is taken from the first occurrence of each atom type. That is, if input atom number one is type 1 with a certain radius, and input atom number seven (for example) is also type 1 but with a different radius, only the radius of input atom number one will be used.

The **Maximum distance as fraction of radii sum** field specifies the upper distance limit for each type of bond. This will be the sum of the radii of the two atom types, multiplied by the number entered in this field. The minimum distance will be 0.2 Angstroms. If you choose to use the current input atom radii, the factor must take account of any reductions in the atomic radii from values which cause the atoms to almost touch.

If the **Delete old bonds** box is not checked, the new bond list will simply be added to the old list.

The **All pairs/Cation-anion only** radio buttons allows skipping many superfluous combinations, i.e. atoms which never bond with each other. In the RADII file, each atom is assigned a code indicating whether it is a cation (1), an anion (-1), non-metal (0) or

inert (3). A "non-metal" is considered to be able to bond with all other types except inert atoms (rare gases). At the time of generating bonds, the codes for the two input atoms in question are added together, and any resulting values with absolute value greater than 1 are rejected. The codes in the RADII file are by default set up primarily for inorganic structures, and if you want to use this option for organic structures, they may need to be modified.

Whether or not this option is used, superfluous bonds can still be removed in the Bonds dialog in the **Input1** menu.

In the **Bond radii** group of radio buttons, you can choose to make the bond radius a fraction of the radius of the smaller atom of the two in the bond; or to enter a constant radius for all bonds. A constant radius value of 0.0 will result in single-line bonds.

The **Default Colors** button will call up a dialog similar to that for individual input bonds (Bond Data), but the atoms types, distance limits and radius will be missing.

If the **Hydrogen bonds** box is checked, a list of Specifications will be used to set up bonds for atoms involved in hydrogen bonding. This will result in two input bonds for each pair (H-other) which may be involved in hydrogen bonding. If the **Hydrogen bonds** box is not checked, any bonds involving hydrogen should be of the normal covalent type.

3.2.2.7.3 Hydrogen Bond Specifications

Dialog Box: Hydrogen Bond Specifications [Generate Bonds Dialog]

The current hydrogen bond specifications are given in the list box - edit the variables for the selected specification in the edit boxes on the right.

If the **Hydrogen bonds** box in the Generate Bonds dialog is checked these specification will be used to set up bonds for atoms involved in hydrogen bonding. As ATOMS considers each possible pair of atoms in the input list, it will test the type numbers against those in this list

If one member of the pair has type number 1 (hydrogen), 99 (deuterium) or 98 (tritium), and the other member of the pair has one of the type numbers in this list, hydrogen bonds will be set up. If both members of the pair have type numbers indicating hydrogen, no bonds at all will be set up. Note that atomic numbers in this list (non-hydrogen) do not need to be atomic numbers, but hydrogen itself (and deuterium and tritium) must have the default atomic numbers.

Two separate input bonds will be set up for each hydrogen-other pair: a short or strong bond in which the other (the atom in this list) is the hydrogen donor in a hydrogen bond; and a long bond or hydrogen bond itself in which the other atom is the acceptor. For normal, strong (non hydrogen) bonds between H and the other atom, the minimum

distance is 0.2 Angstroms and the maximum bond distance is the minimum distance (**Min**) in this table. For hydrogen bonds between H and the other atom, the minimum bond distance is the minimum distance in this table and the maximum bond distance is the maximum distance (**Max**) in this table. That is, the **Min** value is the boundary between donor bonds and acceptor bonds, and the **Max** distance is the longest possible acceptor bond.

The **Intermol** (Intermolecular) flag determines whether bonds will be considered to be intermolecular (see Bond Data dialog) for purposes of locating molecules.

Any input bond specifications set up with this option can always be edited through the Input Bonds dialog.

3.2.2.8 Atoms - Global, Variables Tab

Dialog Box: Atoms - Global: Variables Tab [Input1 Menu**]**

This applies to input atoms, not generated atoms. Select the atoms to be modified in the Which Tab.

3.2.2.9 Atoms - Global, Which Atoms Tab

Dialog Box: Atoms - Global: Which Atoms Tab [Input1 Menu**]**

This tab specifies which atoms will be changed: it applies to input atoms, not generated atoms. You can change parameters for all atoms, for all atoms of a given type, for a sequence of atoms, or for all atoms in a given fragment (if there is more than one fragment - see Multiple Structures) in the **Transform** menu.

Randomize. This allows you to modify only a certain fraction of the input atoms chosen, on a random basis. This is intended primarily for representing solid solutions - you can modify the colors and/or sizes of individual input atoms. Before doing this, it will normally be necessary to do the Generated to Input option in the Transform Menu, so that all atoms become input atoms. If only atoms on a certain site are to be modified, it may be necessary to change the atom type of this site before transforming Generated to Input.

A solid solution with only two types of atom is straightforward, but more than two occupants will require some pre-calculation and repeated use of this dialog. Since all atoms present are affected, the fraction which is entered in this dialog must be with respect to the new occupant and those occupants already present, not the final fraction. For example, suppose you want to show four occupants, each with occupancy factor 0.25. The first occupant is already present. When adding the second occupant, for example changing the color, the fraction should be 0.5, because this gives the correct

ratio of occupant 1 and 2. To add the third component, this dialog must be repeated and the fraction is 0.3333, and for the fourth and last occupant the fraction is 0.25.

Select the variables or attributes to be changed in the Variables Tab.

3.2.2.10 Atomic Vectors

Dialog Box: Atomic Vectors [Input1 Menu**] [** Input Atoms dialog**]**

The vectors can be cylinders or single lines; if cylinders, all will have the same radius.

The **Scale factor** should be in whatever units are necessary to convert the given lengths of the vectors (specified in the **Vector Tab** of the Revise Atom dialog) to suitable lengths in Angstroms. The length of the vector is measured from the surface of the atom to the end of the line or the cylindrical portion, except for double ended vectors (see below) in pen plots, in which the length is measured from the surface of the atom to the center of the sphere on the positive end..

You can choose to use the colors of each individual atom, or the color specified in this dialog.

If the **Single-end, no arrow** radio box is not checked, the vectors will be single lines or cylinders extending in one direction from the atom. The termination is a disk in Standard display mode or a hemisphere in 3D display mode. If the Single-end, arrow radio box is checked, the end will be marked with a cone (arrowhead) except in pen-plot output, in which the positive ends will be marked with a sphere. If the **Double-ended** box is checked, the vectors will extend in both directions from the atom, and the positive end will be marked with a cone (arrowhead).

The **Radius increment for arrow** gives the absolute increment in Angstroms of the radius of the base of the cone over the radius of the vector. The length of the arrow is determined by the **Length/radius** value. Likewise, the **Radius increment for sphere** (pen-plot only) gives the absolute increment in Angstroms of the radius of the sphere over the radius of the vector.

Vectors are drawn by adding pseudo-atoms to the list of generated atoms, and adding pseudo-bonds between these pseudo-atoms and the real atom to which the vector is attached. Thus if the length, orientation (Revise Atom dialog, Vector tab) or single/double-ended status is changed ***the structure must be recalculated***, rather than just replotted. Also, since the length is computed as the visible cylindrical part of the vector, if you change atomic radii the vector lengths will change unless the structure is recalculated. In this dialog (Atomic Vectors), changing the scale factor will require recalculation, as will changing the vector radius, since this affects the length of the visible part of the vector (although this effect is slight).

3.2.2.11 Vibrational Modes

Dialog Box: Vibrational Modes [Input1 Menu]

See the Import File dialog for general aspects of importing atomic-structure data files.

This dialog controls.MOT vibrational displacement files (see Import VIBRAT (.MOT) files and Coordinating ATOMS and VIBRATZ) written by the VIBRATZ program (or the original VIBRAT - Dowty, Phys Chem Minerals (1987) 14:67). When these files are read in the infomation is converted into a standard ATOMS data file, and also a special.MDT modes file which contains the atomic displacements and other information for each vibrational mode. When you re-read the.STR file, the.MDT file is read in also; if this fails, you can read it in using one of the options in the **Modes file** group in this dialog. The title of the.MDS file should already be present in the edit box so you can edit it and click the **Read Named File** button, or use the **Browse** button to find it.

The **Read.MOT file for motions only** button will read the atomic motions, but will ignore other information in the.MOT file. This allows you to set up the drawing once in terms of atom sizes, colors, etc., and retain all this if you decide to recalculate the vibrational modes in VIBRAT.

The mode which is in the.STR file and which is displayed when you first read and calculate the file is the one which was selected when the.STR file was last saved.

After selecting a new mode, you will need to recalculate the structure (Calculate command in the File menu, or the Dialog Bar), not simply replot, since new vectors involve generating new pseudo-atoms and pseudo-bonds.

To see on the screen or output which vibrational mode is being displayed, select the **Print title on plot** option in the Title/Axes dialog in the Input1 menu.

.MOT files from versions of VIBRAT previous to 1997 do not transmit the lattice-type information which is necessary for display of the unit cell. Insert the correct Bravais-lattice symbol if necessary with the **Lattice** combo box. This does not affect the atoms, bonds and displacements.

VIBRATZ data for a crystal can be imported in either of two ways; showing the atoms in the primitive unit cell as a molecule; or using the normal ATOMS boundary options for crystals (see Import VIBRAT (.MOT) files).

VIBRATZ uses two types of atoms for crystals or infinite polymers: *primary* atoms, which are just those in the primitive unit cell; and *secondary* atoms, which are those required to complete the bonds and angles of the complete set of internal coordinates (i.e.

force constants). Molecules do not require secondary atoms. For a crystal, the atoms of the primitive (not Bravais) unit cell are listed in the.MOT file, but the coordinates are given in the standard Bravais cell..

If you have imported the.MOT file as a molecule, not a crystal, this distincion is preserved. The structure is treated as a molecule, that is there is no symmetry and no lattice translations. Sometimes there may be more secondary than primary atoms. You have the option to show the secondary atoms in just the same way as the primary atoms; to mark the secondary atoms with a triangle; or to omit the secondary atoms altogether. If you omit the secondary atoms, the bonds to them will also be omitted.

If you have imported the.MOT file as a crystal, there are no secondary atoms. If the unit cell is non-primitive the Bravais cell is filled out (i.e. you do not see only the atoms in the primitive cell), and all atoms which are translationally equivalent are displayed in the same way.

To specify the details of the vectors which represent the atomic displacements, including the scale factor, go to the Atomic Vectors dialog in the Input1 menu.

Animate Motions. This section controls animated display of the vibrational motions.

The **Screen** button will produce an animated display in the current Graphics window. Clicking the mouse or hitting any key will terminate the animation. In Windows, the Full-Screen mode can also be animated with CTRL-A.

Frames/cycle applies to screen display only - it controls the speed, larger values giving slower speed.

The **Movie** button will bring up the Movie dialog and allow writing of "video" files, .AVI for Windows or .MOV for Macintosh (not available for Linux).

3.2.2.12 Cavity Parameters

Dialog Box: Cavity Parameters [Input1 Menu**]**

This dialog controls the Cavities display mode which uses the 3D system capabilities - if your system does not support 3D display the Cavities display mode is not available. It is applicable to crystals only (not molecules or polymers). The display mode is selected in the Dialog Bar - Left or the Display Mode option in the Display Menu.

Grid spacing. This is the approximate spacing in Angstroms between sample points - the actual spacing may be slightly reduced from this value to give an integral number of points across the unit cell. This should be considerably smaller than the radius of the smallest atom. Values of 0.1 to 0.4 are reasonable. Time of the calculation is proportional to the cube of this number.

Particle radius. This is the radius of the sphere which is presumed to exist in the cavities. The volume shown is that enclosing possible centerpoint locations of this sphere. If this radius is zero, the volume shown will simply be that not occupied by the atoms of the structure.

Show cell faces. If this box is checked, the surface where the cavity volume crosses the unit-cell faces is shown in a different color (next paragraph). If not checked, it may be possible to see completely through a channel, although this requires that the channel be fairly straight. The inner surface is then given a different color (next paragraph).

List Coords [Coordinates]. This will list the fractional coordinates of all grid points which can accomodate the sphere of the specified Particle radius. The listing is made to a text file, CAVVAL.ATD, and this file is then displayed in a Text window (see Types of Windows).

Colors - Outer surface and Cell faces/Inner. The first color is for the outer or exterior surface of the cavities, inside the unit cell. If the **Show cell faces** box (above) is checked, the second color is for the surfaces where the cavities cross the unit-cell faces. The cell-face surfaces may be especially important in judging the continuity of the cavities. If the **Show cell faces** box (above) is not checked, the second color is for the inside or inner surface of the cavities themselves. The material parameters used (3D Parameters/Materials, Input2 menu) are those for polyhedra. As for polyhedra, the specular component is usually best kept small.

In VRML files the viewer controls the color of inner surfaces - it is impossible to specify the color without redrawing the surface (i.e. there is only one color per surface in a VRML file). Some viewers may make the inner surfaces the same color as outer surfaces (there may be a switch specifying that surfaces are "double sided"), some may make them black and some may make them transparent. For VRML files it is safest to check the **Show cell faces** box above.

Offset (fraction of unit cell). This allows the boundaries of the crystal volume shown to be offset by a fraction of the unit cell (axis length). The offset is always in a positive direction, and the lower and upper boundaries are offset by the same amount. The **Offsets** shift the boundaries of the volume shown, not the unit cell itself or the unit-cell **Displacements** in the Axes/Unit Cell option.

Number of unit cells. You may display multiple integral unit cells in any of the axis directions. The extra unit cells extend in the positive directions of the axes. You cannot display fractions of unit cells.

Porosity. This is the fraction of the volume of the unit cell which can accomodate the given size particle. The value shown is for the the last plot (which could be printed or file

output, rather than screen display). To get true porosity, set the **Particle radius** to zero.

Changing the **Grid spacing** or **Offset** requires a recalculation of the grid, and thus you must select **Calculate** in the Dialog Bar - Left or **File** menu. Changing other parameters only requires Replot.

3.2.3 Input2 Menu (Graphics Window)

Note: if the screen is narrow, this may be a submenu in the **Input** menu.

Crystal Edges - This controls the display attributes (color, etc.) of the edges defining the exterior crystal shape, if present.

Perspective - Controls drawing in perspective versus straight projection.

Stereopairs - Controls automatic drawing of stereopairs.

Rims - Controls presence or absence of rims on atoms and bonds and edges on polyhedra.

Linewidths - Controls widths of lines used as edges, etc.

Shading - Controls three-dimensional shading.

Background Color - Controls background color (ignored for b/w display or output).

Crystal Axes - Controls display of crystal or structure axes.

Unit Cell - Controls display of the unit cell, which may be drawn as edges or solid (translucent) faces.

Ellipsoid Parameters - Controls the drawing of ellipsoids and stick bonds in the Thermal Ellipsoids and 3D display modes.

3D Parameters - A pop-up submenu, controlling aspects of the 3D Display mode.

---- General - Some overall parameters.

---- Lighting - Number, direction and/or location of lights.

---- Material - The way the atoms, bonds and polyhedra reflect or emit light.

---- Fog (Fading) - Aids the illusion of depth.

---- Polyhedra - Some aspects of polyhedra specific to the 3D drawing mode.

PDB (Protein) Display - A pop-up submenu (no dialogs), controlling which atoms are plotting in Protein Data Bank structures.

----**All Atoms**
----**Omit All Hetatoms**
----**Omit Water**

Initial Orientation - Controls the orientation which can be imposed after calculation and before first viewing.

Scaling - Controls scaling modes and factors.

Centering and Displacements - Controls displacements and automatic centering of the image.

Calculation Output - Controls the listing of the analytical results of the calculations such as atom locations, bonds, etc.

Atom/Bond Plot States - Allows changing the plotting or non-plotting status of generated atoms and intermolecular bonds.

3.2.3.1 Crystal Edges and Faces

Dialog Box: Crystal Edges and Faces [Input2 Menu**]**

This dialog controls the appearance of the display crystal shape. The Crystal Forms for Display dialog in the **Input1** menu controls the actual generation of the faces which make up this shape.

Display. **Crystal** means the edges which define the external boundary faces. **Atoms** means the atomic structure including bonds and polyhedra. If you are drawing a molecule or polymer, crystal edges are not normally shown, but you can nevertheless display a crystal shape if desired.

Edges Only/Faces Only/Both. In 3D display modes the actual planes of the crystal faces can be shown, instead of or in addition to the edges between faces. Set the **Opacity** and color of the faces in the group at the bottom of the dialog.

Dash length and dash ratio. The dashes are used for back edges of crystals and in display of Crystal Axes and Unit Cell. Length or repeat distance is in inches/centimeters,

and the length factor is the actual length of the solid part divided by the repeat distance. Note that when using Frames in output the dash length remains the same - it may be desirable to decrease the length for very small plots.

Back edges - those not visible if the crystal is opaque - may be specified as none (not shown at all), dashed or solid.

Lines/Cylinders. In 3D display modes the edges may be shown as lines or cylinders of the specified width.

Colors, Patterns, Pen numbers. Front edges are those which are visible; back edges are not visible in an opaque crystal. Widths of lines are set in the Line Widths dialog in the Input2 Menu). See Input Colors/Patterns/Pens for general aspects of input.

For alternate ways of drawing unit cells, and problems sometimes encountered with crystal edges, see Drawing Crystal and Unit-Cell edges.

3.2.3.2 Perspective

Dialog Box: Perspective [Input2 Menu**]**

If perspective is not in effect, or turned off, the drawing is simply a perpendicular or orthographic projection down the observer *x* axis. If perspective is on, the drawing is projected from a point (*xp+xo, yo, zo*), where *xp* is the perspective distance and *xo, yo* and *zo* are the projection offsets (below), perpendicularly onto the plane (*xo*, *y*,*z*), that is a horizontal plane passing through the structure center. Scaling applies to the projection plane, but obviously fixed scaling has limited intrinsic meaning. Generally the scaling modes **Universal Maximum** or **Each View Maximum** (set in the Scaling dialog in the Input2 menu) should be used when perspective is in effect. The perspective distance is the distance *xp* of the projection point from the projection plane, or in other words the distance from which the structure is viewed (distance from the center of the structure to the eye). Smaller distances will accentuate the "perspective"; larger distances will cause the plot to appear more like a straight-on projection. The perspective distance should be considerably larger than the distance of the furthest atom from the center (or the plane *x=xo*) in the positive *x* direction. If atoms come within about 1 Angstrom of the *x* coordinate of the eye they will be omitted, but many of such atoms would be off scale (sideways) anyway.

Projection Offsets. During calculation the midpoint of the structure is determined - this includes all atoms, but does not include crystal edges, unit cell or axes. When projecting in Perspective viewing, the coordinates of this midpoint, *xo, yo* and *zo* are used as the coordinates of the projection point (*xp+xo, yo, zo*), where *xp* is the perspective distance. This insures that the projection is never oblique to the projection plane. This is equivalent to the Automatic Centering option in previous versions of ATOMS. Although arbitrary

specification of the offsets is no longer allowed, you can attain almost any attitude of the structure by suitable rotations. Note that the structure can be displaced in the plotting area with the Centering and Displacements dialog (**Input2** menu). In effect, the projection direction moves along with the structure. If you also have structure axes or a unit cell (Display of Axes and Unit Cell dialogs, Input2 menu) which are separated from the structure, they will be projected obliquely, according to their distance in Angstroms from the structure center; that is, if you are looking down, say, the a-axis in the structure itself, structure axes placed to the side will not have that axis exactly parallel to the view direction. You can rotate to effect a compromise between the two orientations.

3.2.3.3 Stereopairs

Dialog Box: Stereopairs [Input2 Menu]

When stereopair display is on, two images of the structure will be drawn. The upper part of this dialog pertains to non-Anaglyph display modes, in which each image centered in one half of the plot area. The left or left-eye image will be rotated by the stereopair **Rotation angle** clockwise from the normal orientation, and the right-eye image will be rotated the same amount counter-clockwise. If shading is active the illumination vector will be rotated along with the structure. The stereopair rotation angle is typically about 3 degrees, although the proper angle may vary depending on the perspective distance, the actual viewing method, etc.

The **Stereopairs on** check box applies only to separated-image stereopairs drawn in non-Anaglyph display modes.

If the hard copy of stereopairs is to be viewed directly or with a small viewer, a frame size in the dot-matrix or pen plot of 4 to 5 inches across will give a distance between the two images about equal to the normal interocular distance. If you want a pair of images larger than a single page, you can use the Stereopair Rotation in the **Rotation** menu to rotate the images separately, if shading is in effect; if shading is not in effect, ordinary rotation on z is sufficient..

Few people can directly view a stereo pair as shown on the full screen because the images are considerably further apart than the eyes. However, if a negative rotation angle is used, some people can view the image by crossing their eyes.

The lower half of the dialog pertains to the Anaglyph display mode, selected in the **Display Mode** command in the **Display** menu, or the **Dialog Bar - Left**. In this type of display, there are two skeletal images of two different colors, superimposed. Generally red/blue with a black background works best for the screen, while red/green with a white background works best for printed output. However, depending on the color of the glasses, red/cyan may work better for either.

The stereopair **Rotation Angle** for anaglyphs is separate from that for separated-image

stereopairs, since a smaller angle is usually better (e.g. 2 degree instead of 3). The angle for anaglyphs should always be positive, whereas that for separated-image stereopairs may be negative for cross-eyed viewing.

---- Windows only ----

Anaglyphs in 8-bit (256-color) screen modes are not drawn correctly, because the colors are not added correctly for areas of red/green or red/blue overlap. If possible, switch Windows to a "true color" (16-, 24- or 32-bit) mode to get a correct drawing.

---- Macintosh only ----

The Macintosh adds colors correctly even in 8-bit screen modes.

---- End Macintosh only ----

Colors are not added or mixed correctly for labels in anaglyph mode.

3.2.3.4 Rims/Edges

Dialog Box: Rims [Input2 Menu]

In the Standard and Thermal Ellipsoid display modes, this controls the drawing of rims and edges for all the atoms, polyhedra and bonds. Colors and shades for rims and edges are entered in the input for atoms, polyhedra and bonds. Note that edges for polyhedra include edges that appear in the front, as well as those forming the outline.

Generally, rims should be turned on for all types of black-and-white images. They should usually be off for atoms and bonds with color shading with 8-bit or greater pixel depth, although you may wish to show polyhedron edges. Color images with black dithering, such as 4-bit raster files, usually look better with rims. Rims in color images should usually be black or a dark color.

Rims are never used in the 3D display mode.

3.2.3.5 Line Widths

Dialog Box: Line Widths [Input2 Menu]

The widths are in inches or centimeters. If the value is 0.0, the lines will be only one dot wide. For black-and-white display and output, one-dot lines will always be solid black, while wider lines can have gray shades or patterns.

If the **Use individual** box is checked for atoms, bonds or polyhedra, the individual line widths entered for each in the dialogs of the **Input1** menu will be used instead of the

overall values in this dialog.

When reading older files written with ATOMS for the Macintosh or for Windows V3.0, in which the line widths are in dots, the conversion to floating-point is made using the resolution values for the current printer.

Note that line widths in 3D Display Mode are always one pixel. You can use cylinders of any desired diameter instead of lines for Crystal Edges, Crystal Axes or the Unit Cell (also 3D General dialog in the Input2 menu).

3.2.3.6 Shading

Dialog Box: Shading [Input2 Menu**]**

For 8-bit screen display and raster files, the number of shading zones determines the nature of the 256-color palette generated by ATOMS and the number of colors available for shaded atom, bond and polyhedron fills. If the number of zones is 16 or fewer, you can use all 16 colors from the 16-color palette, except black, and there are 16 gradations of each color. If the number of zones is greater than 16, you should use only the first 8 colors in the palette numbered from 0 to 7, each of which has 32 gradations. See Colors, Palettes and Dot Patterns for more details.

Darkness angle (degrees). For an isolated object in a vacuum, the intensity of illumination should vary from maximum to minimum as the angle varies from 0 to 90 degrees. However, this would be a very "hard" illumination, and ATOMS allows for a "softening" or diffusing of the illumination in two alternative ways, by darkness angle or by darkest shade. The darkness angle, or the angle at which the illumination becomes zero or minimal, can vary from 90 to 180 degrees.

Darkest shade (fraction). This option "softens" the shading by allowing the presumed illumination of the darkest zone to be other than zero. Small values of this fraction, such as 0.1 or 0.2, are usually appropriate. It is 0.0 by default.

Use initial pattern numbers. Each atom, bond or polyhedron type is given a fill pattern number or gray shade for use in black-and-white screen displays and dot-matrix images, and this is used if shading is turned off. If shading is on, the shading normally starts from pattern zero, white. However, if the initial-pattern-number option is on, this pattern is used as the initial pattern number, for maximum illumination, other zones then increasing in darkness from this pattern number rather than from zero.

This option can be useful for spherical atoms, which all show the same shading zones, but is less successful for stick bonds and polyhedra, which will show different shading depending on their orientation.

Front-back fading. The initial or unshaded colors of atoms, bonds and polyhedra can be made to darken with depth (decreasing x coordinate). The foremost atom (greatest x coordinate) is considered to have full illumination, and illumination drops off to the rear according to the fading factor. The unit of fading is fraction of full illumination per Angstrom. If the structure has already been calculated, the factor for complete fading (black at the rearmost atom) is shown.

3.2.3.7 Background Color

Dialog Box: Background Color [Input2 Menu**]**

The best color for background may be neither white nor black - sometimes gray brings out shading and front-to-back fading better. The background for black-and-white display and output is always white.

Using colors other than white, black or gray for background may result in increased size of Raster or bitmap files and PostScript files in 3D modes. In some cases a simple run-length-encoding method is used for compression of these files, and this fails for 24-bit RGB (true color) files when the three components are not identical. That is, for a row of white pixels the sequence of bytes is 255, 255, 255, 255... whereas for a row of red pixels it is 255, 0, 0, 255, 0, 0...

3.2.3.8 Display of Crystal Axes

Dialog Box: Display of Crystal Axes [Input2 Menu**]**

Either of two types of axes may be drawn, *Movable* and *Corner* axes. Movable axes may be located anywhere in the drawing with the **Displacement** parameters - these parameters are in structure coordinates (Angstroms). The arms of the axial cross are two-ended, showing both position and negative ends. Corner axes are placed in a fixed position (in screen or drawing coordinates, inches or centimeters) relative to one of the corners of the drawing. They show only one arm of each axis, which is oriented as far as possible toward the interior of the drawing.

In the 3D display mode, the axes can be either lines or cylinders with the specified radius (which can also be set in the General sub-option of the **3D Parameters** command in the **Input2** menu). The axes are not shown in Stereopairs in non-3D display modes since they do not have a definite location in space, but they are shown in stereopairs in the 3D display mode

The **Scale factor** refers to the distance from the center to either end (one end for corner axes). Thus a scale factor of 0.5 gives lines equal in total length to the axes. In non-3D display modes, the axes are always shown in front of the atoms and faces.

The **Labels**, if selected, will be on the positive ends of the axes for movable axes.

Use PostScript font. This allows you to enter a character string for PostScript fonts supported by a PostScript printer if such fonts do not appear in the standard system font dialog called up by the **Font** button. This character string usually specifies the weight (normal, bold) and slant (italic, oblique) of the font, but not the size, which is specified in the **Font** dialog. Certain PostScript typefaces are standard, and should be present on most PostScript printers.

Movable axis settings.

If the **Dashed** box is checked, the c axis is shown solid, the b axis is dashed with the dash length and interval set in the Preferences dialog in the Settings menu or the Crystal Edges dialog in the Input2 menu, and the a axis is dashed with half these intervals.

If the **One-ended** box is checked, only the positive ends of the axes will be shown, otherwise both ends will be shown.

If the **Include in scaling** box is checked the axes will not go off-scale in either the **Universal** or **Maximize for each view** scaling modes (Scaling dialog, Input2 menu).

The **Displacements** can be used to separate the structure and axes. Note that you can also move the structure with the Centering and Displacements command in the **Input2** menu. The Scale Grid can assist in these displacements. In 3D display mode, the axes may interpenetrate with the structure, and the x-coordinate or front-back displacement is also relevant. Unlike the Unit Cell, the crystal axes are not fixed with respect to the structure, rather their location is specified in observer coordinates (see Coordinate Systems), with respect to the center of the structure.

Clicking in the plot area after clicking on the **Locate with Mouse** button will determine the y and z (across and up) coordinates, all that is required in non-3D display modes; in 3D display mode the x (front-back) coordinate will be unchanged and can be set independently.

Projection - Orthographic/Perspective. If Perspective (Input2 menu) is off, the axes are always projected by the orthographic method, in the same way as the structure. If Perspective is on, the projection point is always on a perpendicular to the projection plane (screen or paper) passing through the approximate center of the structure. If the **Perspective** radio button in this group is chosen, the axes are projected from the same point, as a three-dimensional object. This means that if the axes are displaced from the center of the structure, they are viewed obliquely, and it may not be obvious that they are in parallel orientation with the structure. This can be confusing to the observer who is not aware of the complexities of perspective projection. If the **Orthographic** radio button is selected, the axial cross is projected orthographically, which usually is more satisfactory. If the axes are at or near the center of the structure, there is little or no difference

between the two methods.

