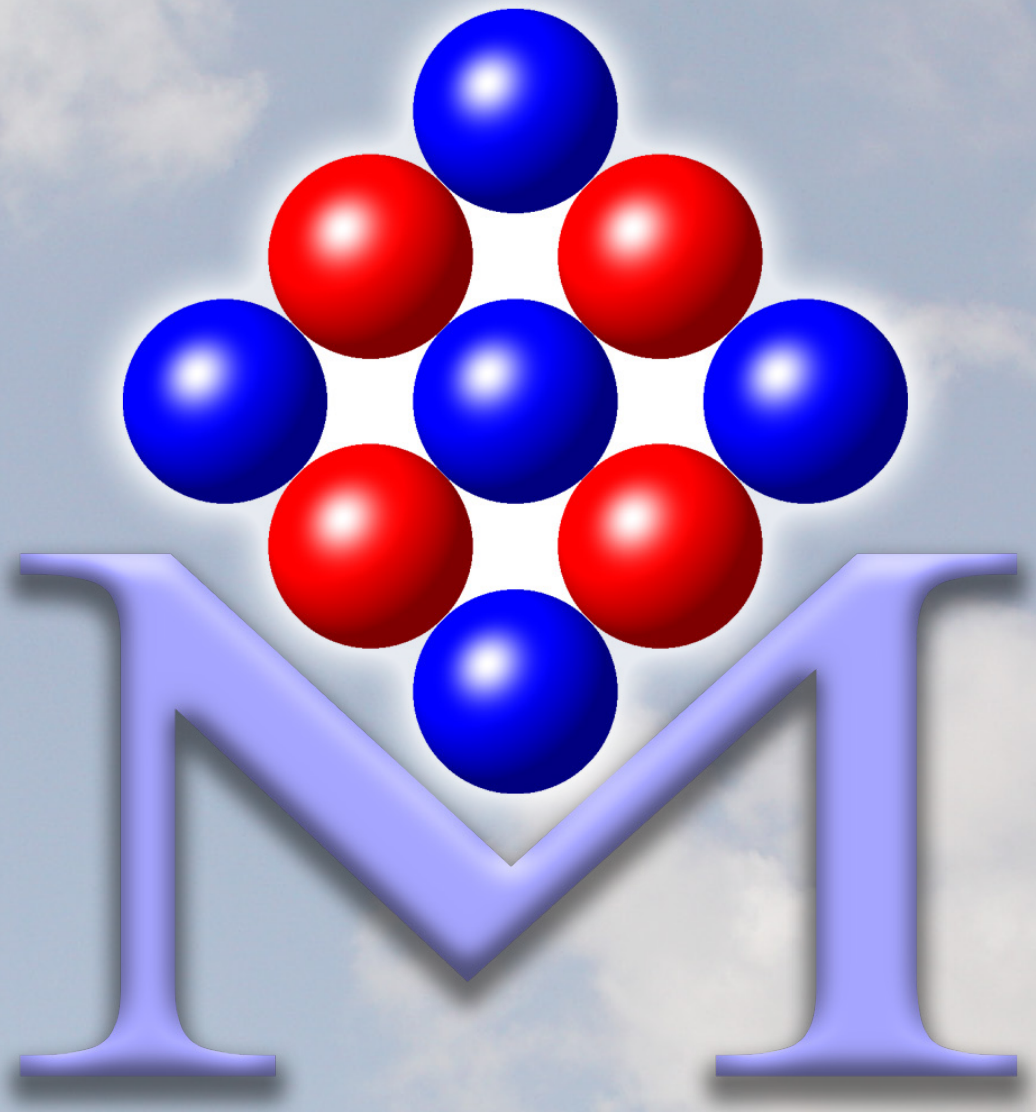
# CrystalMaker®

## Interactive Crystal & Molecular Modelling



# User's Guide

CrystalMaker X for Mac & Windows

NEW EDITION for version 10.5

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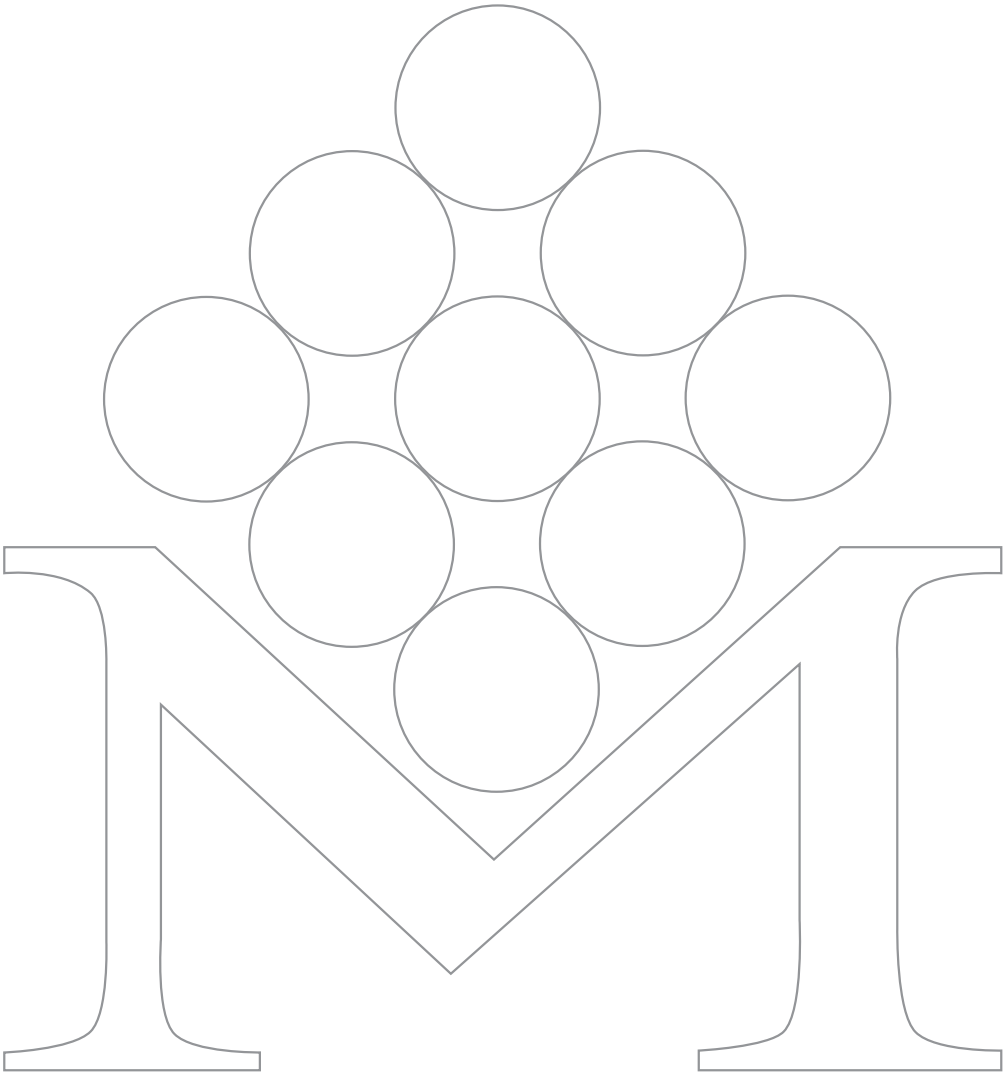
Interactive Crystal & Molecular Modelling



# User's Guide

# CrystalMaker®

# USER'S GUIDE

CrystalMaker Software Limited
Oxford • England

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# Preface

Welcome to CrystalMaker® X: a brand-new program, designed to make the world of crystal and molecular structures accessible and fun. CrystalMaker lets you design new structures and relax them, import data from a myriad of different file formats and generate instant, beautiful models—or simply browse extensive libraries of structures from our integrated Structures Browser. When used with our companion software, CrystalDiffract® and SingleCrystal™, you can combine structure generation with diffraction pattern predication and analysis.

## The Origins of CrystalMaker

CrystalMaker arose out of a deep-seated passion to bring crystal structures and their properties to life: shaking the dust off traditional—and static—teaching models.

Our vision was to harness the *transforming* power of computer, providing *dynamical* models which encourage interactivity. We would enable users to learn through play: developing their own, individual, *visual understanding* of complex arrangements of atoms in crystals. This is beauty at a sub-microscopic level, which echoes (and ultimately causes) the same beauty one observes in a hand specimen of a crystal.

CrystalMaker has since developed into a far more powerful tool for research, as well as teaching. Our aim is to provide a pleasant and efficient workflow—but above all, to encourage users to *explore*, *understand* and *enjoy* the nano-scale world.

## Modelling the Nanoscale

CrystalMaker is a tool for understanding the positions of atoms in a three-dimensional crystal or molecule. At the simplest level, one could visualise these as spheres in space. A slightly more helpful approach would be to plot spheres with "space-filling" radii corresponding to the relevant atomic radii, to see how some structures pack together.

It may be useful to illustrate the