Corner axis settings.

The axes may be located in any of the four corners, at the specified **Displacement** in both directions from the corner. If the title is printed at the bottom, the displacement will be from the title instead of the corner.

In Perspective projection, corner axes are always drawn as for the **Orthographic** projection option for movable axes, above. This means essentially that they indicate the orientation at the center of the drawing, not that of their actual position.

3.2.3.9 Display of Unit Cell

Dialog Box: Display of Unit Cell [Input2 Menu **]**

For alternate ways of drawing unit cells, and problems sometimes encountered with crystal edges, see Drawing Crystal and Unit-Cell edges.

The unit cell is a simple box, with front and back edges having the colors specified. No distinction is made between "front" and "back" edges. In non-3D display modes, the unit cell is shown in front of the structure, like the structure axes, while in 3D display mode it has a definite location in space and may interpenetrate with the structure depending on the **Displacements**.

In non-3D display modes, only the edges may be shown, while in 3D modes faces may be shown as opaque or translucent planes.

Edges may be **Dashed** in non-3D modes only. The dash length and interval are set in the Preferences dialog in the Settings menu or the Crystal Edges dialog in the Input2 menu.

If the **Include in scaling** box is checked the unit cell will not go off-scale in either the **Universal** or **Maximize for each view** scaling modes (Scaling dialog, Input2 menu).

For non-primitive lattices, you can choose either the **Bravais** or **Primitive** cell; the primitive cell will have the same shape as that generated by the Default Unit Cell boundary option (if a primitive cell is selected in that option also).

In 3D modes the edges may be shown as lines, which are always one pixel wide, or as cylinders with the specified radius. In non-3D modes edges are always drawn as lines - the width is set in the Line Widths dialog (Input2 menu).

The unit cell is not shown in Stereopairs in non-3D display modes since it does not have a definite location in space, but it is shown in stereopairs in the 3D display mode.

In 3D display mode, and in perspective viewing in non-3D display modes, the unit cell applies to only one location in three-dimensional space. Change this location with the **Displacements** button, which calls the Unit-Cell Displacements dialog.

See Input Colors/Patterns/Pens for general aspects of color input.

3.2.3.10 Unit-Cell Displacements

Dialog Box: Unit-Cell Displacements [Unit Cell dialog]

The unit cell drawn with the Unit Cell dialog (Input2 menu) has its origin at particular coordinates in the structure coordinate system. The displacements from 0,0,0 are in fractions of the current cell vectors, which may be either primitive or Bravais vectors. The current vectors, in terms of components in the axes used for atomic coordinates (normally the Bravais cell edges), are listed; these are trivial unless you have chosen a primitive cell for a non-primitive Bravais lattice. If you have chosen the -0.5 to 0.5 suboption of the Default Unit Cellboundary option, the boundary volume is centered on the origin, so the displacements -0.5, -0.5, -0.5 will cause the unit-cell outline to coincide with the edges of the boundary shape. For the 0 to 1 suboptions use the displacements 0, 0, 0.

3.2.3.11 Ellipsoid Parameters

Dialog Box: Ellipsoid Parameters [Input2 Menu]

This dialog controls plotting parameters for the Thermal Ellipsoid and 3D display modes, set in the Display Mode sub-menu in the Display menu or in the Dialog Bar - Left

The following parameters are those which are in the various instruction series of ORTEP.

NPLANE - drawing of ellipses
= 0, no ellipsoid components
= 1, boundary ellipse only
= 3, principal ellipses only
= 4, boundary + principal ellipses

NDOT - back side of principal ellipses
< 0, solid line back side
= 0, back side omitted
= 3, 4 dots on back side
= 4, 8 dots on back side
= 5, 16 dots on back side
= 6, 32 dots on back side

NLINE - forward principal axes and shading (cut-out octant)
= 0, no forward axes or shading
= 1, forward principal axes only
= N, forward axes + (N-1) line shading

NDASH - dashed reverse principal axes
= 0, no reverse axes
= N, dashed reverse axes with N dashes

NBOND - bond type for stick bonds
= 0, no bonds
= 1, 2, 3, 4, 5 give lines at 180, 90, 45, 22.5 or 11.25 degrees apart, bonds ending at ellipsoids
= -1 to -5, same, bonds ending at atom centers

TAPER - bond taper. The bond radius is

R = R0 +- TAPER * ABS(COS(THETA))

where theta is the angle between the bond and the view direction. The bond radius R0 is set in the Bond Data dialog (**Input1** menu).

SCAL2 - ellipsoid probability scaling factor.

This controls the size of ellipsoids. A value of 0.76 gives 10% probability, 1.54 gives 50% probability, 3.36 gives 99% probability, etc. See the table below for sample values - for more complete values, consult the table in the original ORTEP instructions.

DISP - retrace resolution.

When lines are retraced to emphasize certain ellipsoids or make the width a function of depth, this is the separation.

A0 and A1 - depth function parameters.

Lines may be retraced to give wider lines for closer ellipsoids.

dR(x) = AO + A1 * x

where dR is the width of the line and x is the height in Angstroms.

Use b/w shades. If this box is checked, ellipsoids in black-and-white display and output will be filled with the b/w shade or color specified in the Input Atom Data dialog (Input1

menu). If it is not checked, they are filled with white before drawing ellipsoid components.

Show iso as spheres. If this box is checked, isotropic atoms are shown as spheres (i.e. circles in non-3D display) without the principal planes which can give a false impression of anisotropy.

Default radius. This is the *mu* value which is given to atoms with no valid entered temperature factors; it is 0.1 by default.

If DISP is 0.0, lines are not retraced. For one-dot lines on typical screens, DISP should be about 0.01 inch, but it can be much smaller for printed output. Note that x is measured from the zero of coordinates, not the rear-most atom

Line widths for atoms are set independently in the Line Widths dialog (Input2 menu), and the value of DISP should take account of these settings if wide lines are used.

For color display and output, depth is probably best shown by front-back fading of color (Shading dialog, Input2 menu) rather than line retracing.

3D Mode. If the **Show in 3D mode** box is checked, and if temperature factor data have been entered, atoms will be shown as ellipsoids in the 3D Display Mode. If NLINE is greater than 0, the "forward axes" or cutout octant is shown as in ORTEP (except in 3D files - see below). If NPLANE is greater than 1, the trace of the principal planes will be shown as stripes or three-dimensional bands just outside the ellipsoids. The **Width of principal- plane stripes** gives the width of these bands. The **Radius Factor for stripes** gives the height or extent to which the curves for the principal planes are outside the ellipsoid itself; this should always be larger than 1.0. By increasing this factor and decreasing SCAL2, the principal planes can be made to dominate the representation, as elliptical disks.

For direct screen and print rendering, the bonds between ellipsoids are the same size as shape as in ORTEP drawing, and the TAPER parameter is applicable. In 3D files (VRML and POV-Ray), bonds are always strictly cylindrical. Also in these files, the ellipsoids are always complete and do not have the cutout octant as possible in ORTEP drawing. When Polyhedra are present, and ligand atoms are not shown at the corners, bonds to these corners are always cylindrical, not tapered. Note that the option to show corner atoms as spheres of constant size is not applicable to the 3D mode - such atoms are either absent, or shown as thermal ellipsoids. Of course, the atoms could be converted to isotropic temperature factors of appropriate size.

The SCAL2 parameter above determines the size of the ellipsoids as in the Ellipsoid drawing mode. Apart from SCAL2, TAPER, NLINE and NPLANE the ORTEP parameters above are not applicable to 3D drawings.

The 3D Material parameters used for both the cutout octant and the principal-plane bands are those for polyhedra - this is to avoid distracting specular reflections from large flat surfaces (although polyhedra may be assigned large specular reflection components as well).

Polyhedra in Ellipsoid mode (non-3D) group. In the Ellipsoid display mode, you can either show polyhedra with flat, opaque faces (last option), or you can show the ligand-ligand "bonds" which are the edges of polyhedra, and also the central-ligand bonds. Both of these types of "bonds" are as defined in the Polyhedra input in the Input1 menu, not the Bonds input. The ligand-ligand "bonds" or edges will have the fill and edge colors which are specified for the given polyhedron in the Polyhedron Data dialog, and the central-ligand "bonds" will have the edge and fill colors of the central atom (Input Atom Data dialog). Both these bond types will have a uniform radius, as specified in the edit box.

The intersections of the solid polyhedra with the corner ellipsoids are not solved exactly, but approximated assuming the corner atoms are spheres. The size of these spheres is determined by the settings in the Polyhedra dialog (Input1 menu). This approximation will be less acceptable as the ellipsoids deviate further from sphericity.

All the atoms involved in polyhedra, except for the central atom in the case of solid polyhedra, will be shown as elllipsoids.

The central-ligand and ligand-ligand "bonds", if used, must be added to the bond list during calculation, so changes in this option may require Recalculation, rather than just replot.

Partial Table of Probability and SCAL2 values

Probability	SCAL2
0.1	0.7644
0.2	1.0026
0.3	1.1932
0.4	1.3672
0.5	1.5382
0.6	1.7164
0.7	1.9144
0.8	2.1544
0.9	2.5003
0.95	2.7955
0.99	3.3682
0.999	4.0331
0.9999	4.5943

3.2.3.12 3D Light Sources

Dialog Box: 3D Light Sources [Input2 Menu **]**

There may be as many as 8 light sources in the 3D drawing mode, and each may have a different color.

Each light may be either **Directional**, in which case all rays are parallel in a given direction; it may be **Positional**, in which case all rays emanate from a given point; or it may be **Ambient**, in which case the rays bathe all objects uniformly - there is no directional quality. If the light is **Directional**, the x, y and z coordinates in the **Position/Direction** box give the direction vector. If the light is **Positional**, the coordinates give the location of the light source, in Angstroms in the Observer coordinate system. Ambient light is neither directional or positional and these coordinates are not used.

There may be only one ambient light.

Each light has only one color. For non-ambient lights, the diffuse and specular components have the same color and intensity. The absolute values of the RGB components determine the intensity of the light - for example, 0.2, 0.2, 0.2 gives a white light of one/fifth the maximum intensity.

Since the colors and Material properties for each atom, etc. are specified individually, the

Ambient, Diffuse and Specular Colors should normally be white (1.0, 1.0, 1.0). However, they can be changed for special effects or to correct color distortions in display or output devices.

The color of a given object is the resultant of the colors of the various lights, the color specified for the object itself in the dialogs of the **Input1** and **Input2** menus, and the Material coefficients. See Lighting Equation for details.

Attenuation. The incident intensity from a light source is itself subject to attenuation according to the equation

$$Ii = Ii(0) / (Kc + Kl\ d + Kq\ d^2)$$

Where d is the distance of the point in question from the (positional) light and Kc, Kl and Kq are the **constant**, **linear** and **quadratic** attenuation coefficents respectively. Constant attenuation is essentially a brightness coefficient. Values larger than 1.0 simply darken the scene. Values smaller than 1.0 may add a white component and/or increase the specular contribution. **Linear** and **quadratic** attenuation apply only to Positional lights.

3.2.3.13 3D General

Dialog Box: 3D General [Input2 Menu **]**

In the 3D drawing mode, crystal edges (Crystal Edges and Faces dialog), structure axes (Crystal Axes dialog) or unit-cell edges (Unit Cell dialog) may either be lines or cylinders. If they are lines, the width is set in the Line Widths dialog (**Input2** menu). Rims of atoms and bonds and edges of polyhedra are never shown, so the relevant values are for edges (which include axes and unit cell) and bonds (which include skeletal bonds. Width of lines in VRML files cannot be controlled. Wide lines in 3D generally do not look good, so if width is to be more than one pixel, cylinders are better.

Spheres (atoms) and cylinders (bonds or vectors) are actually drawn as assemblages of planar polygons, the number of which is determined by the **Subdivisions...** setting (below).

If the **Thermal ellipsoids** box is checked, and if temperature factor data have been entered, atoms will be shown as ellipsoids in the 3D Display Mode. Some of the parameters in the Ellipsoid Parameters dialog may need to be adjusted - see that dialog for further details.

Subdivisions per quadrant... Spheres or ellipsoids (atoms) and cylinders (bonds or other lines) are drawn as assemblages of flat faces, and this parameter determines the fineness of the subdivisions. The default value of 5 may need to be increased for very large atoms. This parameter replaces the **Slices** and **Stacks** parameters in V4.0 of ATOMS - in V4.0 files, values of **Subdivisions** will be obtained from the sphere **Slices**

number. The Slices for spheres and cylinders number is 4 times the Subdivisions, and Stacks for spheres is 2 times the Subdivisions. Cylinders have only one stack. Ellipsoids are distorted spheres (it could also be said that spheres are special ellipsoids) and they use the same subdivision parameters.

Bonds between ellipsoids, which are drawn in ORTEP style, have either 4 or 8 Subdivisions per quadrant, according to whether the value entered is less than, or equal to or greater than 6.

3.2.3.14 3D Fog

Dialog Box: 3D Fog (Fading) [Input2 Menu **]**

Fog in the 3D drawing mode is similar to fading (Shading dialog) in the Standard drawing mode - it contributes to the illusion of depth by changing the color as a function of distance from the eye. It blends the specified foreground color for the atom, bond or other object with the given background or other specified color, on a pixel-by-pixel basis.

This can be according to one of three equations, selected with the radio buttons in the upper left of the dialog.

Linear: f = (end - z) / (end - start)

Exp: f = exp[-density * z]

Exp2: f = exp[(-density * z) ^2]

where z is the distance from the eye and f is the fraction of the initial color, the remainder being the fog color specified in the lower part of the dialog. Note that the color in this case is specified by RGB components varying from 0.0 to 1.0 (floating point) rather than 0 to 255.

ATOMS sets the parameters **start** and **end** at the foremost and rearmost atoms, or calculates the density, using the specified **Fraction of intensity at rear**. That is, the foremost atom will always have the pure (non-fogged) color (f = 1.0), and the rearmost atom will have the specified fraction (f) of the pure color and the remainder the fog color.

For example, if the rearmost atom is to blend into the background, i.e. disappear, set the **Fraction of intensity at rear** at 0.0 and check the **Use background** radio button. If the fog color is not the current background (Background Color dialog, Input2 Menu), it will usually be black (0.0, 0.0, 0.0).

Fog or fading may also be referred to as depth-cueing.

3.2.3.15 3D Material Properties

Dialog Box: 3D Material Properties [Input2 Menu]

In the 3D drawing mode the material properties of objects determine the way the objects interact with the light sources.

The color observed at a given point is a resultant of the light source(s) (3D Lighting) and the material properties; that is, the RGB coefficients of the **Ambient**, **Diffuse** and **Specular** components of the light source(s) are multiplied by the specified colors of the objects, and by the material coefficients in this dialog, then the results are limited to the range 0.0-1.0. See Lighting Equation for details.

Ambient light has no direction or origin and is considered to bathe all objects uniformly. Having a significant ambient component causes non-illuminated parts of objects to be other than black. It thus "softens" the illumination in a somewhat similar way to the **Darkest Shade** and **Darkness Angle** parameters (Shading dialog) in the Standard display mode. Note that there must be a separate ambient light to show this component.

Diffuse color is usually the main component of the appearance of objects. The intensity of the color is dependent on the angle between the light ray and the normal to the surface in question.

Specular reflection only occurs when the normal to the surface in question is close to bisecting the angle between the incident light and the vector from the point on the surface to the eye. It produces bright highlights on a curved surface. The larger the

Shininess coefficient, the smaller will be the bright specular highlight on a curved surface. The shininess coefficient has a maximum of 128 because of computational restrictions, but values on the order of 5-30 are usually realistic.

In ATOMS, specular reflection is always white, that is it does not depend on the color of the object, only the color of the light source(s). Specular reflection does not work well for polyhedra because faces at the reflection angle will give an essentially solid white appearance, rather than a bright spot. This is because the angle is calculated for the corners of the face, and interpolated for each point in the interior of the face.

When thermal ellipsoids are shown in the 3D mode (see Ellipsoid Parameters), the material parameters used for both the cutout octant and the principal-plane bands are those for polyhedra - this is to avoid distracting specular reflections from large flat surfaces.

Emission is similar to ambient, except that there is no dependence on the color of any light source. A high value of emission makes an object look like is is glowing.

3.2.3.16 3D Polyhedra

Dialog Box: 3D Polyhedra [Input2 Menu]

This dialog specifies some special ways of displaying polyhedra in the 3D display mode which are not available in non-3D modes.

The **Polyhedron Mode** can be:

1) **Completely opaque.** This is similar to Standard display mode (but edges cannot be shown);

2) **Skeletal, no bonds** or **3) Skeletal, with bonds**. The skeletal modes show the ligand-ligand bonds or polyhedral edges, with the central atom as a sphere.

4) **Translucent, no bonds** or 5) **Translucent, with bonds**. The polyhedron faces may all be translucent, in which case objects behind show through, or you may check the **Back faces opaque** box, in which case the interior may be seen, but nothing behind the polyhedron. Complete translucency may be confusing if there are many polyhedra, i.e. polyhedra behind polyhedra.

Translucency may increase computation time. Support for translucency may depend on the platform and output mode. VRML files do not support **Back faces opaque**. Viewers for these files may not support translucency.

The **Opacity** (1.0-transmission) for the translucent modes may be specified, but again system software and file viewers may not support a complete range.

Ligands may be shown as spheres, or only as intersections of the ligand-ligand bonds.

Planar polyhedra are shown as plates with a finite thickness, with or without the central atom.

3.2.3.17 PDB (Protein) Display Parameters

Dialog Box: PDB (Protein) Display Parameters [Input2 Menu]

The first radiobox, **Display hetatoms**, applies to all display modes, not just the special Protein Display Mode. You can omit all hetatoms, or water (HOH) only.

The remainder of the settings in this dialog apply to the special Protein Display Mode.

This mode, which is a 3D mode only, only works on data imported from PDB files. It displays the bonds between protein backbone atoms as cylinders, with the radius specified in this dialog. By default, other atoms in the amino acids or residues are omitted, but you

can specify a limited number of individual residues to draw in the ball-and-stick mode in this dialog. Hetatoms (non-residues) are always drawn as ball-and-stick.

The bonds drawn in this mode must be specified in the Bonds dialog in the Input1 menu. At a minimum to show the backbone there must be carbon-carbon and carbon-nitrogen bonds. Any other bonds among hetatoms and non-backbone atoms in the residues must also be specified. Usually this can be done by selecting automatic bonds in the Bonds dialog or during importing.

This mode relies on the atomic labels and residue information derived from PDB files and cannot be used without importing data in that format.

The **Radius of sticks** gives the size of the skeletal or stick bonds between backbone atoms - it does not apply to bonds involving hetatoms or non-backbone atoms in the residues.

Show complete residues - by number. This allows showing non-backbone atoms and associated bonds in the specified residues. Atom and bond attributes are as specified globally in the Atoms and Bonds dialogs in the Input1 menu. Note that even if a residue is selected for "full" display in this option, the backbone atoms in that residue are still shown in the standard protein way (as skeletal sticks).

In the edit box, give the residue sequence number and chain letter together, separated by spaces, commas or semicolons. You can get these numbers and letters by clicking on the atoms, or from the Atoms dialog in the Input1 menu. Thus

5A 12B

indicates that residue 5 of chain A and residue 12 of chain B are to be drawn fully. A number without a letter will be read as chain A.

3.2.3.18 Initial Orientation

Dialog Box: Initial Orientation [Input2 Menu **]**

Any initial Cartesian rotations specified here will be be applied to the x, y and z structure Cartesian axes (see section IV-4) in that order after the atoms are located and boundaries determined and before the structure is first displayed. If initial clinographic viewing is in effect, the clinographic rotations are applied after these initial rotations.

If the **Clinographic viewing** box is checked, the clinographic rotation (see Coordinate Systems) will be applied at the end of the calculation, after any initial Cartesian rotations. It may be turned off with the Clinographic Viewing command in the **Rotation** menu (or the ClinographicViewing command in the **Display** menu).

When exiting, ATOMS checks to see if the orientation has changed from the initial orientation defined in this dialog. If so, you have the option of saving the current orientation. This orientation will be converted into initial rotations on x, y and z, plus initial clinographic viewing if that is in effect.

Summary of orientation operations. ATOMS first sets the *c* structure axis parallel to the *z* viewer axis, and the *a* * structure axis (perpendicular to *b* and *c*) parallel to *x*. This is the *original* orientation. Next, if the Slice boundary option is in effect, the slice is oriented with the slice plane parallel to *yz*, and the orientation vector parallel to *z*. Then the initial Cartesian rotations, if any, are applied. Finally, the clinographic rotations, if selected, are applied. This is the *initial* orientation.

3.2.3.19 Scaling

Dialog Box: Scaling [Input2 Menu **]**

Scaling and displacement operations do not apply to the actual values of atom and corner coordinates and face coefficients, which are permanently set (in Angstroms) by axis lengths and fractional coordinates and the central distances of the faces. Rescaling and displacement apply only to the plotting coordinates in screen, dot-matrix or pen-plotter displays.

Scale mode. There are three modes of scaling:

----Maximize size for each view. In this mode, the structure is scaled in each orientation so that it is just smaller than the viewing area. The actual scale will therefore change whenever the structure is rotated. Hard copy is scaled the same way and what you see is essentially what you get. Note that the **Rescale factor** (below) is now applied - this has the effect of reducing or enlarging the size of the viewing area as used for determining the scaling.

----Universal maximum. In this mode, the structure is scaled so that its maximum dimension is just smaller than the minimum dimension of the plotting areas; thus, rotations can be made without changing the scale and without going out of bounds. Again, hard copy is scaled the same way and what you see is essentially what you get. Note that the **Rescale factor** (below) is now applied - this has the effect of reducing or enlarging the size of the viewing area as used for determining the scaling.

----Fixed scale factors. This suboption allows you to set the scale to a fixed number of inches or centimeters per Angstrom for the dot-matrix and/or pen plot, or simply to reduce or enlarge the image from the automatic scaling modes.

Rescale factor. This factor is always applied in the **Maximize size for each view** and **Universal maximum** modes. When you "zoom" or rescale with the scaling buttons in

the Dialog Bar - Right, this changes the rescale factor (rather than changing to the **Fixed** scale mode, as in pre-V4.2 ATOMS).

Scaling for the screen and normal printer output (Print command in the **File** menu) depends on the resolutions (dots per inch or centimeter), which are obtained from the software drivers for these devices. Resolution for the printer may often be reset in the Page Setup dialog in the **File** menu. The resolution for the Pen Plotter is set in the Pen Plotter Settings dialog, and that for a direct PostScript printer is set in the Postscript Settings in the **Settings** menu.

The Dialog Bar - Right allows "zooming" or incremental adjustment of the scale factors in the **Fixed** mode, or the **Rescale factor** in the other modes.

3.2.3.20 Calculation Output

Dialog Box: Calculation Output [Input2 Menu **]**

This output gives information on the results of the initial calculation, including locations of all atoms, all faces generated, and atoms involved in bonds and polyhedra. It is regenerated every time you use the Calculate command in the **File** menu.
Output. Output, if selected, is sent to a file with title **infile**.ATD, where **infile** is the name of the input file. The.ATD file will be in the same directory as the.STR file (data directory). You can elect to show this file on-screen in a Text window, which is a standard edit window - see Types of Windows.

Note that the output referred to here gives the original atom locations without any rotations whatsoever, while the **List Generated Atoms** command in the **File** menu gives current Cartesian atom locations.

The listings of generated atoms give a symmetry number (Symm.) which can be correlated with the list of symmetry operations, or equivalent positions of the general equipoint, in the Listings/Input/Symmetry listing (File menu). This number, in roman numerals, can be shown as a superscript on the Atoms Label (Display menu).

Bond lengths and angles. Bond angles are part of the normal bond output, so in order to get angles, you must also check the **Bonds** box. You have the option of calculating the angles on all atoms, or only on one atom of each symmetry-equivalent set (input atom) which occurs in the final atom list. ATOMS will find the generated atom which is closest to the zero point.

Note that angles will only be calculated for bonds which have been specified for display, and angles will only be calculated for atoms within the boundaries specified in the Boundary option. Angles within polyhedra will not be calculated. If the boundaries of the structure are not large enough, you may not get a complete set of bonds and angles on any given atom. Specifying the Default Unit Cell boundary option will not guarantee that

you get a complete set, unless you select the third suboption in that dialog, which completes the coordination of all atoms in the unit cell.

Bond lengths and angles about any input atom can can be obtained immediately with the **Coordination** button in the Input Atoms dialog (**Input1** menu).

3.2.3.21 Centering/Displacement

Dialog Box: Centering/Displacement [Input2 Menu]

Automatic centering will center the structure in the current viewing area. This is done for each view, and any displacements entered under **Constant Displacements** are ignored.

In most cases, the easiest way to scale and position a drawing onto a printed or typed page is to use the frame options in the **Print** command or other options in the **File**. However, the displacements in this section can be used to position the drawing within the frame defined in those suboptions.

The displacements are used only in plotting and are not actually part of the atomic coordinates. Note that the center of rotation is not changed by these displacements - that is, the structure is always rotated about its own zero of coordinates. Thus any desired rotations should always be made before using displacements.

The Dialog Bar - Right allows centering of the viewing area on a particular projection point in the structure. Displacements made in that dialog will affect the displacements in this dialog (**Centering/Displacement**), and may be removed here.

The **Set Center** button in the Dialog Bar - Right also allows centering of the viewing area on a particular projection point in the structure.

The Scale Grid command in the **Display** menu is useful for showing the actual scaled location of the structure and in estimating displacements.

For perspective viewing, the projection is made from a point related to the zero of the observer coodinate system. If the displacements in Centering/Displacement are large, it may be desirable to enter offsets in the Perspective dialog, or to select Automatic Centering of the projection point in that dialog.

Note that the projection point for perspective viewing is independent of the Centering/Displacement settings, although this point may also be centered automatically (see the Perspective dialog).

3.2.3.22 Reset Scaling/Centering

Dialog Box: Reset Scaling and Centering [Input2 Menu]

This dialog allows reversion to the Scaling and Centering/Displacement modes and settings in effect before various interactive changes, or selection of the default settings (Universal Maximum scaling and Automatic centering).

Current makes the current settings permanent - after this these settings will be the "Last" settings.

Last returns to the values set in the last calculation, or the last reset with this dialog. Current settings are erased.

Default selects Universal Maximum scaling and Automatic centering, so the structure should remain the same size and completely in view at all times.

Cancel will exit the dialog without any change - the current and last settings will be preserved.

You can always adjust the settings in the Scaling and Centering/Displacement dialogs in the Input2 menu.

This dialog can be called from the DialogBar-Right with the Reset Scaling button.

3.2.3.23 Atom and Bond Plot States

Dialog Box: Atom/Bond Plot States [Input2 Menu]

This is primarily intended for restoration of generated atoms that have been marked as non-plotting with the Generated Atom Data dialog which comes up when an atom is identified by clicking with the mouse pointer in the Graphics window. However, you can also select a range of atoms by number to mark for non-plotting. If the end number is zero, it will be made equal to the start number, i.e. only one atom will be affected.

The **Intermolecule/fragment bonds** combo box (only displayed if there are bonds between molecules or fragments) gives several options for display of inter-molecule or interfragment bonds. If **Highlighted** is selected, such bonds are shown in normal colors while all other atoms, bonds, etc. are dimmed. Other possible highlighting of molecules or fragments is ignored.

Changes in plot states will only be shown after using the Replot command in the **Display** menu.

See Deleting Atoms and Generated Atom Data.

3.2.4 Display Menu (Graphics Window)

Replot - Replots the image (does not recalculate).

Color - Switches the screen between black-and-white and color.

Atom Labels - Controls automatic labeling of atoms, using input labels.

Bond Labels - Controls automatic labeling of bond distances.

Angle Labels - Controls automatic labeling of interbond angles.

Scale Grid - Superimposes a scale grid for location of the structure or parts thereof.

Mark Atoms - Draws a small box at the location of specified types of atoms.

Clinographic Viewing - Switches clinographic viewing on and off.

DialogBar - Left - This is a control bar which is fixed on the left side of the Main window.

DialogBar - Right - This is a control bar which is fixed on the right side of the Main window. It contains some frequently-used controls.

DialogBar - Fragments - This controls placement and orientation of individual structure fragments, if present.

Powder Diffraction - Produces a simulated powder diffractogram or a list of reflections.

Precession Pattern - Produces a simulated precession photograph of a given net.

3.2.4.1 Display Mode Sub-Menu

Sub-Menu - Display Mode [Modes menu]

This sub-menu switches between the five (or six) types of display supported by ATOMS. Note that switching between four of the five modes requires only replotting, but switches involving the Thermal Ellipsoid mode require recalculation. Whichever is required is done automatically.

Graphics on either Macintosh or Windows can be either 2D (or non 3D), which use the standard system software for drawing in two dimensions; or they can be 3D, which uses the system software (OpenGL) for drawing three-dimensional objects. The Standard, Skeletal, Thermal Ellipsods and Anaglyph modes are 2D, while the 3D, 3DSkeletal and Cavities modes are 3D.

Standard**.** This is the main display mode in ATOMS, which supports ball-and-stick, interpenetrating atoms, polyhedra and wire-frame representations, ranging from simple schematic drawings to fully-shaded three-dimensional drawings.

Skeletal and 3DSkeletal. Skeletal or wire-frame representations can be drawn in either non-3D or 3D display. The 3DSkeletal mode may be faster on the screen, but because all 3D output is by means of bitmaps printing may be slower. In either mode, there are two choices for the method of representation. In the "Bond colors" method, atoms are shown as small dots, except those in polyhedra; all bonds are shown as lines with the bond color, and polyhedra are shown by lines joining the corners (outlining the faces). In the "Atom colors" mode there are no dots for atoms, and rather than showing bonds in the color specified in the Bond Data dialog, they are shown half-and-half in the two atom colors. Also, polyhedra are converted to central-ligand bonds and ligand-ligand (corner-corner) lines are not shown. The choice between these two modes of representation is in the Preferences dialog in the Settings menu.

Thermal Ellipsoids. This mode shows thermal ellipsoids in the style of ORTEP, the classic plotting program by Carroll K. Johnson. Note that ellipsoid may also be drawn in the 3D mode.

3D**.** Although a fully shaded drawing done in the **Standard** mode may have a highly 3-dimensional appearance, this option, which uses special system software not available on all machines, allows a number of extra options in terms of lighting and material properties and correctly draws interpenetration of crystal edges, axes and unit cells with the structure. Switching into this mode requires loading the system software, which may take a few seconds. Thermal ellipsoids may be drawn in combination with polyhedra, which is not possible in either the Thermal Ellipsoids or Standard modes.

Anaglyph**.** This is a special type of stereopair display which must be viewed with colored glasses. Rather than completely separate left- and right-eye images, as in the stereopair option in the other display modes, there are superimposed images in two different colors, red/green, red/blue or red/cyan. The representation is the same as in the **Skeletal** mode, bond colors option.

Cavities. This shows the cavities or "open space" in a single unit cell, using the current atomic radii. This mode uses the 3D system capabilities - if your system does not support 3D display (e.g. 68K Macintosh or Windows 3.1) the Cavities display mode is not available.

Protein. This mode, which is a 3D mode only, only works on data imported from PDB files. It displays the bonds between protein backbone atoms as cylinders, with the radius specified in the Protein Display Attributes dialog. By default, other atoms in the amino acids or residues are omitted, but you can specify a limited number of specific residues to draw in the ball-and-stick mode in the Protein Display Attributes dialog. Hetatoms (non-residues) are always drawn as ball-and-stick.

The choices in this submenu are also in the Dialog Bar **-Left** which is controlled from the

Display menu.

3.2.4.1.1 Standard Display Mode

This is one of the modes which can be selected in the Display Mode submenu in the **Display** menu, or in the Dialog Bar**- Left**.

This mode is actually very flexible, and supports representations ranging from very schematic line drawings to fully three-dimensional. The settings in the Rims, Linewidths, and Shading commands in the **Input2** menu have an especially great influence on this mode.

The main alternative to Standard mode is 3D Display mode, which gives a more realistic appearance in full color, but is not generally suitable for schematic drawings.

3.2.4.1.2 Skeletal and 3DSkeletal Display Modes

There are actually two skeletal drawing modes, Skeletal and 3D Skeletal. The appearance in the two modes is virtually identical. Even if you are not otherwise using the 3D display mode, the 3DSkeletal mode may be preferable in that redrawing may be faster, since it is not necessary to sort drawing objects back to front. The relative speed of the two modes may depend on your graphics display hardware.

In either or both of the skeletal drawing modes, there are two alternative modes of skeletal viewing, as selected in the Preferences dialog (Operation tab) in the Settings menu.

In the **Bond colors** or "old" mode, all atoms are shown as small dots, except those in polyhedra; all bonds are shown as lines using bond colors (either fill or edge colors as selected in the Preferences dialog), and polyhedra are shown by lines joining the corners (outlining the faces). The lines indicating polyhedron edges use the polyhedron fill colors.

In the **Atom colors** or "new" mode (new in ATOMS 5.1) the bonds are shown in the colors of the two atoms (fill color), half-and-half. Polyhedron edges are not shown; instead the central-ligand bonds are shown.

During rotation with the mouse cursor, the skeltal mode may optionally be used to represent the structure while the button is down - this is selected in the Preferences dialog. If you are in the 3D display mode, 3DSkeletal will be used during rotation.

This drawing mode can be selected in the **Display Mode** submenu of the **Display** menu, the Dialog Bar - Left.

See also the Anaglyph drawing mode.

3.2.4.1.3 Thermal Ellipsoid Display Mode

In non-3D display, ATOMS shows thermal ellipsoids in the style of ORTEP, the classic plotting program by Carroll K. Johnson. Display parameters, controlling the way the atoms and bonds are drawn, are the same as in ORTEP. However, the ORTEP plotting commands, including atom generation, are not used. Atom generation is done by the usual Boundary methods of ATOMS, and bonds are set up in the usual way (Bonds dialog in the Input1 menu). Bond radii used are the same as those specified in the Bond Data dialog. The ORTEP parameters which actually affect the configuration of the ellipsoids and bonds are set in the Ellipsoid Parameters dialog in the Input2 Menu.

Atoms and bonds are drawn generally from back to front, as in the Standard display mode, the height of bonds being taken at the midpoint. From V5.1, ATOMS has an additional algorithm which should eliminate most inaccuracies in overlap relations which resulted from strict back-to-front drawing. The true relations will be always be shown in the 3D display mode.

Note that thermal ellipsoids may also be shown in the 3D display mode. The option to show them or not is in the Ellipsoid Parameters dialog, and also the 3D-General dialog (Input2 menu)

Thermal ellipsoids in pen-plot or HGPL-file output are not supported at this time.

Switching between Standard, Skeletal, Thermal-ellipsoid, 3D and Anaglyph display modes is done with (a) the Display Mode sub-menu in the **Display** menu; or (b) a box in the Dialog Bar, which is turned on and off in the **Display** menu.

Temperature factor data may be entered and edited for individual atoms in the Atom Data Dialog (**Input1** menu), or temperature factors may be read in with the Import File formats (**File** menu), including the original ORTEP format, or with atom parameters in free-form style through the Input Atoms dialog (**Input1** menu). ATOMS supports all of the temperature factor types used in ORTEP, although most data published now are of type 0 or 8 for anisotropic temperature factors, or 6 for isotropic factors (and also type 10 for isotropic U, which is not a standard ORTEP type). ATOMS will save temperature factor data in its data files only if there is at least one atom with non-zero B11 or U11 coefficient.

When converting to the **Input=Generated** mode (Generated to Input command in the **Transform** menu), the temperature factors of all generated atoms are converted to eigenvectors and eigenvalues in the Cartesian system and stored in that way instead of as beta or U coefficients. Therefore, temperature factors cannot be modified once the conversion has been made. (It would be possible to modify the values in the.STR file, but it is not likely this would be worth the trouble). The Thermal Ellipsoid mode is not supported for multiple structure fragments.

3.2.4.1.4 3D Display mode

This drawing mode can be selected in the **Display Mode** submenu of the Display menu, or the Dialog Bar - Left**.**

Although a fully-shaded ATOMS drawing in the Standard display mode has an excellent 3-dimensional appearance, the term "3D drawing" is used to denote a method of drawing which is different in several respects. ATOMS uses the OpenGL software package for both Windows and Macintosh.

In this type of drawing, the surfaces of three dimensional objects such as spheres and cylinders are converted to an assemblage of planar polygons. Then each polygon is drawn essentially independently. The critical difference from non-3D modes is that a *depth buffer* is used in 3D imaging. This is an array of integers, one for each pixel in the display or output (or that portion which is currently being drawn). Each element, representing a pixel, holds the relative *x* coordinate (in the ATOMS observer coordinate system) of the foremost object or polygon. The color for this object is retained in the *color buffer*, which is a similar array representing pixels; this array is actually the image itself. Whenever a polygon is drawn, each pixel which it contains is compared against the depth buffer; if the *x* coordinate of the pixel is greater, or closer to the observer than what is in that element of the depth buffer, the color for this pixel in the new polygon replaces the value in the color buffer. That is, the depth buffer keeps track of the front surface of the drawing, and ensures that only this front surface (not any hidden surfaces) are kept in the color buffer or image itself. It is also possible to have transparent or translucent objects, through which hidden surfaces may show partially, by mixing the color of the latest object with the color which is already in the buffer.

Actually, the "double buffer" method is normally used, the color buffer being kept in an area of memory and then copied to the screen memory when the drawing is completed. This is usually faster than drawing directly to the screen.

The non-3D display modes of ATOMS do not use a depth buffer: the atoms, bonds and polyhedra are sorted from back to front and drawn in that order (except for the Anaglyph mode). When necessary, the intersections of objects are solved analytically and only the required portions of each are drawn.

Using a depth buffer has the advantages that it is not necessary to solve analytically for intersections, nor to sort the objects with respect to depth (unless some objects are translucent). This may save considerable time, especially for complex drawings, since the time for sorting tends to increase exponentially with the number of objects. Since analytical solution of intersections is not necessary, it is possible to place essentially any objects into the drawing. in any location. This overcomes the problem in ATOMS non-3D display modes of sometimes-incorrect drawing of crystal edges or unit-cell edges which intersect with atoms, bonds and polyhedra. The 3D method allows more complex

shading and lighting effects, such as specular highlights and multiple light sources. For a completely 3-dimensional image, on a computer which has sufficient memory, the 3D display mode is superior to the ATOMS Standard display mode.

However, there are disadvantages to the 3D method. The depth buffer may result in excessive memory requirements even for the screen (but some 3D accelerator cards may have special memory for the depth buffer). The 3D method is not very suitable for black-and-white drawings, which typically are simplified, showing mutual intersections of atoms with bonds and polyhedra as lines or curves; such intersections simply are not drawn in the 3D method. Both Windows and Macintosh implementations currently have some severe limitations in terms of printing. It is necessary to draw each image into a bitmap and then copy that bitmap to the printer. Because printers have much higher resolution than the screen, this causes even higher memory requirements, and for reasonable sized printed drawings it is usually necessary to do the printing in bands or segments.

The **3D Display** mode itself is for drawing atoms, bonds and polyhedra as three-dimensional objects. The same system software is also used for the 3DSkeletal mode and the Cavities mode. During rotation using the mouse when in **3D Display** mode, the drawing mode may optionally be switched to 3DSkeletal while the mouse button is down. This is controlled in the Preferences dialog in the Settings menu.

3.2.4.1.5 Anaglyph Display Mode

This drawing mode, selected in the Display Mode command in the **Display** menu or the Dialog Bar - Left, is a type of stereopair display. Rather than using separated images, as in the Stereopairs option in the other display modes, the two images are superimposed, but each is in a different color - either red/green, red/blue or red/cyan. The only type of display which is currently supported is the same as the Skeletal display mode, that is atoms are shown as small dots and bonds and polyhedra as lines.

Stereoscopic glasses, with the left lens red and the right lens either blue or green, are required to view the image. Such glasses may be purchased where comic books are sold, among other places.

The settings for the Anaglyph mode are in the Stereopairs dialog in the **Input2** menu. Generally red/blue with a black background works best for the screen, while red/green or red/cyan with a white background works best for printed output. The anaglyph mode seems to work better with a smaller rotation angle than the separate-image stereopair mode - for example 1.5 instead of 3 degrees.

For anaglyphs to work properly, the operating system must be able to blend pixel colors in the appropriate way. For example, in printed output, where red and green areas overlap the result must be black, not the color of the line which was drawn last. This is not possible in PostScript, so anaglyphs do not work properly in PostScript output. In metafile or PICT (Picture) output, the program which receives the file may not be able to

interpret the command which sets the blending mode. Color blending does not seem to work properly for labels.

----Windows only ----

Anaglyphs for Windows in 8-bit (256-color) screen modes are currently not drawn correctly, because the colors are not added correctly for areas of red/green or red/blue overlap. If possible, switch Windows to a "true color" (16-, 24- or 32-bit) mode to get a correct drawing.

---- Macintosh only ----

The Macintosh adds colors correctly even in 8-bit screen modes.

3.2.4.1.6 Cavities Display Mode

Parameters for this display mode are set in the Cavity Parameters dialog, Input1 menu.

This display mode shows the surface enclosing the centerpoint locations of a given-sized particle (sphere) within the structure. By setting the particle size to zero, you can show the actual reciprocal of the crystal structure.

There are two steps to the location of this surface. First (grid calculation), the unit cell is sampled at the given **Grid spacing** and **Offset**, to get the distance to the surface of the nearest atom. This calculation need not be repeated unless the unit cell, atom coordinates or atom radii, or the **Grid spacing** or **Offset** are changed. Second (surface evaluation), at plot time the surface which outlines the given **Particle radius** (i.e. a three dimensional contour surface) is drawn. Multiple unit cells are drawn by duplicating the surface segments in the central unit cell, which increases drawing or rendering time, but not grid calculation or surface location time.

The grid calculation uses the current atom radii (Atoms dialog, Input1 menu). Presumably these are full ionic, covalent or van der Waals radii. The radii can all be changed by a factor with the Atoms-Global dialog (Input2 menu).

Since a single unit cell is sampled from 0 to 1, and offsets and multiple cells extend in the positive axis directions, automatic centering should normally be selected in the Centering/Displacement dialog (Input2 menu).

The calculations involved in this mode are essentially independent of those involved in the other display modes. If you want to switch between Cavities mode and other modes, to compare the the actual structure with cavities, it may be helpful to set the Boundary Option and other conditions to match.

When showing a single unit cell with no offsets, the Boundary should be set to Unit Cell, **0-1 inclusive**. It is usually helpful show the unit cell edges with the Axes/Unit Cell option (Input2 menu). The unit-cell **Displacements** (button in the Axes/Unit Cell dialog) should all be set to zero.

When displaying in Cavities mode with multiple unit cells and/or offset unit cells, showing the actual structure with the same boundaries requires using the Enter Forms boundary option. Symmetry for the faces should be None, and the bounding faces should be those of the unit cell, at central distances which are suitable fractions (to take account of **Offsets**) and/or multiples of the d-spacing. The d-spacing is printed out for each form after it is entered. If the boundary is initially set up for Unit Cell (previous paragraph), and then switched to Enter Forms, the appropriate faces will be entered and the central distances/d-spacings given. Note that **Offsets** will require negative central distances. For example, if the Cavities volume is offset by 0.25 on the a-axis, the bounding faces cutting the a-axis should be (100) at central distance 1.25d and (-100) at -0.25d (where d is d-spacing).

Note that atoms with small radii have little influence on the configuration of cavities, and such atoms can usually be omitted. For example when doing silicates using ionic radii, silicon atoms may be omitted. Even using covalent or van der Waals radii the silicon atoms do not greatly influence the configuration of cavities. Of course if the **Particle radius** is set to zero, the locations of omitted small atoms may show up as isolated cavities, but this may be minimized by setting the **Grid spacing** to a value larger than the small atoms. Thus omitting small atoms improves the speed of the calculations in two ways; directly by reducing the number of atoms considered in the grid calculation step; and indirectly by allowing larger grid spacing.

Cavities-mode drawings may be saved as VRML Files. Rotation of a small Cavities-mode drawing may be faster in a VRML viewer than in ATOMS, primarily because the viewer saves all the individual polygons comprising the surface in memory, and does not have to calculate them for each view. However, for large drawings storage of all this information may cause the viewer to use virtual memory, which can bring the entire process essentially to a halt.

There are two zeolite structures set up for Cavities mode in the /SAMPLES sub-folder, LINDE_L.STR and ZSM5.STR. Open these files and switch to the Cavities display mode.

Using Stereopairs (Input2 menu) is usually very helpful in Cavities mode.

The ray-tracing program POV-Ray can be used to make a very smooth-appearing cavities drawing. To do this, select POV-Ray in the File menu and be sure the **Spheres** box is checked.

3.2.4.1.7 Protein Display Mode

This mode, which is a 3D mode only, only works on data imported from PDB files. It displays the bonds between (all) protein backbone atoms as cylinders, with the radius specified in the Protein Display Attributes dialog. By default, other atoms in the amino acids or residues are omitted, but you can specify a limited number of specific residues to draw in the ball-and-stick mode in the Protein Display Attributes dialog. Hetatoms (non-residues) are always drawn as ball-and-stick.

The bonds drawn in this mode must be specified in the Bonds dialog in the Input1 menu. At a minimum to show the backbone there must be carbon-carbon and carbon-nitrogen bonds. Any other bonds among hetatoms and non-backbone atoms in the residues must also be specified. Usually this can be done by selecting automatic bonds.

This mode relies on the atomic labels and residue information derived from PDB files and cannot be used without importing data in that format.

The amino acids or residues are shown in the shapely color scheme as used by RasMol (www.openrasmol.org). This display mode shows more detail (more atoms) than the "backbone" mode of RasMol because a main objective is to be able to focus on some of the groups of hetatoms and show their bonding to the amino acids when necessary.

3.2.4.1.8 Full-screen 3D mode

---Windows only

The **Fullscreen 3D** mode switches to full-screen display, in 3D mode. The main reason to do this is to take advantage of full-screen, full-color stereoscopic viewing using shutter glasses - the software and hardware for these glasses will only work in full-screen mode (see below for details).

The projection method is always perspective, and the perspective distance is set in the Perspective dialog. However, when operating with shutter glasses, the effective perspective distance may also be affected by a setting of the display-card driver, which may in turn be controlled by hot keys.

When in full-screen mode the following controls are in effect:

ESC key exits full-screen mode and returns to whatever viewing mode was in effect before.

Left button down and moving the mouse causes rotation exactly as in the normal windowed mode..

Right button down and moving the mouse down causes structure movement ("panning")- the centering offsets (Centering/Displacement dialog) are changed. This has the same effect as the **Set Center** button in the DialogBar-Right.

CTRL-x, **CTRL-y** and **CTRL-z** start rotation around the x, y or z Cartesian axes. The rotation increment and delay (if any) are set in the Continuous Rotation dialog. Halt the rotation with the same keys, or by exiting this mode with **ESC**.

Plus "+" and **minus** "-" keys change the scale ("zoom" or "dolly"), just like the **Rescale** buttons in the DialogBar-Right.

CTRL-a turns on animation of the vibrational motion, if the current file has been imported as a VIBRAT (.MOT) file. The mode and speed of rotation are controlled in the Vibrational Modes dialog in the Input1 menu. Turn of animation with the same key.

Rotation and vibrational animation can not currently be done at the same time - turn off vibration in order to rotate the structure and vice-versa.

Full-screen, full-color stereoscopic viewing with shutter glasses. These glasses, with driver software for Windows operating systems, can now be bought for well under $100 from many vendors. It is claimed that most recent graphics cards are supported in one way or another, but the most complete support is for nVidia cards, the stereo drivers for which are available for free online (www.nvidia.com). The requirements and general procedure for shutter-glasses viewing are as follows.

1) You must have a cathode-ray-tube (CRT) monitor. Flat-screen monitors will not work because the refreshing mechanism is different.
Stereo only works in 3D (OpenGL) mode, not ATOMS Standard mode.

2) You must install the stereo software driver for your particular graphics card onto the computer. You may also need an up-to-date driver for the card itself. For nVidia cards, install the latest standard (non-stereo) driver for your card, and then the (separate) stereo driver, according to the instructions at www.nvidia.com. For other cards you will need a third-party stereo driver, which may be provided with the glasses. The driver must support OpenGL.

3) Install the glasses (or the wireless station), typically by inserting a "dongle" where the monitor cable plugs into the computer (graphics card).

4) Turn on the Full-Screen mode in ATOMS, then turn on the stereo mode, usually by using a "hot key". It may be best to turn stereo on after entering full-screen mode in ATOMS, and turn it off before exiting.

Flickering in stereo mode is caused by a monitor refresh rate that is too slow. This

usually may be reset in the Windows Display control panel and/or in the stereo driver software. On switching into full-screen mode, ATOMS first tries the current screen size, bit-depth and refresh rate. If this fails, then it tries successively smaller screen sizes. If you get a message saying that the switch into full-screen mode has failed, you can try changing the bit-depth (for example from 32- or 24-bit to 16-bit) or the refresh rate in the Windows Display control panel or in the stereo driver software.

The Website www.stereo3d.com has some basic technical information about shutter-glasses stereo, but the information on specific hardware and vendors may be out of date because the technology and marketing are currently moving very rapidly.

Caution: use shutter glasses or other hardware and driver software at your own risk - stereo drivers may have a tendency to crash your system. SHAPE software is not responsible for any damage to your hardware or software through use of these devices.

3.2.4.2 Cursor Mode Sub-Menu

Cursor Mode Submenu [Display Menu**]**

In **Atom ID** (identification) mode, clicking on the left (or only) mouse button will identify atoms and give bond lengths and angles - see Atoms at Cursor. The cursor in this mode is a cross. Clicking and dragging with the right mouse button (Windows) or control+button (Macintosh) will switch temporarily (as long as the button is down) to the the **Rotate** mode, below.

In **Rotation** mode, clicking and dragging rotates the structure. In most of the window, rotation will be around the y and z Cartesian axes, in the plane of the screen. Clicking and dragging near the left or upper edges will rotate about the z axis, perpendicular to the screen. The cursor is a quadruple arrow when rotating on x and y, and a circular arrow when rotating on z.

The Cursor Mode can be selected either in the Display menu or the Dialog Bar - Right.

3.2.4.3 Replot Command

Replot Command [Display menu**]**

This command redraws the image in the graphics window which is currently active without recalculation. The active window may be the main graphics window (containing the structure image), the Powder or Precession diffraction patterns.

Changes in most items in the Input2 Menu can be put into effect with this command (although these dialogs all have an automatic replot check box). It can also be used after some changes in the items in the Input1 menu, such as colors and bond radii. For

changes which affect atom locations and atoms involved in bonds and polyhedra, or changes in thermal ellipsoids, use the Calculate command in the **File** menu. Changing atomic radii does not require recalculation as long as stick bonds are not changed to interpenetration or vice-versa.

When the **Auto** button in the Dialog Bar - Left is checked, replot is automatic whenever you click one of the axis rotation buttons.

3.2.4.4 Color Command

Color Command [Display menu**]**

This switches between full-color and black-and-white screen display (all types of output such as printing, metafiles, etc. have independent color switches). Screen displays with more than 16 colors may show true gray-scale rather than the dithering which is used in actual black-and-white output. You can set the default or start-up status of this switch in the Preferences dialog in the **Settings** menu.

3.2.4.5 Atom Labels

Dialog Box: Atom Labels [Display Menu**]**

You can show either labels or generated atom numbers. The labels will use the atomic labels entered in the Revise Atom dialog, up to 6 characters. You can specify fewer characters with the **Max. letters** item. The labels will be stripped of trailing blanks and centered on the projection of the atomic center, unless the **Offset**s are non-zero.

If the **Scale** box is checked, in printed output or output to a file, the labels in that output will be scaled to approximately the same relation to the drawing itself as on the screen. This is a very approximate process, and trial-and-error adjustment may still be necessary to get the desired label sizes in output. The option applies to all types of lettering on the plot, not just atom labels.

If the **Background** is opaque, each letter will lie on a small block of the designated color; this usually makes the labels easier to read. Other programs which read ATOMS output files may not be able to reproduce these opaque blocks in Metafile or PICT files output. Labels are not supported for Pen Plot output.

Sequence. The labels may be plotted immediately after each atom, or all at once after all atoms have been plotted. The first usually looks better, but some labels will usually be partly or completely obscured.

Use PostScript font. This allows you to enter a character string for PostScript fonts supported by a PostScript printer if such fonts do not appear in the standard system font dialog called up by the **Font** button. This character string usually specifies the weight

(normal, bold) and slant (italic, oblique) of the font, but not the size, which is specified in the **Font** dialog. Certain PostScript typefaces are standard, and should be present on most PostScript printers.

The label positions are correct for stereopairs, and labels for central atoms of polyhedra will appear suspended in the interior of the polyhedra.

Show symmetry number (roman). If this box is checked, each atom label will have a superscript, in roman numerals, giving the number of the symmetry operation which generated the atom, or in the case of atoms in special positions the first operation generating that atom. This is the method for designating symmetry operations (or equivalent positions) mandated by *Acta Crystallographica*. The symmetry operations or positions in "xyz" form (as given in the International Tables) can be listed out with the Listings/Input option in File menu. The symmetry numbers in roman and arabic numerals for generated atoms can also be listed with the Listings/Generated Atoms option in the File menu, and in the Calculation Output option in the Input2 menu. Note that no superscript will be given to atoms generated by the first symmetry operation (x, y, z or identity), and roman numeral "i" will be given to atoms generated by the second operation, and so on.

The order of space-group symmetry operators may be changed to some extent, giving different symmetry numbers and roman superscripts. To do this, switch to the Custom symmetry option and rearrange the list of operations. The list of operations can also be edited in the saved .str file with a word processor. Operations will always be listed in groups, related by a center of inversion, and by Bravais lattice centerings.

With **Atoms to omit**, you can elect to omit labels for certain classes of atoms, such as non-plotting atoms (those in incomplete polyhedra, or deleted by the user) which are deleted by default.

Individual generated atoms can be omitted or deleted, by clicking on the atom and unchecking the **Labels** checkbox in the Generated Atom Data dialog. This type of deletion is like deleting atoms themselves (see Deleting Atoms) - when you save a file, a list is made of the generated atoms for which labels are deleted. Labels which have been deleted in this way can all be restored with the **Restore All** button in this dialog. Also, you can delete all labels with the **Delete All** button, then restore selected atoms individually with the Generated Atom Data dialog. Starting with V4.0, the lists of deleted atoms and labels use a code containing the unit-cell, the symmetry operator etc., rather than an arbitrary sequence number, so that changing the boundary conditions will not usually make the list invalid (although some deleted atoms or labels may no longer be within the boundaries). However, changing the symmetry will make the list invalid.

Labels on individual atoms can be moved onscreen with a special cursor mode controlled by the **Move Labels** button in the Dialog Bar - Right. The **Zero Displacements** button

in this dialog will remove the displacements on all atom labels.

Use the color options in this dialog, not the color options in the Font dialog to set the color of the letters. Letters are always solid black in black-and-white display or output. See Input Colors/Patterns/Pens for general aspects of color input.

Note that in 3D display mode the labels have an absolute position in space, including the *x* (front-back) coordinate. They are arbitrarily plotted a short distance in front of each atom if the **after each** sequence is selected. If the **after all** sequence is selected, they are drawn in a single plane in front of all atoms.

3.2.4.6 Bond Labels

Dialog Box: Bond Labels [Display Menu**]**

You can specify the number of figures to the right of the decimal with the **Decimals** item. The labels will be stripped of trailing blanks and centered on the projection of the center of the bond (midpoint between atom centers), unless the **Offset**s are non-zero.

If the **Background** is opaque, each letter will lie on a small block of the designated color; this usually makes the labels easier to read. Some other programs may not be able to reproduce these opaque blocks in Metafiles or PICT files output. Labels are not supported for Pen Plot output.

Sequence. The labels may be plotted immediately after each atom, or all at once after all atoms have been plotted. The first usually looks better, but some labels will usually be partly or completely obscured. Some offset may be required.

Use PostScript font. This allows you to enter a character string for PostScript fonts supported by a PostScript printer if such fonts do not appear in the standard system font dialog called up by the **Font** button. This character string usually specifies the weight (normal, bold) and slant (italic, oblique) of the font, but not the size, which is specified in the **Font** dialog. Certain PostScript typefaces are standard, and should be present on most PostScript printers.

If the **Scale** box is checked, the letters in the labels in printed or file output will be rescaled to keep the same approximate proportions with respect to atoms, bonds, etc. as in the screen view.

Use the color options in this dialog, not the color options in the **Font** dialog, to set the color of the letters. Letters are always solid black in black-and-white display or output. See Input Colors/Patterns/Pens for general aspects of color input.

Individual bond labels may be "deleted", or marked for non-plotting, by clicking on the

two atoms in succession and unchecking the **Bond Label** box in the Generated Atom Data dialog. The **Show All** button in this dialog will restore all bond labels to visibility, and the **Delete All** button will mark them all for non-plotting.

Labels on individual bonds can be moved onscreen with a special cursor mode controlled by the **Move Labels** button in the Dialog Bar - Right. The **Zero Displacements** button in this dialog will remove the displacements on all bond labels.

Note that in 3D display mode the labels have an absolute position in space, including the *x* (front-back) coordinate. They are arbitrarily plotted 0.5 Angstroms in front of the center of the bonds, but they may still actually intersect or interpenetrate with the bond in some cases.

3.2.4.7 Angle Labels

Dialog Box: Angle Labels [Display Menu]

Angles are labeled with their values in degrees. A circular arc is drawn between the two central-ligand bonds defining the angle, and the label is drawn over the midpoint of this arc. Note that this arc is 3-dimensional, and its projection may not be circular. The radial position of arc and label are defined with the **Fraction of short bond** edit box. If this value is 0.5, for example, the arc will be drawn half-way out from the central atom to the atom at the end of the shorter bond.

Angles are located automatically, from the **Specifications** (below). Note that the location is done in the calculation, not plotting, so changing the specifications will require Recalculation (Dialog Bar - Left or File menu).

Drawings should be kept simple when this option is used, as only a limited number of angle labels will be intelligible. Typically this option would be used in conjunction with the Sphere boundary option, to illustrate the coordination of a single atom.

The **Blank interval** causes the bond to start and end short of the actual center line of the bonds. Using this interval may improve the appearance, especially if stick bonds, instead of line bonds, are used.

You can specify the number of figures to the right of the decimal with the **Decimals** item. The labels will be stripped of trailing blanks and centered on the projection of the midpoint of the arc, unless the **Offset**s are non-zero.

If the **Background** is opaque, each letter will lie on a small block of the designated color; this usually makes the labels easier to read. Some other programs may not be able to reproduce these opaque blocks in Metafile or PICT file output.

If the **Scale** box is checked, the letters in the labels in printed or file output will be

rescaled to keep the same approximate proportions with respect to atoms, bonds, etc. as in the screen view.

The **Linewidth** gives the width of the arc, which is always a line even in 3D display mode. The line will have the same color as the letters; this color can be specified in this dialog. [Macintosh only] In the 3D display mode on the Macintosh it is not possible to set linewidths - all lines are one pixel wide.

Use PostScript font. This allows you to enter a character string for PostScript fonts supported by a PostScript printer if such fonts do not appear in the standard system font dialog called up by the **Font** button. This character string usually specifies the weight (normal, bold) and slant (italic, oblique) of the font, but not the size, which is specified in the **Font** dialog. Certain PostScript typefaces are standard, and should be present on most PostScript printers.

Use the color options in this dialog, not the color options in the **Font** dialog to set the color of the letters. Letters are always solid black in black-and-white display or output. See Input Colors/Patterns/Pens for general aspects of color input.

Specifications. These are given in terms of coordination of a single central atom. Angles will be found around all atoms of the given **Type**. The **Maximum Angle** can be used to exclude near-180-degree angles in octahedra, for example. The angles are located at calculation, not plot time, so changing specifications will require Recalculation (Dialog Bar - Left or File menu).

"*Deleting* " *angle labels*. All angles around the atoms of the specified type(s) will be located. However, individual angles can be "deleted", or actually marked for non-plotting. This is done by clicking successively on the three atoms in the order outer-central-outer. In the Generated Atom Data dialog, there then appears an **Angle** checkbox. Unchecking will cause non-plotting of the angle. A list of the non-plotting angles is saved in the data (.str) file. The **Show All** button allows restoration of all non-plotting angles, and the **Delete All** button marks all angles for non-plotting. Individual non-plotting angles can be restored by clicking on the atoms and checking the **Angle** box in the Generated Atom Data dialog.

Labels on individual angles can be moved onscreen with a special cursor mode controlled by the **Move Labels** button in the Dialog Bar - Right. The **Zero Displacements** button in this dialog will remove the displacements on all angle labels.

Angle labels are not supported for Pen Plot output.

Note that in 3D display mode the labels have an absolute position in space, including the *x* (front-back) coordinate. They are arbitrarily plotted 0.5 Angstroms in front of the arc, but they may still actually intersect or interpenetrate with the arc in some cases.

3.2.4.8 Scale Grid

Dialog Box: Scale Grid [Display Menu**]**

This option allows you to locate and size the structure, so that it can be rescaled or displaced. It will draw a square grid at the given absolute intervals. The center of coordinates is shown by a star at the center of the screen, and the current location of the center of the structure by another star. These two center points differ only if you have entered displacements or turned on automatic centering with the Centering/Displacements dialog in the **Input2** menu. The grid is removed only by replotting with the **Grid plotting on** box unchecked.

See Input Colors/Patterns/Pens for general aspects of input

3.2.4.9 Mark Atoms

Dialog Box: Mark Atoms [Display Menu**]**

This will draw a box of the given size around the center of of each of the selected type of atom. This is especially useful in locating atoms which you have previously marked as non-plotting.

See Input Colors/Patterns/Pens for general aspects of input.

3.2.4.10 Clinographic Viewing

Clinographic Viewing Command [Display menu**]**

This turns clinographic viewing on and off, with automatic replot. See also Clinographic Viewing in the **Rotation** menu, which does the same thing without automatic replot. Set the inital state of clinographic viewing in the Initial Orientation dialog in the **Input2** menu.

See also Coordinate Systems.

3.2.4.11 General Planes

Dialog Box: General Planes [Display Menu**]**

3D Display mode only.

This allows insertion of general planes.

The planes are defined in terms of corners (points) in fractional coordinates on the structure (crystal) axis system. The points must define a convex planar polygon in correct order. The planes are two-sided, so the sequence 1-2-3-4 is equivalent to 4-3-2-1.

Complete parallelogram. If this box is checked and there are only three points, a fourth point will be added such that side 3-4 will be parallel to 2-1 and 4-1 will be parallel to 3-2. If the box is not checked, three points will define a triangle.

3.2.4.12 General Lines or Cylinders

Dialog Box: General Lines or Cylinders [Display Menu**]**

3D Display mode only.

This allows not only general lines or cylinders, but customized "bonds" to be drawn.

The lines or cylinders are defined in terms of two points in fractional coordinates on the structure (crystal) axis system.

If the **Radius** is 0.0, lines will be drawn (if allowed in the particular type of display or output) - otherwise cylinders will be drawn.

If you have clicked with the mouse on two atoms (see Identifying (Picking) Atoms), you have the option, in the Generated Atom Data dialog, of defining a "bond" between the current atom and the last one. You will be referred to this dialog, and the "bond" will be kept in the list of lines/cylinders, not in the Bonds dialog in the Input1 menu.

3.2.4.13 Dialog Bar - Left

Dialog Bar - Left

This is actually a special type of Control Bar, which resides on the left side of the Main window. It can be turned on or off with the **Dialog Bar - Left** command in the **Display** menu.

The upper part controls rotation of the structure in simple ways (for more ways to rotate or align the structure, see the commands in the Rotation menu). The current orientation is shown at the top. The a, b and c axis labels are attached to the positive ends of the axes, and the part of the axes extending forward (positive x) are drawn with heavier lines. The rotation buttons below this are for rotation on x, y and z, respectively; positive angle (clockwise looking outward on the axis) is on the left, and negative rotation on the right. The angle of rotation is in the box below the buttons. The initial value of this angle is set in the Preferences dialog in the **Settings** menu.

If the **Auto** box is checked, the drawing is replotted immediately after each click on a rotation button. If it is not checked, the rotations are accumulated into a matrix, and the drawing is not replotted until you click on the **Replot** button lower in the dialog (or select **Replot** from the **Display** menu).

The buttons beneath A**uto** duplicate some common commands, all from the File menu except **Replot**, which is also found in the Display menu. You can use **Open** to start up ATOMS by reading in a file.

Replot - Replots the image (does not recalculate).
Calculate - Reproduce atoms within specified boundaries and locate bonds and polyhedra.
Open - Open an old ATOMS data file.
Import - Open a crystallographic or molecular data file from other sources.
Import - Open a crystallographic or molecular data file from other sources.
Save - Save an ATOMS data file.
Save as - Save an ATOMS data file with a new name
Print - Print out the graphics image.

The Combo box at the bottom of the dialog controls the Display mode - this duplicates a submenu in the **Display** menu. The options are Standard, Skeletal/3DSkeletal, Ellipsoid, 3D,Anaglyph, Cavities and Protein. A button in the DialogBar - Right also selects the Full-Screen 3D mode.

The **Animate** button, present when you have read in a .MOT file from VIBRATZ and have atomic-motion data for vibrational modes, will start an animated (moving) display. Exit the animated mode by clicking the mouse or hitting any key. Speed and other parameters of this display are set in the Vibrational Modes dialog in the Input1 Menu. That dialog also controls making movies or "video" files.

3.2.4.13.1 Import File

Dialog Box: Import File [Dialog Bar - Left]

This offers a selection of file types to import, including CCDC FDAT, SHELX-93, CIF, DBWS/LHPM Rietveld, ICSD, ORTEP, XTLVIEW, VIBRAT,PDB, RIETAN, GSAS, AM MINERAL, FULLPROF and Free-Form.

The boundary option in most cases can either be Default Unit Cell, suboption as selected with the **Default** radio button, or Locate Molecules in Crystal.

Multiple occupancies are not permitted in ATOMS, and when more than one atom is found to be in the same position (same fractional x, y and z coordinates) the second and subsequent occurences will be deleted.

There is a limit of 500 input atoms in most cases.

3.2.4.14 Dialog Bar - Right

Dialog Bar - Right

This is actually a special type of Control Bar, which resides on the right side of the Main window. It can be turned on or off with the **Dialog Bar - Right** command in the Display menu.

Cursor Mode. In **Atom ID** (identification) mode, clicking on the left (or only) mouse button will identify atoms and give bond lengths and angles - see Atoms at Cursor.

The cursor in this mode is a cross. Clicking and dragging with the right mouse button (Windows) or control+button Macintosh) will switch temporarily (as long as the button is down) to the the **Rotate** mode, below.

In **Rotate** mode, clicking and dragging rotates the structure. In most of the window, rotation will be around the y and z Cartesian axes, in the plane of the screen. Clicking and dragging near the left or upper edges will rotate about the z axis, perpendicular to the screen. The cursor is a quadruple arrow when rotating on x and y, and a circular arrow when rotating on z.

The **Clino** (clinographic) **View** checkbox will switch viewing with the Clinographic rotations.

The **Set Center** button defines a new center point - use this to "focus" or "zero in" on a specific area or point in the plot. After clicking on this button, an dialog informs you that the next mouse click in the graphics window will define a new center point. After clicking on a point, the drawing will then be displaced so that that point will be at the center of the viewing area. It may be more useful to think of the result as the viewing area being centered on the point selected. Displacements set in this way may be changed in the Centering/Displacement dialog in the Input2 Menu.

With the **Rescale** buttons, you can "zoom" in or out. The actual factor applied is 1/(1+x) for down scaling, and (1+x) for up scaling, where x is the amount in the edit box converted from percent to a fraction. In the **Maximize size for each view** and **Universal maximum** modes this changes the **Rescale factor**, which may be reset manually in the Scaling dialog in the **Input2** menu. When in the **Fixed** scaling mode, the actual scale factors for screen, print and pen plot are changed. This behavior is a change from pre-V5.0 ATOMS, in which rescaling always changed to the Fixed mode.

Orientation buttons. These buttons will actually remove accumulated rotations and return to either the original orientation or the initial orientation. They perform the same functions as the Remove Rotations option in the Rotation menu.

The *original* orientation means the orientation before any rotations, including the alignment of a slice, and the rotations of the Initial Orientation dialog in the **Input2** menu, have been made. This gives the standard orientation of the crystal (the first one in the case of multiple crystals) with respect to the reference Cartesian coordinate system. The *initial* orientation is that attained after the rotations just listed have been made, if any of them were actually used. See also Coordinate Systems.

Delete Tool. This allows "deleting" (see Deleting Atoms and Atom Labels) groups of atoms by creating a polygon with the mouse. All atoms within the projection of the polygon can be marked for non-plotting.

The **Show All** button allows immediate restoration of all atoms marked as non-plotting. See the Atom/Bond Plot States dialog (Input2 menu) for more options regarding non-plotting atoms.

Move Labels. Individual atom, bond and angle labels on generated atoms can be moved from their centered position. This button turns on and off a special cursor mode (for the left button only) in which clicking and dragging labels will move them. This should not be done until the very latest stages of preparing a drawing, since rotations are liable to make the changed locations invalid. All label displacements can be removed for each type of label in the dialogs in the Display menu.

The **Inter. bonds** (inter-molecule bonds) combo box (only displayed if there are bonds between molecules or fragments) gives several options for display of inter-molecule or interfragment bonds. If Highlighted is selected, such bonds are shown in normal colors while all other atoms, bonds, etc. are dimmed. Other possible highlighting of molecules or fragments is ignored.

The **Reset Scale** button calls the Reset Scaling and Centering dialog. This allows reversion to the last setttings, before interactive changes with the **Set Center** or **Rescale** buttons (above), or in the **Fullscreen 3D** mode.

---Windows only

The **Fullscreen 3D** mode switches to full-screen display, in 3D mode. The main reason to do this is to take advantage of full-screen, full-color stereoscopic viewing using shutter glasses - the software and hardware for these glasses will only work in full-screen mode (see below for details).

The projection method is always perspective, and the perspective distance is set in the Perspective dialog. However, when operating with shutter glasses, the effective perspective distance may also be affected by a setting of the display-card driver, which may in turn be controlled by hot keys.

When in full-screen mode the following controls are in effect:

ESC key exits full-screen mode and returns to whatever viewing mode was in effect before.

Left button down and moving the mouse causes rotation exactly as in the normal windowed mode..

Right button down and moving the mouse causes structure movement ("panning")- the centering offsets (Centering/Displacement dialog) are changed. This has the same effect as the **Set Center** button in the DialogBar-Right.

CTRL-x, **CTRL-y** and **CTRL-z** start rotation around the x, y or z Cartesian axes. The rotation increment and delay (if any) are set in the Continuous Rotation dialog. Halt the rotation with the same keys, or by exiting this mode with **ESC**.

Plus "+" and **minus** "-" keys change the scale ("zoom" or "dolly"), just like the **Rescale** buttons.

CTRL-a turns on animation of the vibrational motion, if the current file has been imported as a VIBRAT (.MOT) file. The mode and speed of rotation are controlled in the Vibrational Modes dialog in the Input1 menu. Turn of animation with the same key.

Rotation and vibrational animation can not currently be done at the same time - turn off vibration in order to rotate the structure.

See Full-screen mode for information on setting up stereo view with shutter glasses.

3.2.4.15 Dialog Bar - Fragments

Dialog Bar - Fragments

This is actually a special type of Control Bar, which resides on the right side of the main Graphics window. It can be turned on or off with the **Dialog Bar - Fragments** command in the Display menu.
Frag (Fragment) This selects the fragment to be operated on.

Rotate. Each of the six buttons will rotate the selected fragment about one of the Cartesian observer axes (see Coordinate Systems) by the angle in degrees entered in the edit box below. The arrows in the lower four buttons indicate motion of the front of the structure.

Translate. Pressing the **Translate** button will move the selected structure by the distance in Angstroms entered in the edit box, along one of the Cartesian observer axes

(**Cart** x, y or z) or one of the structure (crystal) axes (**Struct** a, b or c) of the main structure as selected by the radio buttons.

Use a negative distance to move backward along one of the axes.

The translations in this dialog affect the actual x, y and z coordinates of the atoms and are thus quite different from the plotting displacements in the Centering and Displacements dialog in the Input2 Menu.

Translations can be removed in the Translate Structure Fragment dialog under Multiple Structures in the Transform menu. This dialog also allow more complex translations.

Rotations made in this dialog can be removed with the Rotate Structure Fragment dialog, Transform menu.

3.2.4.16 Powder Diffraction

Dialog Box: Powder Diffraction [Display Menu **]**

To calculate diffraction, the type numbers for atoms (**Atom Data** dialog) must be valid atomic numbers, or those numbers modulo 100, or must anyway correlate with the table of scattering factors in the SCATFAC.DAT file if you modify that file.

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.

There are four options for wavelength; averaged **K(alpha)**; separate **K(alpha)1 and K(alpha)2**; averaged **K(alpha) and** (separate) **K(beta)**; and a single **Specified 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 (**Beta inten**.). 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 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 Printing, Raster Files and Metafiles or PICT files.

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 using the program CRYSCON (Shape Software).

NOTE: Many of the sample files provided with ATOMS, especially the Basic Inorganic structures, are idealized structure types. They may have a unit cell scaled to a bond length of 1.0, or use arbitrary numbers for types instead of atomic numbers as required for diffraction. *Therefore they will not always give correct diffraction results.*

3.2.4.17 Precession Pattern

Dialog Box: Precession Pattern [Display Menu **]**

To calculate diffraction, the type numbers for atoms (Atom Data dialog), or those numbers modulo 100, must be valid atomic numbers, or must anyway correlate with the table of scattering factors in the SCATFAC.DAT file if you modify that file.

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).

To reproduce actual X-ray precession photographs, the **Do Lorentz-polarization** box should be checked. Omitting the Lp corrections shows the structure factors (squared), and it also allows display of the inner region in the upper levels, which is not recorded in an actual X-ray pattern. The Lp factor becomes very large near the inner and outer edges of the recorded pattern - if the value of this correction is greater than 10.0, an open symbol is used rather than a filled one. Such intensities are not reliable.

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.

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 Printing, Raster Files and Metafiles or PICT files.

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 using the program CRYSCON (Shape Software).

NOTE: Many of the sample files provided with ATOMS, especially the Basic Inorganic structures, are idealized structure types. They may have a unit cell scaled to a bond length of 1.0, or use arbitrary numbers for types instead of atomic numbers as required for diffraction. *Therefore they will not always give correct diffraction results.*

3.2.5 Rotation Menu (Graphics Window)

Cartesian Axes - Rotate on the viewer or reference axes.

Structure Vector - Rotate on a rational structure vector [uvw].

Clinographic Viewing - This turns clinographic viewing on and off, with optional replot

Align Face or Vector - Align the structure with a face in the screen or a vector perpendicular to it.

Stereopair Rotations - Used to draw separate left- and right-eye stereopair views when Shading is on.

Remove Rotations - Remove all rotations made since the calculation or the Initial Orientation.

Current Orientation - Gives the current orientation of the structure with respect to the observer coordinate system.

Continuous Rotation - Sets up continuous timed rotation about any of the observer axes.

Rotation Movie - Write a video or movie file in the.AVI (Windows) or.MOV (Macintosh) format.

3.2.5.1 Rotate on Cartesian Axes

Dialog Box: Rotate on Cartesian Axes [Rotation menu**]**

This rotates the structure on one of two sets of Cartesian axes. If clinographic viewing is off, the structure is always rotated about one of the axes belonging to the observer system: x coming straight out towards the observer, y in the plane of the screen or paper pointing to the right and z upwards.

Each time you click the **Rotate** button, a rotation is added to a master rotation matrix; the number of such rotations is listed at the bottom of the dialog box. When you have finished rotating, click the **Done** button and the master rotation matrix is applied to the structure. If you click **Cancel**, no rotations are applied.

3.2.5.2 Rotate on Structure Vector

Dialog Box: Rotate on Structure Vector [Rotation Menu**]**

This will rotate about a rational structure direction [uvw], regardless of the current display mode or orientation of the structure. If you are drawing a molecule and have used

Cartesian reference axes, the rotation direction is simply a vector with the coefficients u, v and w in the original molecule axis directions a, b and c. The indices or coefficients refer to a coordinate system fixed with respect to the structure (always rotating with it). The indices must be integers, but this is not a bar in practice to rotation about irrational vectors, since the indices may take very large values.

Each time you click the **Rotate** button, a rotation is added to a master rotation matrix; the number of such rotations is listed at the bottom of the dialog box. When you have finished rotating, click the **Done** button and the master rotation matrix is applied to the structure. If you click **Cancel**, no rotations are applied.

3.2.5.3 Clinographic Viewing

Dialog Box: Clinographic Viewing [Rotation Menu**]**

This will switch on and off the rotations of -18.4 degrees on z and 9.5 degrees on y, applied in clinographic display mode. This in effect changes the viewpoint of the observer between the clinographic position, down the vector [621] referred to the observer Cartesian axial system, and a straight-on position, down the x axis. This command is included in the menu for convenience; the same operation is performed by the Clinographic Viewing command in the **Display** menu, although choosing that command always causes a replot.

See also Coordinate Systems.

3.2.5.4 Stereopair Rotation

Dialog Box: Stereopair Rotation [Rotation Menu**]**

If you want to show a steropair which can fit onto one page, it is usually easiest to draw it automatically by turning on the stereopair mode with the Stereopairs dialog in the **Input2** menu. However, you may want to set up and draw each half of the pair manually, if for example each view is to take up an entire page of output. This option rotates the structure and the illumination vector for shading by the requested angle about the z axis. If you are not using shading, ordinary rotation about z (viewer) will suffice.

The left-eye view should be rotated clockwise (positive angle): an angle of about +3 degrees is usually satisfactory, although this may depend on the perspective distance, the type of viewing device, etc. After making a hard copy of this orientation, the rotation should be negated with the **Remove** button. Then make a right-eye view by rotating the negative of the left-eye value; after making the hard-copy, remove the rotation again.

3.2.5.5 Align Face or Vector

Dialog Box: Align Face or Vector [Rotation Menu**]**

This will rotate a specified face (hkl) to lie flat in the screen or paper (face-normal parallel to x observer), or a vector (uvw) to be perpendicular to the screen or paper. To align a face, it is also necessary to specify a vector lying in the face which will be vertical in the screen or paper (z direction). Conversely, to align a vector, it is necessary to specify a face, containing the vector, whose normal will be vertical. If a vector [uvw] lies in a face (hkl), the indices satisfy the condition hu + kv + lw = 0. If clinographic viewing is in effect, it is turned off when the face is aligned, to simplify any subsequent rotations.

You can elect to use the default alignment vector or face, instead of specifying it. The default vector will be the intersection of the face (hkl) with the face (100), whose indices are given by the cross product (hkl)x(100). If the face (hkl) is (100), the default alignment vector will be the vector [001]. For aligning a vector the algebra is just the same, with interchange of face and vector.

When dealing with a molecule or polymer, using a Cartesian axial system, this rotation option can be used to obtain a view down a given vector direction. Use the vector alignment option, although when the structure axes are Cartesian the two cases of aligning a face or a vector are identical. After specifying the initial vector or view direction, if you do not accept the default you must then give another vector, in place of the "face indices", which is perpendicular to the first vector, and which is to be vertical (z direction). If the two vectors are at right angles, their coefficients or "indices" multiplied together (the vector dot product) should equal zero as in the above condition for a vector lying in a face.

3.2.5.6 Remove Rotations

Dialog Box: Remove Rotations [Rotation Menu**]**

This will counteract all rotations made by the dialogs in the **Rotation** menu as well as any made on-screen with dialogs in the **Display** menu, and take you back to one of two settings. The *original* orientation means the orientation before any rotations, including the alignment of a slice, and the rotations of the Initial Orientation dialog in the **Input2** menu, have been made. The *initial* orientation is that attained after the rotations just listed have been made, if any of them were actually used. See also Coordinate Systems.

Summary of orientation operations. ATOMS first sets the *c* structure axis parallel to the *z* viewer axis, and the *a* * structure axis (perpendicular to *b* and *c*) parallel to *x*. This is the *original* orientation. Next, if the Slice boundary option is in effect, the slice is oriented with the slice plane parallel to *yz*, and the orientation vector parallel to *z*. Then the initial Cartesian rotations, if any, are applied. Finally, the clinographic rotations, if selected, are applied. This is the *initial o*rientation.

3.2.5.7 Current Orientation

Dialog Box: Current Orientation [Rotation Menu**]**

This gives the current orientation of the structure in terms of the structure vectors lying in the x (reverse view direction) and z (vertical) axes of the Cartesian observer system (see Coordinate Systems).

3.2.5.8 Continuous Rotation

Dialog Box: Continuous Rotation [Rotation Menu**]**

This option will rotate the image about any of the three Cartesian observer axes (see Coordinate Systems), by the given increment in degrees.

The **Time delay** is the delay after the image is finished before redrawing is started again. The time required to draw the image is not included in this value.

When this option is in effect, the image is drawn into an off-screen bitmap and then copied onto the screen (see the Preferences dialog in the **Settings** menu), rather than drawn directly onto the screen. When continuous rotation is halted, the previous mode of drawing on- or off-screen is restored. Sound is temporarily turned off.

Pressing any key or mouse button will halt the rotation.

3.2.5.9 Rotation or Vibration Movie

Dialog Box - Rotation or Vibration Movie [Rotation Menu**,**
Vibrational Modes dialog]

This will write a movie or video file in.AVI (Windows) or.MOV (Macintosh) format. This files consist of a series of bitmap (raster) images.

Rotation. The structure will be rotated from its current attitude about the selected **Axis**, with the selected **Rotation increment**, until the sum of rotations exceeds the **Maximum rotation**.

Vibration. One vibrational cycle is written - normally this should be displayed as a loop, or in continuous mode. The **Seconds per cycle** determines the duration of the loop, and therefore the total number of frames.

A normal motion picture uses 32 **Frames per second**, but typical computer videos use less than this. In fact, some computers may not be able to handle 32 frames/sec for large images.

Note that movie files may be very large (many megabytes) even if compressed. For Macintosh, the compression mode is automatically selected by the System software, and is supposedly optimal for the resolution (**Pixel size**) selected. In Windows, you are presented with a dialog showing the available codecs (COmpression-DECompression algorithms), and you must select one. Finding the optimal codec may be a matter of trial and error - performance usually varies with the **Pixel size** and the actual number of colors used. Some codecs compress very effectively, but cause degradation of the image - ATOMS images should usually be compressed with a lossless compression method. One codec which has been found to be good for typical ATOMS images is the CorePNG codec. This and other codecs can be downloaded on the WWWeb (Internet).

See Frames for details of the frame and frame units.

3.2.6 Transform Menu (Graphics Window)

Generated to Input - Converts to a special mode, necessary for dealing with multiple structure fragments, and for modifying individual generated atoms.

Locate Groups - Isolate molecules, polymers or other bonded groups.

Multiple Structures - Generate, read in, or manipulate separate structure fragments.

Remove Crystal Symmetry - Converts to a crystal with no symmetry (space group P1). Unit-cell contents will be converted to input atoms, retaining cell parameters (as triclinic). Temperature factors will be converted to isotropic B.

Expand Layers - Expands a crystal structure on certain planes, increasing the length of the selected axis, creating space near the expansion planes, but leaving the actual structure within layers unchanged.

3.2.6.1 Generated to Input

Dialog Box: Generated to Input [Transform menu**]**

This converts the generated atoms (i.e., all those generated by the symmetry operations and translations within the given boundaries) to input atoms, removes all symmetry and boundary conditions, and changes to a special operating mode, called "Input=generated". This is like converting the current generated volume to a molecule with no symmetry.

This option is required before using the Multiple Structures options in the **Transform** menu. It is also a good idea to use this option if you want to delete more than a few generated atoms (see Deleting Atoms).

Temperature factor data are carried over into the special mode as Cartesian eigenvalues and vectors rather than U or beta coefficients, but they can no longer be modified.

However, if there is more than one structure fragment temperature factors are not allowed (they will be deleted).

Orientation radio buttons. You have the option of returning to the original or standard orientation before converting, or taking the current orientation as the new "original" orientation. This orientation will be saved, which was not the case in pre-V4.0 ATOMS.

Some of the following checkboxes may not be shown, depending on circumstances.

Convert molecules to fragments. This will convert molecules or groups located in several different ways to individual fragments. If one of the Molecules in Crystal boundary options has been chosen, all atoms will be in molecules, and each molecule will become a fragment. "Molecules" may be individual atoms, as in CaCO3 structures (assuming Ca-O bonds are not defined or are marked as intermolecular). If another boundary option is used, and molecules or groups are subsequently located with the **Find** button in the Generated Atom Data dialog (which appears when you click on an atom), or with the Locate Groups dialog in the Transform menu, there may be atoms which are not part of molecules or groups. All these "leftover" atoms will be put into a single fragment, in addition to those already located.

Remove non-plotting atoms. Non-plotting atoms are those which have been explicitly marked as non-plotting, either individually or in groups. Also classed as non-plotting atoms in PDB (protein) structures are hetatoms and/or waters which have been omitted from the plot by means of the setting in the PDB (Protein) Display Parameters dialog in the Input2 menu. Atoms in incomplete polyhedra, which may or may not be shown in the drawing (Polyhedra dialog, Input1 menu) are in a separate option below.

Keep thermal ellipsoids. Thermal ellipsoids are not allowed in Multiple Structures, so there is no point in keeping them if additional fragments are to be added.

Omit atoms in incomplete polyhedra. This includes all atoms in polyhedra which have less than the specified number of ligands, i.e. are incomplete because of boundary conditions.

Keep vectors. Atomic vectors are not likely to be useful in Multiple Structures.

3.2.6.2 Locate Groups

Dialog Box: Locate Groups [Transform Menu]

This allows you to isolate individual molecules, polymers or other structural groups in a crystal. You must specify a single "seed" atom, then all other atoms interconnected to this one are located. The interconnection is by bonds specified in the Bonds input, or

polyhedra specified in the Polyhedra input in the **Input1** menu. There must be no bonds (except those marked inter-molecular) from atoms in a group to atoms outside the group, nor can polyhedra connect atoms within and without the group.

If the structure consists of discrete molecules, not polymers, it is usually easier to use one of the Molecules in Crystal Boundary options. These will automatically identify any and all molecules. See Dealing with Molecules, Groups and Fragments for more information on strategy for dealing with groups. Note also that ATOMS V5.1 differs from previous versions in the way groups are identified - several groups can be identified and this identification persists regardless of whether the atoms are marked for non-plotting or not; and groups may be directly converted to fragments with the Generated to Input option (Transform menu).

Creation of a structure file for displaying such groups involves three steps. Note that the **Find** button in the Generated Atom Data dialog (which appears when you click on an atom) is an alternative to step 2 (that is, to this dialog).

1) *Setting the original boundary option*. Before exercising the **Locate Groups** option, the molecules or other groups must be within the boundaries of a structure calculated in the usual way. For example, you can use the Default Unit Cell option, suboption **-1 to 1;** this gives one full unit cell on either side of the origin (for a total of 8 unit cells).

2) *Locating the group(s).* To do the actual isolation of the group, call on this dialog - **Locate Groups** or use the **Find** button in the Generated Atom Data dialog. You must specify an initial or "seed" atom; this can either be a specific generated atom, or an input atom. If you use a generated atom, it will normally be necessary beforehand to use the on-screen atom-location feature (see **Generated Atom Data**) or a print-out from the **List Generated Atoms** command in the **File** menu to find the number of a suitable atom. Actually, when using a generated atom the **Find** button in the **Generated Atom Data** dialog is usually more convenient than using this dialog (Locate Groups). However, this dialog is the only way to use an input atom (see the list in the Input Atoms dialog in the **Input1** menu, or the List Input dialog in the **File** menu). In this case, ATOMS will test all the generated atoms in the equivalent set derived from that input atom, and find the one which is closest to the origin.

When you click on OK, ATOMS makes a temporary list of all atoms in each group.

3) *Saving the Structure*. After you are finished with step 2, you are presented with the Groups Located dialog, which allows a) restoration of the non-plotting atoms, which will *not* undo the process of group location (as in pre-V5.1 ATOMS); b) locating an additional group; or c) converting the generated atoms to input atoms. If you leave the dialog without doing any of these things, the molecule(s) can be highlighted or hidden in various ways.

You may wish to turn on centering with the Centering/Displacement dialog in the **Input2** menu if the group(s) are not near the origin.

The "deletion" of atoms (see Deleting Atoms) or marking for non-plotting, does not directly affect the location of groups. That is, if you mark an atom for non-plotting, neither the atom nor bonds to it are shown in the drawing, but the atom and its bonds still exist for the purpose of locating groups. In order to remove atoms and bonds permanently before locating groups, you must convert Generated to Input (**Transform** menu), selecting the option to remove non-plotting atoms. Or you can convert Generated to Input and then delete the atoms. Then recalculate to reestablish bonds and polyhedra, and proceed with location of groups.

3.2.6.3 Groups Located

Dialog Box: Groups Located [Transform Menu**]**

This dialog appears after you have located one or more groups with the Locate Groups dialog.

If you click on the **Done** button, the last and other groups can be displayed in various ways according to the radio buttons;

---**Highlight the last group -** really means dim all atoms not in this group.
---**Hide all except the last group** - atoms not in the last group selected will be marked as non-plotting.
---**Hide all except groups** - atoms not in any group will be marked as non-plotting.

Highlighting and hiding can be reversed with buttons in the Generated Atoms Data dialog which appears when you click on an atom.

The **Show All** button allows restoration of any non-plotting atoms. In pre-V5.1 ATOMS this would undo the process of group location, but now the atoms in groups are individually marked with the group number.

The **Add** button allows locating an additional group (back to the Locate Groups dialog).

The **Convert** button converts generated to input atoms in exactly the same as in the Generated to Input command in the **Transform** menu. Note that this option now can convert molecules directly to independent structure fragments.

See the Locate Groups dialog for step-by-step instructions on locating groups, and Dealing with Molecules, Groups and Fragments for general aspects of handling groups.

3.2.6.4 Multiple Structures

Dialog Box: Multiple Structures [Transform Menu**]**

Multiple structures fragments can be used to model twinning, epitaxy and certain types of crystalline defects, as well as interactions between molecules. Each structure can be rotated and translated independently; however, there is only one list of bonds and of polyhedra, and both are located throughout the structure as a whole.

Thermal ellipsoids for multiple structures are not supported; temperature factor information is lost if you introduce multiple fragments.

Most operations on individual structures are carried out through this dialog in the **File** menu. However, individual structure fragments can be rotated and translated in some simple ways using the Dialog Bar - Fragments (**Display** menu).

Before more than one structure can be dealt with, each of the structures concerned must be transformed to the "Input=generated" mode with the Generated to Input command in the **Transform** menu.

The **Multiple Structures** dialog gives a list of the current structure fragments. The first fragment is always the main structure. There are two ways to add additional fragments; the **Duplicate** button and the **Read File** button.

If you choose **Duplicate**, the new fragment will have the same orientation and center point as the current fragment. You have the option of inverting the current fragment, that is, negating all the atomic coordinates. All the types of the atoms remain the same, and the lists of bonds and polyhedra are not duplicated. The title is copied to the new fragment (the title for fragment number 1 is that of the structure as a whole).

The **Read File** button calls up the Read Structure Fragment from File dialog. The **Revise** button calls up the Revise Structure Fragment dialog.

After duplicating a structure or reading in an additional structure fragment, you must choose Calculate from the **File** menu in order to locate bonds and polyhedra. The Calculation Output dialog in the **Input2** menu allows you to get a listing of only those bonds and bond angles which involve more than one fragment, i.e. inter-fragment bonds. To get such a list you must have some sort of calculation output turned on, and the bond distances and/or angles print-outs turned on also.

You can highlight, dim or omit interfragment bonds with a Combo box in either the Dialog Bar - Right or the Atom/Bond Plot States dialog (Input2 menu). Individual fragments can be rotated or moved with DialogBar - Fragments.

Note that clicking with the mouse on an atom in the drawing on-screen brings up the Generated Atom Data dialog, which lists the bond distance to the last atom, and the bond angle involving the last three atoms.

3.2.6.5 Read Structure Fragment from File

Dialog Box: Read Structure Fragment from File [Multiple Structures dialog]

The file specified must be an ATOMS data file (.STR), and this structure must already have been transformed to the "Input=generated" mode with the Generated to Input command in the **Transform** menu. Structure files from old versions of ATOMS may not be readable through this option - in this case the old file may be read with the **Open** command (File menu) and saved in the current format.

You have the option of inversion, that is negating all the atomic coordinates. All other orientation operations can be carried out with rotations after the file is read in. You have the option of adding the bond and polyhedra lists to the old ones.

ATOMS can use either standard bonds, defined by specifying atom types in the Bond Data dialog in the **Input1** menu, or it can use a connectivity table, which is obtained only from a CCDC FDAT file or PDB file - it cannot use both. Thus if the main (first) structure has normal bonds, and the structure read in has a connectivity table, the connectivity table will be ignored; and if the main structure has a connectivity table, normal bonds in the structure fragment being read in will be ignored. In general, normal bonds are more flexible, and can be derived automatically (see Generate Bonds from Atomic Radii).

3.2.6.6 Revise Structure Fragment

Dialog Box: Revise Structure Fragment [Multiple Structures dialog]

This gives the start and end numbers of the atoms for the current fragment or individual structure - the atoms are all kept in the same master list. The coordinates, colors, etc. of individual atoms are revised through the Input Atoms dialog in the **Input1** menu. The displacement of the current fragment is given in both Cartesian coordinates and coordinates on the structure axes of the current fragment, and the fragment may be moved on either set of axes with the Translate button. The center point, used for rotations, is given in Cartesian coordinates with respect to the zero or center point of the aggregate.

The structure which is in memory when you first add a second fragment provides the overall zero point for translations of individual fragments, and for rotations of the aggregate with the **Rotation** menu or the on-screen rotations in the **Display** menu. However, it is possible to rotate the initial fragment, translate it or reset its center point

with the subdialogs under **Multiple Structures** so that its center point and/or orientation are not the same as that of the aggregate.

There are three main types of coordinate system involved in Multiple Structures dialog:

(1) Fixed or reference Cartesian coordinate systems. These apply to all structures and have fixed orientations. The main observer or reference system has a simple relationship to the screen or paper. When Clinographic Viewing is in effect, rotations can also be done on the Clinographic axial system, which is another Cartesian system rotated by a fixed amount relative to the reference system (see Coordinate Systems).

(2) The aggregate or overall structure axes coordinate system. This is taken originally from the first or main structure, but if the first structure is individually translated or rotated through sub-dialogs in Multiple Structures dialog, it may not be the same. Operations in the **Rotation** menu apply to this coordinate system.

(3) A structure-axes coordinate system for each individual structure. Translations and rotations done with sub-dialogs in Multiple Structures dialog may use these coordinate systems.

Only one set of crystal faces is allowed, and it belongs to the overall structure axes coordinate system. Thus it is possible to rotate the first structure out of proper orientation with the faces. For this and other reasons, rotating structure fragment number 1 individually is not usually advisable.

3.2.6.7 Rotate Structure Fragment

Dialog Box: Rotate Structure Fragment [Revise Structure Fragment dialog**]**

This allows much the same operations as for the overall rotations in the Rotation menu, except of course that only the atoms in the current fragment are rotated, about its own center. The Cartesian Axes, Structure Vector and Align Face/Vector options call up dialogs which are called up from the **Rotation** menu, but in this case only the current fragment is affected. The **Structure Vector** and **Align Face/Vector** options use the structure axes belonging to the current fragment. For orienting fragments, especially crystal structures, the **Align Face/Vector** option is most useful.

If you click on the **Set Default** button, the current orientation of this fragment will be the one which is returned to with the **Remove Previous Rotations** button.

3.2.6.8 Translate Structure Fragment

Dialog Box: Translate Structure Fragment [Revise Structure Fragment dialog**]**

The locations listed at the top are the distances the structure has been moved from its

original position, or since the last time the **Set Current Location as Zero** button has been used.

You can move the current structure on either its own structure axes or the overall observer Cartesian axes. Note that the **Distance** in Angstroms applies only to translation on Cartesian axes; if you use a structure vector, the vector itself must have the proper length, which is expressed as fractions of the original structure axes.

If you click on the **Set Zero** button, the current location of this fragment will be the one which is returned to with the **Remove Previous** button.

3.2.6.9 Reset Rotation Center of Fragment

Dialog Box: Reset Rotation Center of Fragment **[**Revise Structure Fragment dialog**]**

This allows you to change the observer Cartesian coordinates of the point about which the fragment is rotated. This rotation center is initially the same as the origin of the coordinate system for this fragment. If it is changed, the new center will be moved along with the fragment by any translations.

3.2.6.10 Expand Layers

Dialog Box: Expand Layers **[**Transform Menu**]**

This option will expand a crystal structure on certain planes, increasing the length of the selected axis, creating space near the expansion planes, but leaving the actual structure within layers unchanged.. It operates on input atoms, leaving the symmetry unchanged.

Any atoms which are exactly on the expansion planes (for example K atoms in a mica structure) will remain on the expansion planes, and thus bonds from these atoms to other parts of the structure will be lengthened. Bonds connecting structural layers (that is, any bonds crossing the expansion planes) 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. Thus the structure will be expanded on the principal plane or unit-cell face which cuts the chosen axis - this plane is not always perpendicular to the axis. For example if the chosen axis is c, the expansion is on the (001) plane.

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. Support for expansion planes other than unit-cell faces could also be added if necessary.

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.

3.2.7 Settings Menu (Graphics Window)

The Settings Menu (Graphics Window) is identical to the Settings Menu (Startup Window).

3.2.8 Window menu

The Window menu lists all the possible windows in ATOMS - 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 0.4 times the size of the lettering for legends.

3.3 Text Window Menu Bar

Text windows are used for the **Listings** group in the File menu of the Graphics window, by the Coordination button in the Input Atoms dialog in the **Input2** menu, and by the Calculation Output command in the **Input2** menu - see Types of Windows. They are standard text or edit windows. To switch to the ATOMS main graphics window, which has the menus and commands for altering and displaying atomic structure data, use the

Window menu, or click on the Graphics window if it is visible.

File menu - This is a standard File menu which pertains *only* to the special files with extension.ADT named above.

Edit menu - This menu has the normal text editing commands, which again pertain *only* to the special files with extension.ADT.

Window menu - Use this menu to switch to the ATOMS graphic window for most operations on ATOMS data sets, and to set the font for the Text windows.

Help menu - On-line help.

3.3.1 File menu (Text Window)

The commands in this menu apply *only* to Text windows, which are generated by the **List...** commands in the File menu of the Graphics window, by the Coordination button in the Input Atoms dialog in the Input1 menu, or by Calculation Output - see Types of Windows for further explanation.

Close - Closes the Text window, and the file associated with it.

Save - Saves the file associated with the window.

Save As - Saves the contents of the window to a specified file name.

Print - Prints the contents of the Text window.

Page Setup - Set the page size and select the printer.

Exit - Exits ATOMS.

3.3.1.1 Save command (Text Window)

Save command (File menu, Text windows)

When called from Text windows, this saves the (text) contents of the current window in the file whose name is in the title bar. The standard ATOMS files INPUT.ATD, GENATOMS.ATD, FACES.ATD and TOTALS.ATD are in a subdirectory or subfolder (**Output**) to the directory containing the ATOMS program (.EXE) file. They are overwritten each time you request a list of the corresponding type. Thus if you want to save these files, you should probably use the **Save As** command instead of **Save**, give the files new names and put them in the same directory as the structure data (.STR) file. See Types of Windows.

3.3.1.2 Save As command (Text Windows)

Save As command (File menu**, Text windows)**

When called from Text windows, this saves the (text) contents of the current window in the file whose name is in the title bar. The standard ATOMS files INPUT.ATD, GENATOMS.ATD, FACES.ATD and TOTALS.ATD are in a subdirectory or subfolder (**Output**) to the directory containing the ATOMS program (.EXE) file. They are overwritten each time you request a list of the corresponding type. Thus if you want to save these files, you should probably use the **Save As** command instead of **Save**, give the files new names and put them in the same directory as the structure data (.STR) file. See Types of Windows.

To save a text file with its existing name and directory, use the Save command**.**

3.3.1.3 Close command (Text Windows)

Close command (File menu**, Text windows)**

Use this command to close the currently active Text window. ATOMS inquires if you want to save changes to your data file before you close it. If you close a data set without saving, you lose all changes made since the last time you saved it.

The standard ATOMS files INPUT.ATD, GENATOMS.ATD, FACES.ATD and TOTALS.ATD are in a subdirectory or subfolder (**Output**) to the directory containing the ATOMS program (.EXE) file. They are overwritten each time you request a list of the corresponding type. Thus if you want to save these files, you should probably use the **Save As** command, give the files new names and put them in the same directory as the structure data (.STR) file.

3.3.1.4 Print command (Text Windows)

Print command (File menu**, Text windows)**

Use this command to print the contents of a Text window. This command presents a Print dialog box, where you may specify the range of pages to be printed, the number of copies, the destination printer, and other printer setup options.

3.3.1.5 Page Setup

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

---Macintosh only ------

Use the Page Margins dialog to set margins.

3.3.1.6 Page Margins

-----Macintosh only----

This dialog sets the margins for Text Windows. Use the Page Setup dialog to choose page size and orientation.

3.3.2 Edit menu (Text Window)

The Edit menu for Text windows offers the usual commands.

Undo Reverse previous editing operation.
Cut Deletes data from the document and moves it to the clipboard.
Copy Copies data from the document to the clipboard.
Paste Pastes data from the clipboard into the document.

3.3.2.1 Cut command

Cut command (Edit menu)

Use this command to remove the currently selected data from the document and put it on the clipboard. This command is unavailable if there is no data currently selected.

Cutting data to the clipboard replaces the contents previously stored there.

3.3.2.2 Paste command

Paste command (Edit menu)

Use this command to insert a copy of the clipboard contents at the insertion point. This command is unavailable if the clipboard is empty.

3.3.2.3 Copy command

Copy command (Edit menu)

Use this command to copy selected data onto the clipboard. This command is unavailable if there is no data currently selected.

Copying data to the clipboard replaces the contents previously stored there.

3.3.2.4 Undo command

Undo/Can't Undo command (Edit menu)

Use this command to reverse the last editing action, if possible. The name of the command changes, depending on what the last action was. The Undo command changes

to Can't Undo on the menu if you cannot reverse your last action.

3.3.3 Window Menu

The Window Menu in Text Windows is identical to the Window Menu in the Graphics Window. It does have a command for changing the font of all text in the window.

3.4 Help Menu

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

ATOMS 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 ATOMS. For Macintosh, the About dialog is either in the Apple menu (OS 8/9) or the Application menu (OS X).

3.4.1 About command

About command (Help menu)

Use this command to display the copyright notice and version number of your copy of ATOMS.

3.5 Identifying (Picking) Atoms

Identifying (Picking) Atoms

When a drawing is displayed in the ATOMS graphics window, you can identify generated atoms by clicking with the mouse. Generated atoms can thus be marked for non-plotting and later deletion (see Deleting Atoms). If molecules have been located or fragment are present these are also identified.

A mouse click is judged to be "on" a given atom if it is within that atom's radius of its center point. If the atom in question has zero or negative radius (see the Revise Atom dialog in the **Input1** menu for the significance of non-positive radii), then the default radius, set in the Preferences dialog in the **Settings** menu, is used.

The click point may actually be "on" more than one atom; all atoms which project onto the plane (x = 0) within the specified distance of this point are identified, not just the one which is visible at this point. In this case, the Atoms at Cursor dialog comes up, giving a list of the atoms, from foremost to rearmost. Select the desired atom, and click on the **View/Revise Atom** button. This brings up the Generated Atom Data dialog for that particular atom. If the click point is only on one atom, the G**enerated Atom Data** dialog

comes up directly. If the click point is not on an atom, you get an alert to this effect.

The atom(s) which have been identified may be marked by outlining with a contrasting color - see the Preferences dialog in the **Settings** menu.

3.5.1 Atoms at Cursor

Dialog Box: Atoms at Cursor [click in graphics window]

When a drawing is displayed in the ATOMS graphics window, you can identify generated atoms by clicking with the mouse. Generated atoms can thus be marked for non-plotting and later deletion (see Deleting Atoms). If molecules have been located or fragment are present these are also identified.

A mouse click is judged to be "on" a given atom if it is within that atom's radius of its center point. If the atom in question has zero or negative radius (see the Revise Atom dialog in the **Input1** menu for the significance of non-positive radii), then the default radius, set in the Preferences dialog in the **Settings** menu, is used.

The click point may actually be "on" more than one atom; all atoms which project onto the plane (x = 0) within the specified distance of this point are identified, not just the one which is visible at this point. In this case, the Atoms at Cursor dialog comes up, giving a list of the atoms, from foremost to rearmost. Select the desired atom, and click on the **View/Revise Atom** button. This brings up the Generated Atom Data dialog for that particular atom. If the click point is only on one atom, the **Generated Atom Data** dialog comes up directly. If the click point is not on an atom, you get an alert to this effect.

The atom(s) which have been identified may be marked by outlining with a contrasting color - see the Preferences dialog in the **Settings** menu.

3.5.2 Generated Atom Data

Dialog Box: Generated Atom Data [click in graphics window]
[Atoms at Cursor dialog**]**

When a drawing is displayed in the ATOMS graphics window, you can identify generated atoms by clicking with the mouse. With this dialog, generated atoms can thus be marked for non-plotting and later deletion (see Deleting Atoms). If molecules have been located or fragment are present these are also identified.

A mouse click is judged to be "on" a given atom if it is within that atom's radius of its center point. If the atom in question has zero or negative radius (see below and the Revise Atom dialog in the **Input1** menu for the significance of non-positive radii), then the default radius, set in the Preferences dialog in the Setting menu, is used.

The click point may actually be "on" more than one atom; all atoms which project onto the plane (x = 0) within the specified distance of this point are identified, not just the one which is visible. In this case, the dialog Atoms at Cursor dialog comes up, giving a list of the atoms, from foremost to rearmost. Select the desired atom, and click on the **View/Revise Atom** button. This brings up the **Generated Atom Data** dialog for that particular atom. If the click point is only on one atom, the **Generated Atom Data** dialog comes up directly. If the click point is not on an atom, you get an message to this effect.

The atom(s) which have been identified may be marked by outlining with a contrasting color - see the Preferences dialog in the **Settings** menu.

The label, type and atomic radius listed towards the top of the **Generated Atom Data** dialog pertain to the input atoms and cannot be changed here - they are set in the Revise Atom dialog in the **Input1** menu.

The listed Cartesian atomic coordinates are in Angstroms, in the observer Cartesian system (see IV-4). You can change these coordinates if you wish, but if ATOMS is in its normal operating mode this change in position will only be temporary; it applies to a generated atom, which is not saved in the structure file. If the structure is recalculated, the changes are lost. However, you can make such changes permanent by using the Generated to Input conversion in the **Transform** menu. This puts the Input=generated operating mode into effect, and the changes in atomic coordinates are permanent (if the file is saved). When this mode is in effect, input atoms are equivalent to generated atoms.

The fractional atomic coordinates are in the structure axis system. They cannot be changed directly, but will be changed if the Cartesian coordinates are changed (previous paragraph).

If the structure has been converted to the Input=generated mode (Generated to Input in the **Transform** menu), there is an **Edit Input** button. This button brings up the Revise Atom dialog for the current atom. With this dialog, you can change the color, radius, type, etc. of the current atom. Some such changes may require recalculation, rather than replotting. For example, you can change the color of individual polyhedra. Set up an additional polyhedron type, identical to a current type except for color and the type number of the central atom. Then, by clicking on a central atom, you can change the color by changing the atom type number.

Use the Mark Atoms command in the **Display** menu to mark the locations of specified types of atoms, or of atoms which may not currently be plotting.

The **Atom plot type** determines how the atom, and bonds to it, are displayed. The plot type is determined by the absolute value of a plot code, which is set by certain input values and results of the calculation. (this plot code is listed with other data on the generated atoms, with the **List Generated Atoms** command in the **File** menu). The

check box below the plot type may be labeled **Plot atom**, **Plot bonds**, **Plot Atom and Bonds** or **Plot Polyhedron**, or it may be absent altogether. Checking or unchecking this box changes the sign of the plot code; generally positive means plotting and negative means non-plotting.

By unchecking the box, you can make the atom and/or and the bonds to it non-plotting. This action marks the atom as non-plotting but does not remove it from the generated atom list. A list of non-plotting generated atoms is saved in the structure file (see Deleting Atoms). You can cause the non-plotting atoms to be permanently deleted by exercising the Generated to Input conversion in the **Transform** menu; this can be done repeatedly, just for the purpose of deleting atoms.

All atoms marked as non-plotting can be restored, and a specific range of generated atoms can be either restored or marked non-plotting, with the Atom Plot Status dialog in the **Input2** menu.

The effect of the check boxes depends on the atom plot type. The atomic radius of an input atom (see the Revise Atom dialog in the **Input1** menu) in part controls the plot type; if the radius is positive, the generated atoms derived from this input atom are shown as spheres, if they are not part of polyhedra. Display (as spheres) of atoms which belong to incomplete polyhedra is controlled by a checkbox in the Polyhedra dialog (Input1 menu). Display of polyhedron ligands as spheres is also controlled by a checkbox in the Polyhedra dialog. If the input radius is zero (polyhedron atom), the atom is only shown if it is a corner of a complete polyhedron. If the radius is negative (wire-frame atom), the atom is never shown as a sphere, but its bonds may be shown. The plot codes are derived as follows.

Non-plotting atom (plot code 0). These atoms never plot. This code is assigned to atoms with input radius zero, and which should be either central atoms or ligands of polyhedra, but which belong to incomplete polyhedra - that is polyhedra with an insufficient number of ligands or no central atom.

Spherical atom (plot code 1). This type is always shown as a sphere. The check box below **Atom plot type** is labelled **Plot Atoms and Bonds**. Positive (+1) plot code (box checked) means the atom and all bonds to it are plotted, negative (-1) means they are not plotted.

Central atom of polyhedron (plot code 2). This type is never actually shown itself; The check box below **Atom plot type** is labelled **Plot Polyhedron**. Positive (+2) plot code (box checked) means the entire polyhedron is plotted, negative (-2) means it is not plotted. Checking or unchecking not only changes the sign of the plot code for the central atom, but also that of all the ligands (see next item). This means that all the bonds from spherical or wire-frame atoms (codes 1 and 3) to the ligands become plotting or non-plotting respectively.

Polyhedron ligand (plot code 3). If the atom input radius is positive, this type of atom may be shown as a sphere, as controlled by the checkbox in the Polyhedra dialog (Input1 menu). If the input radius is zero, these atoms may never be shown as spheres, only as corners of polyhedra. The check box below **Atom plot type** thus can be labelled either **Plot Atom and Bonds** or **Plot Bonds**. Whether the polyhedron as a whole is shown or not is controlled by the central atom (see above). The **Plot Atoms/Bonds** box controls all bonds from this ligand to spherical atoms (code 1), ligands of other polyhedra (code 3) or wire frame atoms (code 4).

Ligand or wire frame (plot code 4). The check box below **Atom plot type** is labelled **Plot Bonds**. This type of atom is never plotted itself. However, the **Plot bonds** check box is active and controls whether the atom is visible, since it controls all bonds to the atom.

Atoms in incomplete polyhedra (plot code 5). If the input radius of either the central atom or ligands of polyhedra is positive, and an insufficient number of atoms is found to complete the polyhedron (because of boundary conditions), these atoms will be given plot code 5. The display of such atoms as spheres is controlled by a check box in the Polyhedra dialog (**Input1** menu). Note that if input radius of polyhedral atoms is zero, atoms in incomplete polyhedra will be given plot code zero, and will never be plotted. This saves computation time because the bonds to these atoms are not located.

For polyhedron ligands, the **Plot Atoms/Bonds** check box is generally best left alone, except for the case of ligands shared between polyhedra. In this case, if the **Plot Polyhedron** box for the central atom of one of the polyhedra is unchecked, this unchecks the **Plot Atoms/Bonds** box for all of its ligands (i.e. changes the plot code from +3 to -3). If there are non-polyhedron bonds, i.e. bonds from a spherical atom or a wire-frame atom, to a ligand which is shared between the non-plotting polyhedron and a polyhedron which is still plotting, they will not be shown. You can correct this condition, restoring these bonds to plotting, by checking the **Plot Atoms/Bonds** box of the shared ligands. Note that changing the status of the central atom will undo changes of the status of the ligands.

Deletions or restorations of atoms and attached bonds with the check boxes does not take effect immediately, only after replotting of the drawing. Replotting is automatic if the **Replot** box is checked; otherwise select the Replot command in the **Display** menu.

Label. This box is checked by default, so that turning on atom labels with the Atom Labels dialog in the Display menu will produce a label for each atom. Deleting or omitting labels is similar to deleting atoms (see above); it only applies to generated atoms. Deleted labels can be restored with the **Restore Deleted** button in the Atom Labels dialog in the Display menu.

The distance to the last atom selected with this dialog is printed out near the bottom, if a

different atom was selected. There will be a **Bond Label** checkbox, and unchecking this box will suppress plotting of the label. All labels can be restored with the **Show All** button in the Bond Labels dialog. A list of non-plotting bond labels is kept in the data (.str) file.

The **Bond** button can be used to make a custom "bond" between the current atom and the last one. If you click on this button, you will be shown the General Lines or Cylinders dialog, and the "bond" thus defined will be kept in that list, not in the Bonds dialog in the Input1 menu.

The bond angle involving the last three atoms selected is also printed out, if three appropriate atoms have been selected. If this angle is one of those which satisfy the specifications in the Angle Labels dialog, there will be an **Angles** checkbox. Unchecking this box will supress plotting of the angle label. All labels can be restored with the **Show All** button in the Angle Labels dialog. A list of non-plotting angles is kept in the data (.str) file.

The **Align** button will use the last three atoms selected (those which define the angle) to realign the entire structure (generated atoms). These atoms will be aligned in the y-z plane (screen or paper). If the atoms are number 1, 2 and 3 in the order selected (last one selected is 3), then the 2-1 vector will be vertical, parallel to z, and the 2-3 vector will be in the y-z plane, clockwise from z (looking down x).

If Atomic Vectors are present and if the structure is Input=generated, the direction may be reversed with the **Invert Vector** button. The drawing must be recalculated, not just replotted, to see the reversal.

For Protein Data Bank (PDB) structures, the **Protein** button will bring up a listing of the protein-specific attributes of the selected atom.

The three lines at the bottom of the dialog give the distance from the current atom to the last atom selected, the angle defined by the current atom and the last two, and the dihedral angle involving the last four atoms. See Construct Molecule from Z-Matrix for the definition of the dihedral angle and the sign convention.

Molecule/Group options.

If molecules have been located or individual structure fragments are present (allowed only in the Input=generated boundary/operating mode), you can control their display with the buttons at the bottom of the dialog. **Highlight** means that the selected group appears in normal colors while all other atoms are dimmed. **Hide** means that atoms in the group are marked as non-plotting (see above)

If molecules have not been located with one of the Molecules in Crystal

boundary options, you can locate them with the **Find** button. Molecules or groups to be located or isolated must have all their atoms connected by Bonds or Polyhedra, and the must be no bonds (except those marked as intermolecular in the Bond Data dialog) or polyhedra interconnecting molecules. For more information on locating and manipulating groups, see Dealing with Molecules, Groups and Fragments, and the Locate Groups dialog (Transform menu).

3.5.3 Protein Attributes of Atom

Dialog Box: Protein Attributes of Atom [Revise Atom: Basic Tab**] [** Generated Atom Data**]**

This dialog is used only when the atom data are obtained from a Protein Data Bank (PDB) file. It gives the parameters which are specific to protein structures - none of these parameters are set in ATOMS. See the PDB literature for explanation.

3.6 Select Color

Dialog Box: Select Color [various dialogs].

This dialog allows color selection from the current 16-color palette, and also allows selection of a custom color. The **Custom** button calls up a system standard color-picking dialog.

The red, green and blue values are given below each color box, to the right of the radio button. These values are on a scale of 0-255, as used by Windows.

It is usually best to use one of the 16 colors in the palette, because 1) the 256-color or 8-bit display palette is derived from these colors, and shaded atoms, bonds and polyhedra will be forced to one of these colors anyway at plot time; and 2) display and output are usually more satisfactory when simple colors, such as those in the default palette, are used.

The default colors selectable in this dialog may be changed in the Palette dialog (Settings menu).

4 Reference

Topics here are of general interest or may be referred to in several dialogs.

4.1 Atom Parameter Files

Atom Parameter Files (Free-Form or.inp)

This type of ASCII or text file may be used in either the Input Atoms dialog in the Input1

menu, or the the **Import** option in the **File** menu (Import Free-Form), to read in atomic coordinates alone, or to supply complete structure information. ATOMS itself does not write.inp files, but they are written by the program CRYSCON (Shape Software) which can be used to perform various types of crystallographic conversions, such as sub/supercell, change of origin, change of symmetry, etc. Listings of atomic coordinates from almost any source can be used as the basis of a free-form file.

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 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.

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. When a free-form file is read through the Input Atoms dialog in the Input1 menu, current values are kept if the corresponding line is absent.

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-Maughin 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 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.

FORM lines. These lines contain the three indices and the central distance for each form. When the file is read in, you will have the option of using these forms in the Enter Forms boundary option.

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 ATOMS 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, but they are all converted to upper case after

input. This is a required field.

2) **COO** - This actually denotes three floating-point fields giving the fractional atomic coordinates for crystals, or the absolute coordinates for molecules. 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

4) **RAD** - This is the radius used when the atom is plotted as a sphere. FLOATING-POINT

5) **RMC** - This is the color for the atom rim or edge, in terms of three RGB components 0-255. 3 INTEGERS

6) **FLC** - This is the color for the atom fill, in terms of three RGB components 0-255. 3 INTEGERS

7) **RMP** - This is the pattern number or gray shade used in black-and-white display or output. This number is used only for wide lines (see Line Widths). INTEGER

8) **FLP** - This is the b/w pattern number for fills. This is used only if shading is off or the initial pattern number option (Shading) is on. INTEGER

9) **PEN** - This is the pen number used for atom outlines in pen plots. INTEGER

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 ATOMS 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 converted to B values (type 6 in 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. The length may be in any units, as a scale factor is always applied (see the Atomic Vectors dialog). 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 ATOMS.

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 ATOMS, 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 taking the correspoding value from the ELEMENTS file, as discussed in the next section. However, values given in the latest DEFAULT line take precedence over any values read in or derived from the ELEMENTS file. You can turn off defaults, thereby accepting the values on the input atom line or the values in the ELEMENTS file, with a line containing the word DEFAULT and no other keywords.

ELEMENTS files. These files may contain a line for each possible type of input atom. Either of two files may be used: ELEMENTS.COV, with covalent radii, and ELEMENTS.ION, with ionic radii - the choice between the two is made in the Preferences dialog in the Settings menu.

The ELEMENTS files may be modified to change the default parameters. The first field in each line is the atomic number or other designated type number. The second field, or SYM field, consisting of two characters in single quotes, is usually the normal elemental symbol. The remaining fields give the default values for the RMC, FLC, RMP, FLP and PEN parameters. If all fields for each input data line are either read in with one of the fields in the FIELDS line, or given values with a DEFAULT line, the ELEMENTS file is not used. If one or more parameters are missing, then the first two characters of the LAB are matched with the elemental symbol in the ELEMENTS file. If the TYPE has not been read in or specified with a DEFAULT line, it is taken to be the atomic number, and other missing parameters are given values from the proper field in the ELEMENTS file.

4.2 central distance

Central distance. The central distance for a face or form (set of symmetry-equivalent faces) is the perpendicular distance in Angstroms from the center of the structure coordinates to the face in question. Generally, the larger the central distance the less prominent (smaller) the face is.

4.3 Colors, Palettes and Dot Patterns

Color Models.

ATOMS is designed to give the best quality display and output for the most common types of screen display, printers and plotters. However, because these devices vary widely in their capabilities for displaying color, it may be necessary to understand several different color models. The models are best discussed in terms of the number of bits used to represent each pixel in a raster or bit-mapped display or output.

1-bit or black-and-white. This is used for two-color or black-and-white printing and files destined to be printed. Each pixel is either off (white) or on (black). For filled areas dot-patterns with varying percentages of black dots simulate shades of gray. Every input atom, bond or polyhedron has a black-and-white pattern number for rim and fill. For

raster files, ATOMS supplies the patterns in two series, coarse and fine (see below). For printer output in Windows, you can select either the ATOMS patterns or the screen-driver patterns; for Macintosh the ATOMS patterns are always used. Direct PostScript output uses the patterns supplied by the output device.

The dot pattern is used for lines only if wide lines **(**Line Widths dialog in the **Input2** Menu**)** are selected; if lines are one-dot width, they are black. If atoms, bonds or polyhedra are not shaded, that is given variable coloring depending on presumed illumination, then the pattern number can be used without modification as a means of distinguishing different atoms, etc. Generally, if shading is used, it is best to treat all atoms, bonds and polyhedra alike, that is show a white color (no dithering) at maximum illumination. However, it is possible to assign an *initial shade* to each type of atom. (Shading dialog in the **Input2** menu)**.**

8-bit or 256 color. This may be used by older types of screen displays, and it is often advantageous for non-3D drawings in raster files. The 256 colors in these displays (in Windows minus 20 colors set aside for system use) may each be set to any admixture of red, green and blue. ATOMS sets up a 256-color palette designed for displaying shaded atoms, bonds and polyhedra. It is based on 16 principal colors, which can be defined in the Palette dialog in the **Settings** menu. See below (**Palettes**) for further information on palettes.

15-, 16, 24- or 32-bit or RGB color. This is becoming standard for screen displays, and it is used for Postscript color output and for 16- and 24-bit raster files. One-third of the available bits are used to represent each of the color components red, green and blue. For 24- or 32-bit screen displays, there are virtually no restrictions on colors, and any colors and shadings thereof can be rendered faithfully.

In non-3D display modes, for the most part RGB color does not greatly improve the quality of ATOMS drawings over 8-bit color. However, it does remove restrictions in two areas: (1) Any number of separate colors are valid for shaded atoms, bonds and polyhedra, rather than only 15 colors for 16 or fewer shading zones, or 7 colors for 32 zones (see under palettes below); (2) when front-back fading **(**Shading dialog in the **Input2** menu**)** is in effect, the atoms etc. in the rear of the drawing are not restricted to a few of the darker zones in a shading series, as in 8-bit color.

When generating raster files of color images in non-3D modes, it may advantageous to use use 8-bit (256-color) rather than RGB (15-bit through 32-bit) color because the files tend to be much smaller. This is because of the smaller number of bits in the pixels, but also because the run-length encoding used in some file types does not compress RGB files well.

The 3D mode does not use the ATOMS 256-color palette on 8-bit displays, in either Windows or Macintosh. Windows uses a special palette for this mode and the Macintosh

must use the system color table. This often results in dithering, so RGB color should generally be used for 3D modes.

Printing. The choice between 4-bit (standard VGA), 8-bit (256-color) and 15-32-bit display may may a great difference in the appearance on screen, but hard-copy devices such as printers actually use only a very limited number of colors (typically cyan, magenta, yellow and black, although some inkjet printers may use more by mixing inks), simulating more complex colors with dithering. Some degradation of color quality from screen to printed image is to be expected. If color match of the printed output is very poor, check the settings for the printer in the **Print** dialog.

Palettes.

Although Windows and Macintosh programs can specify colors made up of any admixture of red, green and blue components, it is generally a good idea to use simple colors whenever possible, to increase the chances of faithful reproduction on a variety of display and output devices.

16-Color Palettes. ATOMS uses a Main Palette composed of 16 colors for two reasons: to aid in the consistent selection of simple colors; and to form a basis for the 256-color palette used for 8-bit displays or other devices. The first eight colors in the default Main palette are black, white, red, green and blue, and then the binary combinations of red, green and blue which are cyan, magenta (violet) and yellow. The second eight colors are two shades of gray, then the binary combinations of red, green, blue, cyan, magenta and yellow (these six have no universally-recognized names). The colors in this palette are the same as those in the Alternate palette which is used in the DOS versions of ATOMS, but in a different order.

The RGB values in both the 16-color palettes can be changed with dialogs in the **Settings** menu. You can also save and re-read palette files.

256-Color Palettes. The palettes which are used in 256-color screen-display modes are primarily designed for shading. There are two distinct palettes; the first has 15 principal colors, each with 16 gradations from full intensity to almost black, and is used whenever the number of atom shading zones (Shading dialog in the **Input2** menu) is 16 or fewer; the second has only 7 principal colors, each with 32 gradations from full intensity to almost black, and is used when the number of atom shading zones is 32.

The first or "16-zone" palette is made up as follows. The first 15 colors (0-14) start with full-intensity color number 1 (white), and grade with decreasing intensity to near black; the second 15 colors (15-29) start with full intensity color number 2, grading to near black, and so on. When shading is in effect, ATOMS finds the nearest color in the 16-color palette to the color selected in the input for the atoms, bond or polyhedron. Any shading zone of an atom, bond or polyhedron receiving full illumination is given this full-

intensity color and shaded parts are given colors in the series of 15 colors derived from that principal color. The palette defined in this way actually contains only 225 colors.

In the second or "32-zone" palette, the first 31 colors (0-30) grade from full-intensity color 1 to near black, the next 31 from full-intensity color 2 to near black and so on, through color number 7 and its derivatives. When shading is in effect, ATOMS again "forces" the color to one of those in the 16-color palette, but the choices this time are only colors 0-7. As the colors are arranged in the default palette, this results in changing colors 8-15 to 0-7 respectively. Actually, colors 0-7 can be regarded as "simplified" or more basic versions of colors 8-15. The above shaded colors add up to only 217, so colors 8-15 are also added to the palette to be usable for lines and unshaded fills.

Again, if shading is in effect and you are using more than 16 shading zones (Shading dialog in the **Input2** menu), any fill colors for atoms, stick bonds or polyhedra in the range 8-15 will be automatically "downgraded" to colors 0-7.

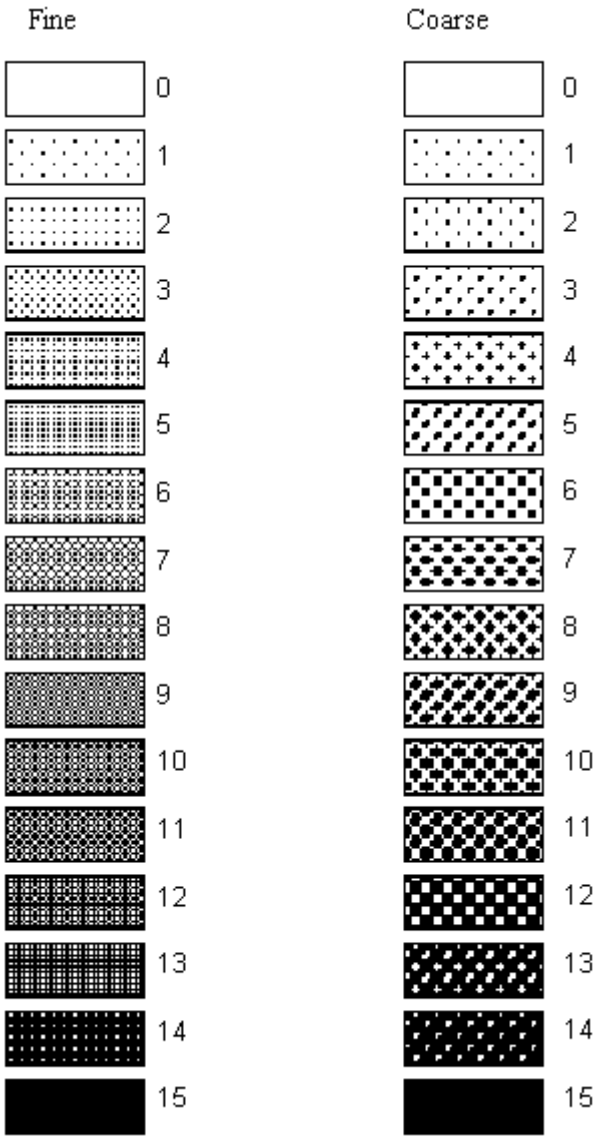
All these complexities and restrictions pertain *only* to 8-bit or 256-color display or raster files. For standard VGA (4-bit) display in Windows, the RGB values are sent to the display driver, which determines in its own way what combination of pixels to mix to represent a given color. This is likewise true for printer and PostScript output. The RGB values are also sent directly to 16-, 24- and 32- bit screen displays, which can presumably render any color without dithering.

Dot Patterns for Black-and-White Display and Output.

The dot-patterns which are the "colors" for atom, bond and polyhedron fills and wide lines in black-and-white printer output (if ATOMS patterns are selected in preference to those supplied by the printer driver in Windows), and which are also used for shading in black-and-white raster files, are shown in the diagram below. The patterns comprise two series of dot-patterns of increasing density with shade numbers 0-15; the choice between them is made in the **Print** or **Raster File** dialogs (**File** menu).

The fine series is recommended for 9-pin or other low resolution dot-matrix plotting, for very small drawings done at high resolution, or for raster files which will be shown on a low-resolution screen. The coarse series contains patterns more like the half-tone screening used in printing. It is appropriate for gray tones and shading in high-resolution dot-matrix plotting. Actually, for shading with 32 zones, there are 32 patterns in the coarse series, only half of which are shown in Figure IV-1. The fine series has only 16 unique patterns even if the number of shading zones is 32, although this could be changed in the SCRPTR file (Direct Modification...).

ATOMS has the ability to use macrosopic hachure patterns on both polyhedra and atoms. In many cases it may be more appropriate to use these patterns to differentiate atoms and polyhedra than to use grey shades.



4.4 Colors/Patterns/Pens for Input

In color display or output, lines may be drawn with different colors, and atoms, stick bonds and polyhedra may be filled with different colors (except in pen plots, in which atoms, stick bonds and polyhedra are always blank or white). In black-and-white display or output, various dot-patterns, simulating shades of gray, are normally used for fills, and for lines if they are wide enough.

This section discusses the common aspects of color/shade input for lines and fills, as occurs in many input dialogs in ATOMS. Depending on the type of display and output involved, any of three different sets of colors or patterns/shades may be used.

(a) For color screen displays, printer, Raster, Metafile or PICT output, actual colors are used. The RGB components, which are numbers ranging from zero to 255 can be directly entered in the edit boxes, but the color is most easily and reliably selected with the **Select...Color** buttons. These bring up the Select Color dialog, presenting the colors of the current main palette. If the color is being selected for a fill, and if shading for the object in question (atom, stick bond or polyhedron) is selected in the Shading dialog in the **Input2** menu, the color chosen here is that at maximum (perpendicular) illumination. If front-to-back fading has been selected in the Shading dialog in the **Input2** menu, the chosen color is that for the foremost atom.

For 16-, 24- or 32-bit color screen displays you have complete freedom to choose colors. For 8- or 4-bit color the fill colors of shaded atoms, bonds and polyhedra may be forced at plot time to one of a limited number of allowed colors. For 8-bit color the number of colors allowed depends on the number of atom shading zones selected in the Shading dialog in the **Input2** menu. See the general section Colors, Palettes and DotPatterns for further information on palettes for the 8-bit color mode.

For best results on a wide range of display and output devices, chose the simplest colors, which are firstly colors 0-7 in the default main palette, and secondly colors 8-15

(b) For black-and-white screen displays and printer, raster or metafile output, either true grays or dot patterns of various densities are used. The codes for these shades or patterns range from 0 for white to 15 for solid black.

The selected pattern is used for fills if shading is not in effect. If shading is in effect, selected in the Shading dialog in the **Input2** menu, the actual fill patterns shown may either start at white for maximum illumination, or at the pattern number selected here depending on the setting of the **Use initial patterns** checkbox in the Shading dialog.

The selected pattern is used for lines only if the width of the line is greater than one dot. The width of various types of lines is set in the Line Widths dialog in the **Input2** menu. Note that rendering of gray-scale for lines in black-and-white printed output is determined by the printer driver, not ATOMS. Many printer drivers do not support gray lines and pattern numbers other than 15 may give either white or black lines.

(c) For pen-plotters the number requested refers to the pen number used in drawing the lines. For atoms, stick bonds and polyhedra, this refers to the outlines; there are no fills in pen plots (the interiors of atoms, stick bonds and polyhedra are always blank). These numbers are not used if the single-pen mode is selected in the Pen Plotter Settings dialog in the **Settings** menu.

When changing the red, green and blue values directly in the edit boxes which appear in many dialogs in ATOMS, the rectangle showing the actual color does not change until

the focus shifts from the current edit field, that is until the mouse is clicked in another place in the dialog.

4.5 Coordinate Systems

Three types of coordinate system are used frequently in ATOMS: the observer Cartesian system; the natural structure system; and a Clinographic system.

The *observer system* is fixed with respect to the display screen or paper of dot-matrix or pen-plotter copy. The origin is at the center of the screen or paper, and the *x* axis points directly toward the observer. The *y* axis points to the observer's right and the *z* axis vertically, both in the plane of the screen or paper.

The atomic coordinates and the parameters of crystal faces if present are given in terms of the natural structure axis system, although in the case of molecules this may itself be a Cartesian system. Once all the atoms and faces have been generated, their coordinates are converted to Cartesian coordinates. Except for crystals using rhombohedral axes, the natural *c* axis is originally placed parallel to the observer *z* axis, and the natural *b* axis is aligned in the *y*-*z* plane (or in crystallographic terminology the *a** axis is parallel to *x*). If rhombohedral crystal axes are chosen, the three-fold symmetry axis is parallel to *z*, and the the vertical plane containing the first rhombohedral axis is aligned in the *x*-*z* plane.

This conversion defines the "original" orientation of the structure. After the location of atoms and faces, and before the initial display, the orientation may optionally be modified by the rotations in the Initial Orientation dialog in the **Input2** menu, by the alignment of a Slice of a crystal, and by clinographic rotation, defined in the next paragraph.

Clinographic Viewing. One of the standard methods of drawing crystals (external morphology) is clinographic projection, in which the crystal is in effect viewed from above and slightly to the right of the a axis, or to be more precise, in towards the center along the vector [621] referred to cubic or Cartesian axes. If the option for clinographic viewing is chosen, after the faces, atoms etc. are found, the structure and its associated Cartesian system are rotated -18.4 degrees on the *z* axis, then 9.5 degrees on the *y* axis.

After the drawing appears, additional rotations may be made either on (1) specified vectors in the natural structure system; (2) the observer Cartesian axes; or (3) if clinographic viewing is on, the rotated Cartesian axes, or *clinographic system.* The clinographic system does not rotate with the crystal; it is always related to the observer system by the two rotations given above.

If clinographic viewing is not on, the clinographic and observer systems have the same orientation, and if the natural structure system is Cartesian or cubic all three systems have the same orientation.

Summary of axial systems:

1) *Observer Cartesian system*. Reference system, fixed with respect to the display screen or paper.

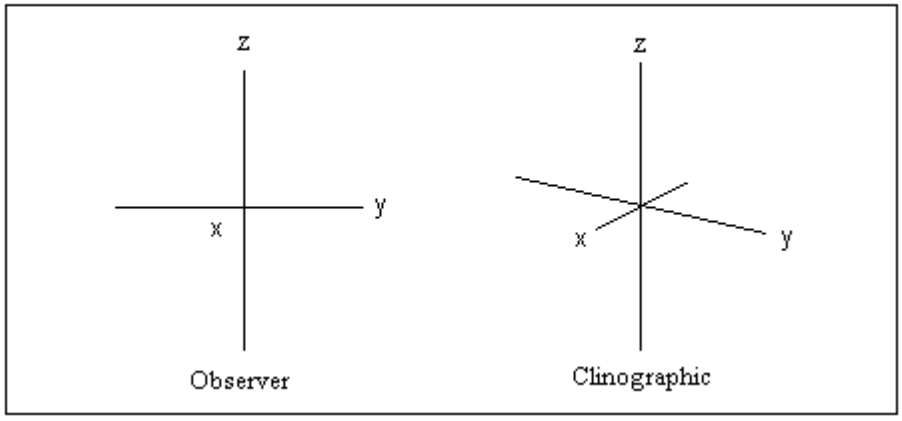
2) *Natural or structure system.* Fixed with respect to the atomic structure. Atom coordinates are initially given in this system. The axes are the unit-cell edges in the case of crystals. Axes may have unequal lengths and may be at angles of other than 90 degrees.

3) *Clinographic system.* Only applies when clinographic projection or viewing is on. Axes are those of the observer Cartesian system, but rotated in a certain manner to avoid a straight-on view of the structure.

If Perspective viewing is not selected, the drawing is a direct projection in the *x* axis direction (observer system). If perspective viewing is selected, the atoms are projected onto the *y*-*z* plane from a point on the *x*- axis at the specified distance in the positive direction (toward the observer).

In ATOMS, *a*, *b* and *c* (or A, B and C) refer to the natural structure axes. The three axes may sometimes have these names although it is conventional in some systems to use *a*1, *a*2 and *a*3 if the axes are equal by symmetry. The letters *x*, *y* and *z* usually refer to the observer Cartesian axes. If it is necessary to refer to the clinographic system, this is mentioned explicitly. The fractional atomic coordinates are also referred to as *x*, *y* and *z*, but these are usually identified explicitly.

Coordinate Systems for Rotations



4.6 Dealing with Molecules, Groups and Fragments in Crystals

Atoms has capabilities to deal with several types of atomic groups, which may be roughly separated into three classes.

1) True Molecules

It is often useful to be able to identify true molecules in crystals. A "true" molecule has strong bonds linking all atoms within it, does not have strong bonds linking its atoms to other molecules or groups, and is limited to a constant number of atoms, i.e. it is not a polymer.

True molecules which are not to be combined with other structures are most easily dealt with initially using one of the special Molecules in Crystals Boundary Options. These boundary options will identify all molecules in the structure regardless of whether or not they cross the formal unit-cell boundaries, and fill out a specified volume using simple translation or crystal faces or a sphere as boundary surfaces, these boundaries being applied to the centers of the molecules. Individual molecules can be identified with the cursor and highlighted or hidden completely (i.e. marked as non-plotting).

Atoms within molecules can be connected to each other with bonds or with polyhedra. Input bond specifications can be marked as inter-molecular, meaning that they will not be used in the molecule search.

Molecules located with these boundary options cannot be deleted, translated or rotated. Colors, etc. cannot be changed for molecules as a whole as opposed to individual input atoms. For these reasons, and because the molecule-locating algorithm is time consuming, it is often advantageous to use the Generated to Input conversion (Transform Menu). In this conversion, the symmetry and lattice translations are essentially lost, but the molecules can be optionally converted to fragments, which can then be duplicated, translated, rotated and deleted independently. Molecules which have been marked as non-plotting may be optionally deleted during the conversion.

2) Polymer groups

Many crystal structures have polymer units which are continuously bonded in one, two or even three directions (lattice directions). It is often useful to be able to isolate these units, which requires a different approach from true molecules.

Polymer groups in crystals cannot be identified in the Molecules in Crystal Boundary options because the bonding is continuous. To deal with such groups, it is first necessary to define boundaries for the drawing using one of the boundary options which apply to individual atoms, not molecules. Then bonded groups can be located individually in either of two ways: with the **Find** button in the Generated Atom Data dialog which

comes up when you click on an atom in the display; or with the Locate Groups option in the Transform menu. In either case the units identified are limited to the current generated atoms, i.e. those within the current boundaries, whereas the special boundary options in 1) above locate complete molecules regardless of the boundaries. That is to say, in 2) groups may be truncated (which is necessary in the case of polymers) whereas in 1) molecules always maintain their integrity.

Groups identified in this way are not permanent - the groupings disappear when the structure is saved in a file, although if some groups have been hidden, the individual atom numbers will be saved in the list of non-plotting atoms. Having made the desired identification of groups, it may thus be advantageous to use the Generated to Input conversion (Transform Menu), converting groups to fragments which are then saved in the data (.str) file.

3) Structure fragments

ATOMS can combine portions of completely separate crystals and/or molecules (termed fragments). This is most commonly used for epitaxy (crystal on crystal or molecule on crystal), but can also be used for combining molecules, for example to depict chemical reactions. These fragments can be duplicated, translated, rotated and deleted independently.

Fragments can exist only in the Input=Generated boundary/operating mode, which is attained only by going through the Generated to Input transformation (Transform Menu). As explained above, molecules or polymer groups can be converted to fragments, so fragments can represent 1) molecules, as identified with one of the Molecules in Crystal boundary options; 2) polymer (or molecular) groups, as identified with the **Find** button in the Generated Atom Data dialog (after clicking on an atom) or with the Locate Groups option in the Transform menu; 3) completely distinct structures, obtained by reading from files or by one of the other options in the Multiple Structures options in the Transform menu.

It is not possible to identify groups or molecules when in the Input=Generated mode and more than one fragment is present. However, all the atoms can be combined into one fragment with the **Consolidate** option in the Locate Groups dialog (Transform Menu), and you can then start over with identification of molecules or groups. Of course all molecules or groups will have to be identified individually.

Molecules, groups and fragments do not have to contain more than one atom, nor do they have to be electrically neutral. Furthermore, the atoms of fragments are not necessarily connected by bonding. For example, in structures with cations and anion radicals, for example CaCO3, using the Molecules in Crystal boundary options will result in each Ca

atom, as well as each CaCO3 group, being identified as a molecule. The Generated to Input transformation would (optionally) convert each of these molecules to a fragment. On the other hand, if you calculate a CaCO3 crystal using one of the boundary options for individual atoms, then identify each CO3 group (but not Ca atoms) and finally use the Generated to Input transformation, all the Ca atoms will be grouped in one fragment.

4.7 Deleting Atoms and Atom Labels

In ATOMS normal operating mode, there are two types of atoms, input atoms and generated atoms. The input atoms are usually entered and removed in the the Input Atoms dialog. The symmetry and lattice translations, if present, are used to derive the generated atoms from the input atoms; it is the generated atoms which are actually viewed in a drawing. There are basically two ways of removing specific generated atoms from the drawing.

If only a few atoms are to be deleted, they can be marked as non-plotting. Clicking with the mouse on or near the location of an atom brings up either the Generated Atom Data dialog or the Atoms at Cursor dialog, in which selecting an atom brings up the first dialog. Unchecking the **Plot Atom** box will mark the atom as non-plotting. You must replot to actually cause the atom to be removed from the drawing. When the structure file is closed, a list is made of the non-plotting atoms, which will be saved and used the next time the structure is calculated. Starting with V4.0, the lists of deleted atoms and atom labels use a code containing the unit-cell, the symmetry operator etc., rather than an arbitrary generated-atom sequence number, so that changing the boundary conditions will not usually make the list invalid (although some deleted atoms or labels may no longer be within the boundaries). However, changing the symmetry will make the list invalid.

When molecules or fragments are present, the atoms in the entire group can be marked as plotting or non-plotting.

All atoms marked as non-plotting can be restored, and a specific range of generated atoms can be either restored or marked non-plotting, with the Atom/Bond Plot States dialog in the **Input2** menu.

If many generated atoms are to be deleted, it may be better to change to the special Input=generated operating mode. This is done with the Generated to Input command in the **Transform** menu. In this operating mode, all symmetry and boundary conditions are removed, and generated atoms are exactly equivalent to input atoms. The individual atoms can be removed in the Input Atoms dialog. You can click on atoms on the screen and use the Generated Atom Data dialog to get the number, then delete them in the

Input Atoms dialog. Or, you can mark atoms for deletion by unchecking the **Plot atom** box as above, then do the Generated to Input command. This command gives you an opportunity to delete atoms which are marked as non-plotting. It can be repeated as many times as necessary, just for the purpose of deleting atoms in this way.

Deleting angle labels. Angle labels are automatically applied to all groups meeting the specifications in the Angle Labels dialog (Display menu). Individual angles can be deleted (actually, marked as non-plotting) by clicking on the three atoms in succession (outer-central-outer) and unchecking the **Angle** box which appears in the Generated Atom Data dialog.

4.8 Direct Modification of Files

If you modify any data or setup file, be sure never to use tabs.

Data Files. The files written for each structure are of the standard ASCII type. Direct modification of these files is no longer recommended. However, occasion may arise for repairing a damaged file, which can be done with any word- or text-processor or other program which handles ASCII files.

SCRPTR Setup File. There are now only two types of data in the SCRPTR file which should be modified; the dot-patterns and the SHELX commands-to-be-ignored.

There are two sets of 32 dot-patterns (fine and coarse), each consisting of 32 lines of 8 numbers each. Each number can range from 0 to 255, with a binary 1 bit representing a black dot and 0 representing white (or color in the case of 4-bit raster files). Note that earlier versions of ATOMS may have had either 14 (V1.0) or 16 patterns in each series. The fine series, which is first, contains duplicate lines so that there are only 16 patterns for shading, even if the number of shading zones is greater than 16. These patterns could be modified to give 32 distinct shades, although it is doubtful if this would greatly improve the quality of the image.

Patterns can also be modified to give striations, hachures or other patterns for distinguishing unshaded atoms. For example, the sequence "1 1 1 1 1 1 1 1" will give vertical striations, and the sequence "255 0 0 0 0 0 0 0" will give horizontal striations. Such patterns should not be used when shading is in effect. ATOMS now has the ability to show macrosopic hachure patterns on polyhedra and atoms, so pixel-scale patterns are probably unnecessary.

The patterns in the SCRPTR file are only used for raster-file output, and for standard printer output (when ATOMS patterns are selected in Windows); they are not used for the screen.

At the end of the SCRPTR file is a list SHELX commands of four (or fewer) characters each, which are to be ignored by ATOMS when importing SHELX files. The list has ten commands per line, and is preceeded by the number of commands. If you add commands, be sure to change the number.

Although the data for the two 16-color palettes is also in the SCRPTR file, it is easiest to modify palettes with the **Main Palette** and **Conversion Palette** dialogs in the **Settings** menu, or to prepare files to be read in with these dialogs.

ELEMENTS files. These files, ELEMENTS.ION and ELEMENTS.COV supply default types (atomic numbers by default), radii and colors for input atoms read in from an ASCII file. See the next section for information on modification.

SCATFAC.DAT file. This file contains scattering factor data for powder and precession diffraction. The data are by default those for neutral atoms from the International Tables for X-Ray Crystallography (1974, Vol. 4). The ATOMS type numbers of input atoms are keyed to the entries in this table in order of the entries (not by element name). Other values using the same exponential form, for example different valence states, may be substituted. The coefficients are separated by blank spaces and are not confined to particular columns.

The first nine coefficients in each line are the X-ray scattering factor coefficients and the last number is the neutron scattering factor or length.

By default, number 99 in this file is used for deuterium (symbol "D") and number 98 is tritium (symbol "T"). These differ from hydrogen only in the neutron scattering factor.

The atomic type numbers, modulo 100, are used as indices to this table. For example 6, 106, 206 etc will all reference the sixth entry (carbon). Thus entries beyond 100 will be ignored. Any special or temporary entries should generally be placed in numbers 93 to 97.

If you modify any data or setup file, be sure never to use tabs.

4.9 Drawing Crystal and Unit-cell Edges

Drawing Crystal and Unit-cell Edges and Faces

Non-3D Drawing Modes. In the Standard, Skeletal and Thermal Ellipsoid drawing modes of atoms, all objects in the atomic structure itself, namely atoms, bond and polyhedra, are sorted with respect to distance from the eye (perspective projection) or height in the *x* -coordinate (orthogonal projection). Then the objects are drawn in order from back to front. Instead of constructing three-dimensional objects and then projecting onto the plane of the drawing, it is possible in many cases to use simplified two-

dimensional objects (e.g. circle instead of sphere). When objects are actually in bonding relationship the interpenetrations are solved analytically, but this is done only for certain cases where the geometry is very restricted; atom-atom, bond-atom where the bond connects that atom with another; and atom-polyhedron in the case where the atom is a ligand of the polyhedron. For the atomic structure itself, there is no need to solve for interpenetration of, for example, a bond with atoms which are not connected by that bond, or a polyhedron with bonds other than those to its ligands, because such geometries do not exist.

However, for the lines or cylinders which are used to represent the edges of the boundary polyhedron, or the edges of the unit cell, there are no such restrictions on interpenetration geometry; such lines or cylinders may interpenetrate with atoms, bond and polyhedra in any way.

For pen plots and pen-plot files, which use strictly vector methods of drawing, it is not possible to superimpose objects while drawing from back to front, and it is necessary to solve analytically for overlay relationships as well as the same limited interpenetration relationships mentioned in the first paragraph. However, this process is made much faster by the process of sorting and drawing from back to front.

For these reasons, the drawing of lines representing the boundary or other crystal shape (Crystal Forms for Display) in the Standard, Skeletal and Thermal Ellipsoid drawing modes assumes that there is no interpenetration between these lines and atoms, bond or polyhedra. The lines representing edges which would be hidden if the crystal shape were opaque ("back" edges) are drawn *before* the structure; and the lines representing visible edges ("front" edges) are all drawn *after* the structure.

Since it is normally necessary to show a volume of a crystal greater than one unit cell, similar assumptions cannot be made for the special drawing in the Unit-Cell option in the **Input2** menu. The unit-cell edges in this option are thus all drawn *after* the structure. They are intended to show the translational relationships of the structure, not to delimit some particular volume.

These simplifications are primarily intended to cut down on plotting time; they may be removed in the future as processors become faster.

In the Anaglyph drawing mode, which at this time only draws a skeletal view in a single color for each eye, there is no need to sort or to solve for intersections or overlays in any way.

3D Mode. The 3D drawing mode uses a completely different drawing method. Fully three-dimensional objects are drawn in any order, but the height (x-coordinate in the system used by ATOMS) of each pixel is compared with the value in a depth buffer and the color which is already in that pixel is replaced by the color belonging to the new

object only if the new object is closer to the eye at that point (i.e. if the new object overlies all other objects at that point). In this drawing mode there is absolutely no restriction on interpenetration relations - they are drawn correctly as a matter of course. Thus unit cells are drawn in correct 3-dimensional position, not in front of the structure. Crystal edges are also always drawn in correct position, and interpenetrations are exact.

Crystal and unit-cell faces, that is actual surfaces, may also be drawn in the 3D mode. Usually this is most useful if the faces are transparent or translucent. However, full transparency may not be supported by the system software and/or hardware. Absolutely correct transparency would require drawing from back to front, and would again encounter some of the problems discussed above for non-3D drawing modes.

4.10 ELEMENTS Files

These files provide a table of standard or default parameters for input atoms, namely atomic display radii, type numbers and colors. The key to the elements in the table is through the two-character symbol, normally the standard elemental symbol, which is matched to the first two or one characters in the label for the input atom.

The radii may be used when reading in atom parameters from an ASCII file in the Input Atoms dialog (see also Atom Parameter Files), or when importing a data file (Import Files popup of the File menu(Startup) or File menu(Graphics)). Note that when generating bonds automatically (Generate Bonds dialog), by default a different table of radii is used (from the **RADII** file), although the atom display radii can optionally be used.

The single ELEMENTS.DAT in early versions of ATOMS has been superceded by the ionic and covalent equivalents, ELEMENTS.ION and ELEMENTS.COV. One or the other of these is used, depending on the setting in the Preferences dialog in the **Settings** menu, or in the dialogs for import files. The default versions of these files now contain full ionic and covalent radii, and when importing a file or reading atomic coordinates the radii values are multiplied by the **Factor** in the Preferences dialog in the **Settings** menu.

The first field in each line is the atomic number or other designated type number. The second field, or SYM field, consisting of two characters in single quotes, is usually the normal elemental symbol. The remaining fields give the default values for the rim color and the fill color (RGB components 0-255, three numbers for each color), the rim and fill b/w shades (one integer for each, 0-15 for white-black) and pen number. These fields are the same as the RMC, FLC, RMP, FLP and PEN parameters as described in Atom Parameter Files. All these fields are required, in the given order. There is a limit of 150 entries (lines) in the ELEMENTS files.

Modifying the ELEMENTS files. The ELEMENTS files may be modified with a word processor to assign any desired default values to the parameters. It may also be necessary

to do some editing to avoid problems in interpreting the LAB field in terms of elemental symbols, or to change the elemental symbols from English to other language versions. Atomic numbers or types may be duplicated; for example you can have a line with number 53 and symbol I and also one with symbol J.

ATOMS first attempts to match the first two characters in the LAB field with two-character SYMBOLs in the ELEMENTS file. If no match is found, then it tries one-character symbols. For example, it will test the first two characters in the LAB against CA, CD, CL, etc., and only then will it test the first character against C (or C). Thus a carbon atom designated CALPHA would be read as calcium unless the CA line is removed from the ELEMENTS file. The label "C-ALPH" would avoid this problem.

If you only work with a limited number of atom types, it would be best to prepare a shortened version of the ELEMENTS file, to avoid possible conflicts and to shorten search times.

If no match is found in the ELEMENTS file for the first two characters of a LAB field, the values from the first entry in the file are used. Thus if you want to assign the same default values to all atoms, regardless of the LAB field, you can put these values in a single line and remove all others.

You can use appropriate values for the radius to set up for polyhedral or wire frame models. For example, if all Si and O atoms in a silicate are part of silicate tetrahedra, the radii for Si and O could be set to 0.0, which insures that the atoms which are not part of complete polyhedra are not plotted. Likewise for wire-frame models the radii can be set to -1.0, so that only bonds are plotted.

The **Factor** edit field in the **Atomic Radii** group in the Preferences dialog (**Settings** menu) multiplies the radii. For ball-and-stick models a factor of about 0.5 is appropriate, and for interpenetration (space-filling) models a factor considerably larger than one may be required.. Also, you can multiply all radii by a given factor with the Atoms - Global dialog in the **Input1** menu.

Blanks in the SYMBOL field in the ELEMENTS file are ignored.

ELEMENTS.ION uses ionic radius values for the most common ionization state (rare gases use Van der Waals radii, and minimum values of 0.05 are used for atoms which are central atoms of radicals). The radii are mostly from the tabulation of Shannon and Prewitt. Note that V4.0 and later of ATOMS uses full ionic radii, while previous versions had values of 50% for the radii. ELEMENTS.COV has full values of covalent radii, mostly from Pauling.

4.11 File Types

ATOMS uses several different types of auxiliary files, with different extensions. *Structure data files* (.str). These hold the information on individual structures. The Open, Save and Save As commands in the File menu of the Graphics window pertain to these files.

Internal files. These are for ATOMS internal use and should not normally be modified by the user (but see Direct Modification of Files). SCRPTR is the main start-up file which saves current settings. DEFAULTS saves default display variables for use with the New command. PPLOT contains data on pen plotters. CPATOMS.HLP [Windows] or ATOMS HELP [Macintosh] is the help file, which is in condensed format and not modifiable by the user. CIFDIC.SHT is the (shortened) dictionary file used when importing CIF files.

Space-group file. The file HALL.DAT contains space-group information.

Scattering factor file. The file SCATFAC.DAT contains the X-ray scattering factor data for neutral atoms in the exponential form as given in the *International Tables*, Vol. 4, for use in the Powder and Precession diffraction options (Display menu). 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.

Cartesian symmetry files (.sym). These contain Cartesian point-symmetry matrices generated by the auxiliary program SYMGRP.

Palette files (.pal). These contain RGB values for two 16-color palettes which (a) form the basis for 8-bit (256-color) palettes; and (b) are used to convert PC-DOS color numbers to RGB values. They can be modified, read and written with the Palettes commands in the Settings menu.

Atom parameter input files (.inp). These are files supplied by the user, containing at least the atom labels and coordinates, and optionally other parameters. They are read in through the Input Atoms dialog in the **Input1** menu, not the **Open** command in the File menu (Startup) or File menu (Graphics).

Atom parameter default file (ELEMENTS.ION or ELEMENTS.COV). This contains default atom types, radii and colors for use when reading in atom parameters from.inp files. It can be modified by the user to give the desired parameters. By default, ELEMENTS.ION contains standard ionic radii and ELEMENTS.COV contains standard covalent radii.

Radius values for bonds. The RADII file supplies values for generating input bonds. It

also has index values for each element, which optionally may be used avoid superfluous or impossible bonds. The values currently used are 1 for cations, -1 for anions, 0 for "non-metals", and 3 for inert (rare gases). At the time of generating input bonds, the values for the two candidates (input atoms) are added together, and pairs with absolute values greater than 1 are rejected.

Imported data files. These include the following. These files types are sometimes given arbitrary extensions, but any filename can be opened. (1) CCDC FDAT files (.fdt). (2) SHELX refinement input files (.ins). (3) CIF - Crystallographic Information Files (.cif). (4) DBWS/LHPM Rietveld refinement files (.dbw and.lhp). (5) Inorganic Crystal Structure Database (ICSD) files (.ret and.cry). (6) ORTEP data files (.ort). (7) XTLVIEW structure display files (.xtl). (8) VIBRAT motion files (.mot). (9) Protein Data Bank files (.pdb). (10) RIETAN Rietveld files (.xyz). (11) GSAS Los Alamos program system files (.exp). (12) American Mineralogist structure database files (.amc). (13) FULLPROF refinement files (.pcr). (13) Free-form (.inp) files.

Text output files (.atd). These contain the input to and/or results of the ATOMS calculations. The file infile.ATD contains output of the atom-locating calculation on the structure file infile.STR, such as atom locations, atoms in bonds and polyhedra, bond length and angles. INPUT.ATD lists the input data. GENATOMS.ATD lists the Cartesian coordinates of all the generated atoms in their current orientations. FACES.ATD lists attributes of the current boundary and/or display crystal faces. TOTALS.ATD gives totals of various types and the current maxima for these values. BONDS.ATD gives bonds and angles around each or all input atoms. These files may all appear in a Text window, and are saved independently of the ATOMS structure data files.

Graphics output files. ATOMS can write graphics output files of various types: encapsulated PostScript files (.eps); HPGL vector files (.pgl), 3D VRML files and

---- Windows only ----

raster files (.bmp,.pcx,.tif,.png); and Windows metafiles (.wmf or.emf).

---- Macintosh only ----

PICT files (.pic) in either Picture (metafile) or bitmap format and.png raster files.

---- End Windows/Mac only ----

File Locations

ATOMS expects to find certain files in the "home" directory, which is the directory containing the ATOMS program file (CPATOMS.EXE for Windows). These files are

SCRPTR, DEFAULTS, PPLOT, SPCGRP.DAT, CPATOMS.HLP, ELEMENTS, HALL.DAT, CIFDIC.SHT, RADII, SCATFAC.DAT and palette (.PAL) files.

If you are using Cartesian symmetry files (.sym), they should be in the same directory ("data" directory) as the structure file. The data directory is reset whenever you read or write a structure file (.str). Most output files, including EPS, raster, HPGL, metafiles and calculation output files (infile.atd), will be written to the data directory. However, the data files (.atd) from the **List...** options in the File menu are written to the home directory, to avoid cluttering the disks. To save these files permanently, use **Save As** to give them new names in the directory of your choice.

When reading files, the extensions are not mandatory, and you can always use a different extension when saving a file, or specify "all files" when browsing or searching for a file.

---- Macintosh only ----

File and Creator Types

Most output and data text files have file creator 'ATOM' and file type 'TEXT'. The main ATOMS data files (.STR) have file type 'ATDT', to prevent accidental damage by editing with a word processor. However, you can can change the file type to 'TEXT' with a utility program if necessary. Only files with creator 'ATOM' and extension.STR will be opened as data files by ATOMS when they are double-clicked.

Files from previous versions of ATOMS may have different creator and file types.

---- End Macintosh only ----

4.12 Frames

With printed and pen-plot output, you have a choice of using the full page, or confining the output to a *frame*. For Raster Files and Metafiles or PICT files (**File** menu) output always goes to a frame.

If you are using the **Universal** or **Maximize Each View** scale modes (Scaling dialog in the **Input2** menu), the image is scaled to fit in the frame. If you are using the **Fixed** scale mode, the image is clipped to the frame.

In printed and pen-plot 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.

In some cases, you can choose the units for the size and offset of the window; either inches, centimeters or dots (pixels), and you may also be able to specify the nominal dots

per inch or centimeter. The units setting is independent of the overall choice of inches or centimeters in the **Preferences** dialog in the **Settings** menu.

4.13 Lighting Equation

In the 3D drawing mode the material properties of objects determine the way the objects interact with the light sources. The color observed at a given point is a resultant of the light source(s) (3D Lighting) and the Material properties; that is, the RGB coefficients of the **Ambient**, **Diffuse** and **Specular** components of the light source(s) are multiplied by the specified colors of the objects, and by the material coefficients in this dialog, then the results are limited to the range 0.0-1.0.

```
Itotal  =   Ke C                          ;emissive
        + Ia Ka C                         ;ambient
        + Sum(i) [ ( NdotVi ) Ii Kd C ]    ;diffuse
        + Sum(i) [ ( NdotSi )^ns Ii Ks ]   ;specular
```

Where

Itotal is the total intensity as an RGB triplet at any point on an object;

Ia is the intensity (RGB triplet) of the ambient light source (3D Lighting dialog);

Ii is the incident intensity (RGB triplet) at the object of directional or positional light source i (3D Lighting dialog);

C is the assigned color (RGB triplet) of the object (Input Atoms, Bonds, Polyhedra dialogs);

Ke is the emissive material coefficient of the object (3D Material Properties dialog);

Ka is the ambient material coefficient of the object (3D Material Properties dialog);

Ks is the specular material coefficient of the object (3D Material Properties dialog);

ns is the specular exponent or shininess coefficient of the object (3D Material Properties dialog);

N (a vector) is the normal to the surface at the point in question;

Vi (a vector) is the direction of the incident directional or positional light i at the point;

S (a vector) is the bisector of the angle between the light-surface vector (or Vi) and the eye-surface vector;

"dot" signifies the vector dot product.

The incident intensity from a light source is itself subject to attenuation (3D Lighting dialog);

$$Ii = Ii(0) / (Kc + Kl\ d + Kq\ d^2)$$

Where d is the distance of the point in question from the (positional) light and Kc, Kl and Kq are the **constant**, **linear** and **quadratic** attenuation coefficents respectively. Constant attenuation is essentially a brightness coefficient. Values larger than 1.0 simply darken the scene. Values smaller than 1.0 may add a white component and/or increase the specular contribution. **Linear** and **quadratic** attenuation apply only to Positional lights.

Ambient light has no direction or origin and is considered to bathe all objects uniformly. Having a significant ambient component causes non-illuminated parts of objects to be other than black. It thus "softens" the illumination in a somewhat similar way to the **Darkest Shade** and **Darkness Angle** parameters (Shading dialog) in the Standard display mode.

Diffuse color is usually the main component of the appearance of objects. The intensity of the color is dependent on the angle between the light ray and the normal to the surface in question.

Specular reflection only occurs when the normal to the surface in question is close to bisecting the angle between the incident light and the vector from the point on the surface to the eye. It produces bright highlights on a curved surface. The larger the **Specular** material coefficient, the smaller will be the bright specular highlight on a curved surface. The shininess coefficient has a maximum of 128 because of computational restrictions, but values on the order of 5-30 are usually realistic. In ATOMS, specular reflection is always white, that is it does not depend on the color of the object, only the color of the light source(s). For directional lights, specular reflection may not work well for polyhedra because faces at certain angles will give a solid white appearance.

Emission is similar to ambient, except that there is no dependence on the color of any light source. A high value of emission makes an object look like is is glowing.

This equation ignores translucency, which causes colors objects lying at different depths to be blended.

4.14 Space- and Point-Group Orientation

Proper generation of atoms by symmetry requires that atom coordinates be consistent with the orientation of symmetry elements. That is, the people who publish or otherwise report atom coordinates have to assume a particular geometric relationship between the

symmetry elements and the coordinate axes in terms of which the atomic positions are given. In some point and space groups there is only one reasonable choice for the mutual orientation of coordinate axes and symmetry, but in some groups there may be two or more possibilities and ambiguity may arise.

Crystals. The preferred symmetry option for crystals is normally Space-group**,** which reads the symmetry operations from a selection of those in the *Tables*. The main part of the *Tables* themselves (section 4.3 of Volume I, pre-1983 or Chapter 6 of Volume A, post-1983) lists only some of the possible orientations of space-group symmetry for monoclinic and orthorhombic crystals, but the alternate orientations can be generated by ATOMS, as described in the detailed instructions for the Space-group option. The alternate settings are listed in Table 6.2.1 of Volume 1 or Table 4.3.1 of Volume A of the *Tables*.

A consistent orientation of symmetry elements with respect to axes is not always used for space groups in the *International Tables for X-ray Crystallography*. As an example of alternate orientations, consider the point group C_{3v}. The two simplest orientations for the vertical mirror planes are either parallel to the a_1 and a_2 axes, or in between, rotated 30 degrees. These two orientations are embodied in the two space groups $P31m$-C_{3v}^2 (no. 157) and $P3m$-C_{3v}^1 (no. 156). If the same orientation were used for both, one of them would have a *C*-centered Bravais lattice, the avoidance of which the compilers of the *Tables* apparently considered more important than consistent axial orientation.

It is important to realize that these different possibilities exist, especially when using face or form indices from textbooks or the literature; it may be necessary to transform the indices to conform with the orientation used in the structure description.

Molecules. Using the Point Group symmetry option**,** which derives the symmetry operations from space-group listings in the *Tables*, unavoidably makes certain assumptions about orientation. In monoclinic symmetry (point groups *2*-C_2, *m*-C_s, and *2/m*-C_{2h}) the unique axis is taken to be parallel to *c* or *z*, rather than *b* or *y* (as in crystals). In the orthorhombic point group *mm*2-C_{2v} the two-fold axis is assumed to be parallel to *c*. If the atomic coordinates for the molecule are given in terms of a non-standard setting, an alternate to manual rotation of the coordinates before input is to use the Space-group option, specifying a space group in the point group of interest which has the alternate orientation. Some examples of alternate settings related by 30 and 45 degree rotations on the c axis are given in the section on the Space-group option.

4.15 Special Considerations for Molecules and Polymers

While ATOMS can deal equally as well with molecules as crystals, the input contains some options which are extraneous for molecules. The following sections give some guidelines for dealing with molecules and polymers. This is intended only for molecules

which are input as single entities with absolute coordinates, not for molecules which are part of a crystal structure, which can be isolated with the Locate Groups command (**Transform** menu), the **Find** button in the Generated Atom Data dialog, or the special boundary options for molecules in crystals..

1. Coordinate Axes for Molecules.
The type of axial system specified in the Title/Axes dialog (**Input1** menu) may depend on the symmetry of the molecule. Except for cases in which one 3-fold or 6-fold axis is present, i.e. trigonal or hexagonal symmetry, there is no reason not to use Cartesian reference axes. The symmetry may then be specified using the Point-group symmetry option if the molecule is in a standard orientation, or the Space-group or Custom options if it is not. All these options use symmetry operations which are of the type used for crystals.

However, if a molecule has either a 3-fold or a 6-fold axis the full symmetry can be specified by means of crystallographic symmetry operations only if hexagonal structure axes are used. Both trigonal and hexagonal crystal systems by default use "hexagonal axes", that is a_1 and a_2 axes at right angles to the c axis, and 120 degrees from one another. Trigonal crystals may also use rhombohedral axes, which are not applicable to molecules. Cartesian coordinates may be transformed to hexagonal coordinates, and vice-versa, with the following sets of equations (angles in degrees).

$$x_h = (1/a)\, x_C \sin 120 + (1/a)\, y_C \cos 120$$
$$y_h = (1/a)\, x_C \cos 120 + (1/a)\, y_C$$
$$x_C = (a)\, x_h \sin 120$$
$$y_C = (a)\, x_h \cos 120 + (a)\, y_h$$

where a is the length of the hexagonal a axes (or ratio of lengths hexagonal over Cartesian if the Cartesian axes are not of length one). These equations assume that the two c or z axes are parallel and that the a_2, b or y axes are parallel.

Trigonal and hexagonal point groups. If unit Cartesian axes are used and a trigonal or hexagonal point group is selected in the Point Group symmetry option, the standard matrices for this group (derived from the first space group in the point group in the International Tables) are converted from a basis of hexagonal axes to Cartesian axes. This implies a certain orientation of the symmetry elements. If a different orientation is desired, there are two options; you can use a space group with a different orientation, or you can select the Cartesian symmetry option. The Cartesian option requires the preexistence of a file containing the symmetry matrices, which may be generated with the auxiliary program SYMGRP available from Shape software. With this option the symmetry elements may have any desired orientation with respect to the coordinate axes.

2. Boundary Options for Molecules and Polymers.
For an isolated molecule, the boundary option will normally be No boundaries — this

simply accepts all atoms in the original input and those generated by point-group symmetry — no translations (lattice vectors) are applied. Again, if you want to locate a molecule in a crystal structure, see the Locate Groups command in the **Transform** menu, the **Find** button in the Generated Atom Data dialog, or the special boundary options for molecules in crystals.

For a polymer, there are two possible choices. The simplest is to use the **Translation Limits** option**.** This takes all the atoms in the central cell and those generated by translation within the given limits in the directions of the selected lattice vectors (axes). For a one-dimensional (chain) polymer, two of the translations should be disabled and for a two-dimensional (sheet) polymer, three should be disabled. This is certainly the best choice for a one-dimensional polymer.

The other choice is to use the Enter Forms option**,** and manually disable one or two lattice translations. This allows for showing different parts of two-dimensional polymers. For example, consider a trigonal or hexagonal sheet; the Translation Limits option allows for showing only a rhombic slice of the sheet. Suppose that the polymer extends in the *a* and *b* (*x* and *y*) directions; then it can be limited by vertical faces such as (100), (010), etc. to give a slice with hexagonal or trigonal symmetry. Translation in the *c* (*z*) axis direction should be disabled**.**

The above choices again assume that the input is actually for a molecule, and not a crystal. For viewing molecules in crystals, the procedure is different. First, you can import several types of crystallographic files for structures containing molecules using the Isolate Molecules in Crystal boundary option (**Input1** menu). The Free-Form (.inp) import option can be used to read in almost any type of atomic-coordinate information. You can also use the Locate Groups option in the **Transform** menu to isolate individual molecules or polymers.

3. Symmetry for Molecules and Polymers.

Symmetry of molecules is normally described in terms of point groups. The point group symmetry can be provided as crystallographic symmetry operations, or in the form of Cartesian symmetry matrices.

3.1. Crystallographic symmetry operations.

ATOMS can automatically provide the symmetry for the 32 point groups which are also crystal classes, i.e. contain no non-crystallographic symmetry elements such as 5-fold axes. Provided that the orientation of the symmetry elements with respect to the coordinate axes is standard, it is only necessary to give the Schoenflies or International (Hermann-Maughin) symbol for the point group in the Point-group symmetry option. Certain alternate orientations, related to the "standard" ones by a rotation of 45 or 30 degrees on the *c* or *z* axis, can be attained by using the Space-group symmetry option**.** If the orientation is not attainable by either of these methods, appropriate symmetry operations can be entered with the Custom symmetry option.

There is no provision in ATOMS for strictly one-dimensional, two-dimensional or spiral symmetry elements, such as might occur in polymers. Nevertheless, most if not all of the symmetry in polymers may be included with judicious use of space groups, combined with disabling of repetition by translation in one or two dimensions. The space groups which are applicable are those which have no screw axes or glide planes with translation in a non-polymer direction. For example, an ideal silicate chain polymer is completely described by space group no. 28 *Pma*2-C_{2v}^4, with the chain running in the *a* (*x*) direction and the translations in the *b* and *c* directions disabled.

3.2 Cartesian Symmetry Matrices.
This symmetry option is necessary for non-crystallographic point symmetry, that is symmetry groups containing *n*-fold axes with *n* equal to 5 or higher than 6. It can also be used for trigonal and hexagonal symmetry if you want to use Cartesian atomic coordinates. Some symmetry files are provided, namely for the two icosahedral groups and the pentagonal groups; in other cases the Cartesian matrices must be generated before running ATOMS, by using the program SYMGRP, which generates self-consistent point symmetry groups in any orientation.

4.16 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

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

Bold Slanted: Courier-BoldOblique

4.17 Starting ATOMS - Command-Line Processing

Starting ATOMS from DOS command line with data file or import file

---- Windows only ----

ATOMS for Windows can be started from the DOS command line, or other situations where command lines are used. If the name of an ATOMS data file (extension.STR) or an import file is also given, this file will be read in. For example

WXATOMS MYFILE.STR

will start ATOMS and open the ATOMS data file MYFILE.STR.

WXATOMS MYFILE.INS

will import the SHELX input file MYFILE.INS.

ATOMS distinguishes among the different kinds of files by using the file extension (the last three characters in the name, following the dot). It tests first for the ATOMS data file extension.STR, then tests for the extensions for the import file types in the order in which the file types are listed in the File/Import menu (with one exception). The default extensions are as follows:

.INP Free-form Input
.FDT CCDC FDAT file
.INS SHELX input file
.CIF CIF Crystallograpic Information File
.DBW DBWS Rietveld file
.LHP LHPM Rietveld file
.RET ICSD RETRIEVE file
.CRY ICSD CAN/SND file
.CRY ICSD Original CRYSTIN file (must be changed; see below)
.XTL Xtlview file
.PDB Protein Data Base file
.XYZ RIETAN Rietveld file
.EXP GSAS (Los Alamos) Rietveld file
.AMC American Mineralogist structure database
.PCR FULLPROF refinement file
.MOT VIBRATZ atomic motion file

In order to read Original CRYSTIN ICSD files with the command line, the.CRY

extension (or that of CAN/SND files) must be changed within ATOMS, as both file types normally use the same extension.

The extensions, which should always be three characters, can be changed in the dialogs for the individual file types, accessed through the Import item in the File menu (Startup) or File menu (Graphics). The options for importing are also set in these dialogs. Thus to set the file extension and other options, start up ATOMS in Windows and select File/Import and the file type of interest. The extension and options will be saved if you click OK in these dialogs – it is not necessary to actually read a file (that is, you can click Cancel in the File Open dialog).

Note that you must give sufficient information about the PATH so that the ATOMS program file (CPATOMS.EXE) and the data file to be read can be located. If this information in not in the current DOS PATH, and the files are not both in the current directory, path information must be given in the names. For example:

C:\ATOMS60\WXATOMS.EXE C:\ATOMS60\SAMPLES\DDRANE.STR

4.18 Character Sets - sub- and superscripts

ATOMS uses only 1-byte characters (256 possible characters) for the various types of labels and for file input and output. Most types of file containing structural information use only this type of character encoding, not multi-byte characters such as unicode. As latin characters and arabic numerals for chemical symbols are nearly standard worldwide, this should not cause too much difficulty.

ATOMS previously was restricted to the standard ANSI character set, but this restriction has been removed for the Title and atom labels. Thus it is possible to use fonts with non-latin-based character sets (if simplified to 256 characters), and special fonts such as FEBTechnical to display numeric sub- and superscripts and special characters. Such fonts may be selected through the **Font** options in these dialog.

In the Title/Axes and Input Atom Data dialogs (Input1 menu) characters for non-ANSI typefaces should be displayed correctly, but at a fixed font size. The list of input atoms in the Atoms dialog (Input1 menu) may not show non-ANSI characters correctly because this list must be written in a fixed-width font (Courier or Monaco).

Note that superscript 1 (character number 185), 2 (178) and 3 (179) are included in the standard ANSI character set and may be displayed in standard latin fonts such as Times, Courier, Monaco, etc.

To insert special characters into the title or atom labels in ATOMS, it may be easiest to generate these in special system-supplied applications or applets, such as the Character Map in Windows or the Character Palette in Macintosh, and cut-and-paste into the text boxes in the ATOMS dialogs. In some operating systems it may be possible to insert characters by number using specific key combinations.

Special fonts with desired characters may be designed, or standard fonts modified, with commercial font-editing tools. The Private Character Editor in recent releases of Windows does not apply to 1-byte characters.

Atom labels may optionally include special roman-numeral superscripts indicating the symmetry-operator number - this is done automatically and should not require any special font as long as the font selected for atom labels contains the standard latin characters used in the roman numerals.

4.19 Coordinating ATOMS and VIBRATZ

The vibrational-analysis program VIBRATZ and the structure-display program ATOMS are designed to work together. The structure-display capabilities of ATOMS, which has 3-D display and animation of vibrational motions, among many other things, are much greater than those of VIBRATZ.

Communication between the two programs is through the modes (.MDS) binary files, which can be written by either program. These files contain the detailed data for each mode, including atomic motions. These files are designed for quick access to the data for each individual mode, so all the data for all modes does not have to be in memory at the same time.

ATOMS can import the .MOT ascii (text) files written by ATOMS. These also contain detailed data for each mode. As ATOMS imports a .MOT file, it writes a .MDS (binary) file - this should be the same as the .MDS file written by VIBRATZ. Why bother with two different types of file? Because the binary .MDS files are not portable between platforms (e.g. Intel vs. Motorola processor).

ATOMS can also import the main VIBRATZ .VBR data files. The information in these files is not the same as in the .MOT files - the .VBR data files, like ATOMS .STR files, contain complete symmetry information and only the symmetry-unique input atoms, while .MOT files contain all atoms in the molecule or unit cell, without symmetry. The atomic motions in .MDS and .MOT files must refer to all atoms in the molecule or unit cell. Thus, **do not** import .VBR files into ATOMS if you want to display atomic motions.

When importing either type of VIBRATZ file, ATOMS will read the type numbers modulo 100 - for example, atom types number 6, 106, 206 etc. will all be converted to 6 (carbon).

Recommended procedure for using ATOMS to show vibrational motions.

1) If you import an ATOMS (.STR) file into VIBRATZ, it is a good idea to use two different names, for example myfile_orig.STR for the original ATOMS files, and myfile.VBR for the VIBRATZ file. This is because you will use another .STR file, without symmetry, to display the motions.

2) In VIBRATZ, check the .MOT file box in the Control window so that a .MOT file is written during calculation. This will be myfile.MOT.

3) In ATOMS, import the myfile.MOT file. This will rewrite myfile.MDS. The new ATOMS

file will be by default myfile.STR. Set up the boundary (for crystals), display parameters, vectors, etc. as desired. Most parameters dealing specifically with motion display are in the Vectors and Vibrational Modes dialogs in the Input1 menu. The bonds are just those specified in VIBRATZ.

4) If you return to VIBRATZ to recalculate with changed forces, it will rewrite myfile.MDS, which can be read by ATOMS, so ATOMS will remain up to date with the latest VIBRATZ calculations. On the other hand, if you want to preserve the motions for a particular calculation, you can rename the .MDS file, e.g. myfile_1.MDS (you must do this in the operating system). You can switch between different .MDS files in the Vibrational Modes dialog in the Input1 menu. You can also reread the .MOT file, for atomic motions only, in the Vibrational Modes dialog.

5) *Starting a new problem*. Once you have the parameters in ATOMS set up to your liking, before importing a new .MOT file, just read an old ATOMS file with the appropriate settings. When you import a .MOT file, the new ATOMS .STR file will have the same name as the .MOT file. Or, save the desired parameters by selecting Save Defaults in the Settings menu in ATOMS. These parameters can be reread during import, or later through the Settings menu.

6) *Transferring problems across platforms.* The binary .MDS files may be incompatible between platforms (Macintosh and Windows computers write the bytes of numbers in opposite order). Thus you should transfer the ascii (text) files myfiles_orig.STR, myfiles.VBR and myfiles.MOT. When you open the myfiles.STR file in ATOMS for display of atomic motions, use the option in the Vibrational Modes dialog in the Input1 menu to read in the .MOT file for atomic-motion parameters only. This will cause writing of a new myfile.MDS. Rerunning VIBRATZ should also rewrite the .MDS file.

Display parameters in ATOMS. The atomic radii are controlled during import with the choice between covalent and ionic radii, and by the factor which may be applied - for displaying motions the factor should normally be well under 0.5. You can later change radii globally with the Atoms-Global option in the Input1 menu. You can change the default radii and atom colors for import by editing the ELEMENTS.ION and ELEMENTS.COV files. (The file RADII contains a universal table for automatic bond generation - this should not be modified unless there are problems with automatic bond generation). Bond parameters may be set during import, or reset with automatic bond generation (Bonds dialog in the Input1 menu).

When importing a .MOT file, bond specifications are taken directly from the VIBRATZ data. If there is a structure in memory, and if there are bonds (Bonds dialog in the Input1 menu), the radius and colors of all the new bonds are taken from the first old bond - if there are no bonds, radius and colors of the bonds derived from the .MOT file will be standard (radius 0.0, black rim, white fill), or the values of the first bond when defaults were last saved.

5 Tutorials

In addition to the examples selected for tutorials, the subfolder SAMPLES contains some other examples. All example files have the suffix.STR; check the file EXAMPLES.DOC for comments on the examples, including the tutorials.

To start any of the tutorials elect the **New** command from the **File** menu. This will step through most of the dialogs in the **Input1** menu and also the **Input2** menu if desired. Input for each of these dialogs is discussed below. After each of these main dialogs has been completed by clicking on the **OK** button, the **Enter New Data Set** dialog comes up. This gives you the choice to **Continue**, **Abort** or **Revise** the last category of input. This dialog will not be mentioned again, but keep in mind that it comes up after each of the main dialogs described below.

In the input for atoms, polyhedra, bonds etc., there are edit boxes for the pen number. Pen numbers will not be discussed, since for multi-pen plotters the color depends on which pens are placed in each position in the holder.

Note that when you are editing individual entries in the **Input Atoms**, **Polyhedra** or **Bonds** dialog, you can continue to edit items in the list with the **Revise** button; input of these lists is finished when you click on **OK**. When in the **Atom Data**, **Polyhedron Data** or **Bond Data** dialogs which are called up by the **Revise** or **Add** buttons, you can step through the list forwards or backwards with the **Next** and **Last** buttons. When you are editing the last item in each list, the **Next** button becomes the **New** button. The same things hold true for editing boundary or display forms.

You can get Help for any dialog with the Help button.

5.1 Tutorial 1 - Glutaric Acid

This illustrates basic atom and bond input and interpenetrating atoms (space-filling representation). The coordinates and radii were improvised from an illustration in a magazine ad, and are not absolutely realistic.

Dialog - **Title/Structure Axes**. In the **Title** field, enter "Glutaric Acid". In the **Structure axes** combo box, select "unit Cartesian".

Dialog - **Symmetry Option**. Select **Point group from Table**.

Sub-Dialog - **Symmetry - Point Group from Table**. Select the group **mm2 - C2v**.

Dialog - **Boundary Option**. Select **No Boundaries (molecule)**. This brings up a dialog which simply confirms the choice

Dialog - **Crystal Forms for Display**. In the **Display forms** group of radio buttons, select **None**.

Dialog - **Input Atoms**. Click on the **Add Atoms** button.

Sub-Dialog - **Revise Atom**. We will first enter three carbon atoms. For all these atoms, the **Type** will be 6 (the atomic number) and the **Radius** will 0.75. The colors can be selected as desired; however black (RGB components 0, 0, 0) is recommended for rims, and dark gray (85, 85, 85) for fills. These colors can be selected by filling in the RBG fields directly, or by clicking on the **Select...Color** buttons, and choosing from the 16 colors presented there. For **Black-and-white pattern numbers**, 15 is recommended for rims and 2 for fills. All these fields can be entered once, and they will be copied to the next atom.

The fields which will change between atoms are the **Label**, and the coordinates (**x**, **y** and **z**). For the first atom, fill in the fields from the values given for atom number 1 below. Then, if you have filled in the remainder of the fields as described in the previous paragraph, click on the **New** button. For the second atom, all the fields will be the same; replace the values for **Label**, **x**, **y** and **z** for atom 2) below. In like manner continue on to the third carbon atom. Note that these are absolute coordinates, in Angstroms.

Carbon atoms:

1)	C1	0.0	0.0	0.0
2)	C2	0.0	0.943	0.333
3)	C3	0.0	1.886	0.0

Next come three hydrogen atoms. Click on **New** after the last carbon atom. Set the **Type** to 1, and the **Radius** to 0.4. The rim color and patterns can be left as black, but the fill color and pattern should be changed, for example to green (0, 255, 0) and 8. Again, for each new atom you can change only the **Label** and coordinates **x**, **y** and **z** to the values given below.

Hydrogen atoms:

4)	H1	0.52	0.0	-0.233
5)	H2	0.52	0.943	0.566
6)	H3	0.0	2.4	-1.1

Next come two oxygen atoms. Set the **Type** to 8, and the **Radius** to.75. The fill color and pattern can be changed to red (255, 0, 0) and 5.

Oxygen atoms:

7)	O1	0.0	2.794	0.419
8)	O2	0.0	1.794	-0.996

When finished with atom 8), click on **OK**.

Back in the **Input Atoms** dialog, check the list. If there are any mistakes, you can correct them by selecting the atom and clicking on the **Revise** button.

Dialog - **Polyhedra**. No polyhedra will be used, so just click on **OK**.

Dialog - **Bonds**. Click on the **Add Bonds** button.

Sub-Dialog - **Bond Data**. We will add four bonds. Since the atoms will be interpenetrating, the bond radius, colors and patterns will not be used, and there is no need to set these fields. The **Min distance** field can be set to 0.4 or any small number, and the **Max. distance** field can be set to 1.2. Set the fields listed below, clicking on **New** to go from bond 1) to 2) and so on.

	Atom type 1	Atom type 2	
1)	6	6	(C-C)
2)	6	8	(C-O)
3)	6	1	(C-H)

4) 8 1 (O-H)

Back in the **Bonds** dialog, correct any mistaken entries. Click on **OK** when done.

Dialog - **End of Mandatory Input**. At this point you have the choice of continuing with the dialogs in the **Input2** menu, or accepting default values for the parameters in those dialogs. If a structure file was in memory when you started the **New** input, you can also accept the parameters used in that structure (the current values). Let us continue, to insure that the result is the same as the sample file GLUT.STR.

Dialog - **Crystal Edges**. A crystal shape is inappropriate for this molecule, so select **Atoms only** from the **Display** group.

Dialog - **Perspective Viewing**. Do not check the box; perspective viewing adds little to this molecule.

Dialog - **Stereopairs**. You can check the **Stereopairs on** box if you like, although you may need a special viewer to see the screen image in 3D.

Dialog - **Rims**. Check all the boxes. Unshaded color drawings and all black-and-white drawings look best with rims, and shaded drawings in color usually look better without rims.

Dialog - **Line Widths**. Click on the **Set All to 0** button - this will result in widths of one dot in screen display and raster output. Be sure that the **Use Individual** check boxes are off.

Dialog - **Shading**. Uncheck the boxes **Shading for atoms**, **Shading for bonds** and **Shading for polyhedra**. You can switch later to shading.

Dialog - **Background Color**. A light or medium gray, such as (170, 170, 170) usually works best on the screen.

Dialog - **Axes/Unit Cell**. In the **Display** group, select **Neither**.

Dialog - **Thermal Ellipsoid Parameters**. Click on **Cancel** to skip this dialog.

Dialog - **Initial Orientation**. Set the **Initial Cartesian** rotations (**x**, **y** and **z**) all to zero. Check the **Clinographic viewing** box.

Dialog - **Scaling**. Set the **Scale mode** to **Maximize size for each view**.

Dialog - **Centering/Displacement**. Select **Automatic Centering**.

Dialog - **Calculation Output**. In the combo box **Output**, select "No Output".

After the last dialog has been completed, you are asked if you want to save the file. Then a message box appears saying "New input completed - calculate now?". Click on **Yes**, and the drawing should appear quickly.

You can compare the results of this input process with the file GLUT.STR in the SAMPLES subfolder. If there are differences, you can print out the input parameters in either or both files with the **List Input** command in the **File** menu (**Listings** sub-menu).
You can experiment with shading, using the Shading dialog in the **Input2** menu. The shaded drawing will look better if atom rims are turned off in the Rims dialog in the **Input2** menu. Note, however, that if you are using a 256-color display adapter, and if you use 32 shading zones, the carbon atoms become solid black. As explained in section IV-2, the second 8 colors in the 16-color palette are not valid for 32 shading zones. You can use the Atoms - Global dialog in the **Input1** menu to change the fill color for all type 6 atoms to one of the colors in the upper half of the **Choose Color** dialog.

5.2 Tutorial 2 - Diopside

This is a typical silicate crystal. Unless the unit cell is very small, ball-and-stick display is too complicated for most silicates, and showing the SiO_4 groups as polyhedra is usually more satisfactory. The atomic radii used for Mg and Ca are approximately half the ionic radii, which works fairly well as a general practice.

Select the **New** command from the **File** menu. See the start of the Tutorials section for general comments.

Dialog - **Title/Structure Axes**. In the **Title** field, enter "Diopside". In the **Structure axes** combo box, select "monoclinic". For the a, b and c axes, enter 9.746, 8.899 and 5.251, and for beta enter 105.63.

Dialog - **Symmetry Option**. Select **Space group from Table**.

Sub-Dialog - **Symmetry - Space Group from Table**. Enter "C2/c" in the **H-M Symbol** field, and make sure that the radio button for this option is checked. Or, you can select this space group in the list box, clicking on the **Select** button, and it makes no difference which option (H-M, Hall or Number) is selected.

Dialog - **Boundary Option**. Select **Enter Forms**.

Sub-Dialog - **Boundary - Enter Forms**. Set the **Symmetry for boundary forms** to **Center only**. At the bottom of the dialog, **Use individual atom distances** should be unchecked and all the **Lattice translation** boxes should be checked. Now click on the **Add Forms** button.

Sub-Sub-Dialog - **Add/Revise Form**. For each form, enter the indices shown below in the **h**, **k** and **l** edit boxes, and the distance in the **Central distance** box. When finished with each, click on the **New Form** button to go to the next. When done, click on **OK**.

	h	k	l	distance
1)	1	0	0	4.0
2)	0	1	0	7.0

3) 0 0 1 11.0

Back in the **Boundary - Enter Forms** dialog, check the list and correct the entries if necessary with the **Revise** button. When done, click on **OK**.

Dialog - **Crystal Forms for Display**. In the **Display forms** group of radio buttons, select **Same as boundary**.

Dialog - **Input Atoms**. Click on the **Add Atoms** button.

Sub-Dialog - **Revise Atom**.

Atom 1) is silicon. The **Label** should be Si, the **Type** should be 14 (the atomic number) and the **Radius** 0.15 - silicon atoms will not appear by themselves unless skeletal or transparent polyhedra are selected for the 3D display mode. The colors and pattern numbers can be ignored for this reason. The **x**, **y** and **z** coordinates are 0.2862, 0.0933, and 0.2293. When done, click on the **New** button.

Atom 2) is magnesium - Mg and Ca atoms will be shown as spheres. The **Label** should be Mg, the **Type** should be 12 (the atomic number) and the **Radius** 0.36. The x, y and z coordinates are 0.0, 0.9082 and 0.25. The colors can be selected as desired; however black (RGB components 0, 0, 0) is recommended for rims, and red (255, 0, 0) for the fill. For **Black-and-white pattern numbers**, 15 is recommended for rims and 6 for fills. When done, click on the **New** button.

Atom 3) is calcium. The **Label** should be Ca, the **Type** should be 20 (the atomic number) and the **Radius** 0.56. The x, y and z coordinates are 0.0, 0.3015 and 0.25. The colors can be selected as desired; however black (RGB components 0, 0, 0) is recommended for rims, and blue (0, 0, 255) for the fill. For **Black-and-white pattern numbers**, 15 is recommended for rims and 4 for fills. When done, click on the **New** button.

Now enter three oxygen atoms. For all these atoms, the **Type** will be 8 (the atomic number) and the **Radius** will be 0.0 - oxygen atoms only appear as corners of polyhedra, and if they are to be shown as spheres they can be given a uniform radius. The rim color can be black and the fill color cyan (0, 255, 255). For **Black-and-white pattern numbers**, 15 is recommended for rims and 1 for fills.

The fields which will change between atoms are the **Label**, and the coordinates (**x**, **y** and **z**). For the first atom, fill in the fields from the values given for atom number 1 below. Then, if you have filled in the remainder of the fields as described in the previous paragraph, click on the **New** button. For the second atom, all the fields will be the same; replace the values for **Label**, **x**, **y** and **z** for atom 2) below. In like manner continue on to the third carbon atom.

Oxygen atoms:

4)	O1	0.1156	0.0873	0.1422
5)	O2	0.3611	0.25	0.3180
6)	O3	0.3503	0.0176	-0.0047

When finished with atom 6), click on **OK**.

Back in the **Input Atoms** dialog, check the list. If there are any mistakes, you can correct them by selecting the atom and clicking on the **Revise** button.

Dialog - **Polyhedra**. Click on **Add Polyhedra.**

Dialog - **Polyhedron Data**. The only polyhedron will be the silicate tetrahedron, although is is also possible to do Mg octahedra. The **Coordination number** is four, the **Maximum bond distance** can be 1.8, the **Central type** (Si) is 14 and there is only one **Ligand type**, 8 for oxygen; put the number eight in the first **Ligand type** box and be sure the other 6 boxes are empty. The rim color should be black, and the fill color can be yellow (255, 255, 0). Rim pattern should be 15 (black) and fill pattern can be 2. Click on **OK** when finished.

Back in the **Polyhedra dialog**, in the **Show ligands as spheres** group, select the **Use single radius** radio button, with radius 0.2.

Click on **OK** if the single polyhedron entry is correct.

Dialog - **Bonds**. Click on the **Add Bonds** button.

Sub-Dialog - **Bond Data**. We will add two bonds. The **Atom types**, **Max. distance** and rim color are given below. The **Radius** should be set to 0.0 for single-line bonds, which will use the rim color and pattern number - the fill color and pattern are ignored. Rim pattern number should be 15. The **Min distance** field can be set to 0.4 or any small number.
For bond 1), Mg-0, the two types are 12 and 8; the maximum distance is 2.3; and rim color can be blue (0, 0, 255). After entering the values for bond 1), click on **New** to go to 2). For bond 2), Ca-0, the two types are 20 and 8; the maximum distance is 3.0; and rim color can be magenta (255, 0, 255). Click on OK when finished with bond 2)

Back in the **Bonds** dialog, correct any mistaken entries. Click on **OK** when done.

Dialog - **End of Mandatory Input**. At this point you have the choice of continuing with the dialogs in the **Input2** menu, or accepting default values for the parameters in those dialogs. If a structure file was in memory when you started the **New** input, you can also accept the parameters used in that structure (the current values). Let us continue, to insure that the result is the same as the sample file DIOPSIDE.STR.

Dialog - **Crystal Edges**. You can select either **Both** or **Atoms only** from the **Display** group. Set the dash length to 0.2 and the dash ratio to 0.45. colors can be yellow (255,255,0) for front edges and blue (0,0,255) for back edges. Pattern numbers for both front and back edges should be 15.

Dialog - **Perspective Viewing**. Check the box and set the **Perspective distance** to 50.0.

Dialog - **Stereopairs**. You can check the box if you like, although you may need a special viewer to see the screen image in 3D.

Dialog - **Rims**. Check all the boxes. Unshaded drawings look best with rims, and shaded drawings in color usually look better without rims.

Dialog - **Line Widths**. Click on the **Set All to 0** button - this will result in widths of one dot in screen display and raster output. Be sure that the **Use Individual** check boxes are off.

Dialog - **Shading**. Uncheck the boxes **Shading for atoms**, **Shading for bonds** and **Shading for polyhedra**. You can switch later to shading.

Dialog - **Background Color**. A light or medium gray, such as (170, 170, 170) usually works best on the screen.

Dialog - **Axes/Unit Cell**. In the **Display** group, select **Neither**.

Dialog - **Thermal Ellipsoid Parameters**. Click on **Cancel** to skip this dialog.

Dialog - **Initial Orientation**. We want to look almost directly down the c axis, so set the **Initial Cartesian** rotations (**x**, **y** and **z**) to 0.0, 92.5 and 0.0. Uncheck the **Clinographic viewing** box.

Dialog - **Scaling**. Set the **Scale mode** to **Maximize size for each view**.

Dialog - **Centering/Displacement**. Select **Automatic Centering**.

Dialog - **Calculation Output**. In the **Output** combo box, select "No Output".

After the last dialog has been completed, a message box appears saying "New input completed - calculate now?". Click on **Yes**, and the drawing should appear quickly.

You can compare the results of this input process with the file DIOPSIDE.STR in the \SAMPLES subdirectory. If there are differences, you can print out the input parameters in either or both files with the **List Input** command in the **File** menu (**Listings** sub-menu).

5.3 Tutorial 3 - Dodecahedrane

This is a hypothetical cyclic saturated hydrocarbon molecule with carbon atoms at the 20 corners of a pentagonal dodecahedron (Icosahedral symmetry, group *I*), and one hydrogen bonded to each carbon. It illustrates the input of non-crystallographic symmetry using.SYM files, and the use of stick bonds. This drawing will also be done with shading and perspective viewing. See SYMGRP for the generation of the I.SYM file, which in this case is present in both the SAMPLES and the SYMGRP subfolders. Since the Cartesian symmetry file must be in the same directory as the data file, be sure you are in one of these two directories, or move the I.SYM file to the directory you are in. You can switch ATOMS to the SAMPLES subfolder by reading in a file from there. You can also go through the **New** input until you reach the message box "New input completed - calculate now?". If you click on **No**, you can use **Save As** in the **File** menu to save the current file to the SAMPLES subfolder. Then select **Calculate** from the **File** menu.

Select the **New** command from the **File** menu. See the start of the Tutorials section for general comments.

Dialog - **Title/Structure Axes**. In the **Title** field, enter "Dodecahedrane". In the **Structure axes** combo box, select "unit Cartesian".

Dialog - **Symmetry Option**. Select **Cartesian Matrices**.

Sub-Dialog - **Symmetry - Cartesian Matrices**. In the **File name** box, enter I.SYM.

Dialog - **Boundary Option**. Select **No Boundaries (molecule)**. This brings up a dialog which simply confirms the choice

Dialog - **Crystal Forms for Display**. In the **Display** group of radio buttons, select **None**.

Dialog - **Input Atoms**. Click on the **Add Atoms** button.

Sub-Dialog - **Revise Atom**. We will enter only one carbon atom. The **Type** should be 6 (the atomic number) and the **Radius** 0.35. The **x**, **y** and **z** coordinates are 0.0, 0.0 and 1.4. The colors can be selected as desired; however black (0, 0, 0) is recommended for rims, and magenta (255, 0, 255) for fills. For **Black-and-white pattern numbers**, 15 is recommended for rims and 2 for fills. The **Pen number** can be 1, or if you will not be using a pen plotter, just ignore this field.

Click on the **New** button to enter the hydrogen atom. Set the **Type** to 1, and the **Radius** to 0.2. The **x**, **y** and **z** coordinates are 0.0, 0.0 and 2.2. The rim color and patterns can be left as black, but the fill color and pattern should be changed, for example to cyan (0, 255, 255) and 4. The **Label** should be "H" and the **x**, **y** and **z** coordinates 0.0, 0.0 and 2.2.

Back in the **Input Atoms** dialog, check the list. If there are any mistakes, you can correct them by selecting the atom and clicking on the **Revise** button.

Dialog - **Polyhedra**. No polyhedra will be used, so just click on **OK**.

Dialog - **Bonds**. Click on the **Add Bonds** button.

Sub-Dialog - **Bond Data**. We will add 2 bonds. For C-C bonds, both **Atom type 1** and **Atom type 2** are 6. The **Min. distance** field can be set to 0.4 or any small number, and the **Max. distance** field can be set to 1.4. Set the **Radius** to 0.1. The rim color should be black and the rim pattern number 15. Fill color and pattern can be selected to taste, for example red (255, 0, 0) and 6.

For C-H bonds, **Atom type 1** is 6 and **Atom type 2** is 1. The **Min. Distance** field can be set to 0.4 or any small number, and the **Max. Distance** field can be set to 1.0. Set the **Radius** to 0.06. The rim color should be black and the rim pattern number 15. File color and pattern can be selected to taste, for example blue (0, 0, 255) and 6.

Back in the **Bonds** dialog, correct any mistaken entries. Click on **OK** when done.

Dialog - **End of Mandatory Input**. At this point you have the choice of continuing with the dialogs in the **Input2** menu, or accepting default values for the parameters in those dialogs. If a structure file was in memory when you started the **New** input, you can also accept the parameters used in that structure (the current values). Let us continue, to insure that the result is the same as the sample file DDRANE.STR.

Dialog - **Crystal Edges**. Select **Atoms only** from the **Display** group.

Dialog - **Perspective Viewing**. Check the box; and set the perspective distance to 7.5.

Dialog - **Stereopairs**. You can check the box if you like, although you may need a special viewer to see the screen image in 3D.

Dialog - **Rims**. Uncheck all the boxes. Shaded drawings in color usually look better without rims.

Dialog - **Line Widths**. Click on the **Set All to 0** button, although rims will not be used. Be sure that the **Use Individual** check boxes are off.

Dialog - **Shading**. Check the boxes **Shading for atoms** and **Shading for bonds**. Set the **Number of zones** to 32. The **Illumination vector** can be 3.0, -1.0, 1.0 (this vector will be normalized to length one after leaving the dialog). Set the **Darkest shade** to 0.0 and the **Darkness angle** to 110. You can check **Front-back fading** if desired, and set the **Fading factor** to 0.15. This factor should be smaller than the **Factor for complete fading** shown at the bottom of the dialog; however, this factor is not computed until the structure is calculated.

Dialog - **Background Color**. A light or medium gray, such as (170, 170, 170) usually works best on the screen.

Dialog - **Axes/Unit Cell**. In the **Display** group, select **Neither**.

Dialog - **Thermal Ellipsoid Parameters**. Click on **Cancel** to skip this dialog.

Dialog - **Initial Orientation**. Set the **Initial Cartesian** rotations (**x**, **y** and **z**) all to zero. Check the **Clinographic viewing** box.

Dialog - **Scaling**. Set the **Scale mode** to **Maximize size for each view**.

Dialog - **Centering/Displacement**. Select **Automatic Centering**.

Dialog - **Calculation Output**. In the combo box **Output**, select "No Output".

After the last dialog has been completed, a message box appears saying "New input completed - calculate now?". Click on **Yes**, and the drawing should appear quickly.

You can compare the results of this input process with the file DDRANE.STR in the SAMPLES subfolder. If there are differences, you can print out the input parameters in either or both files

with the **List Input** command in the **File** menu (**Listings** sub-menu).

Index

- C -

- D -

- E -

- F -

- G -

- H -

- I -

- L -

- M -

- N -

- O -

- P -

- Q -

- R -

- S -

- T -

- U -

- V -

- W -

- X -

- Z -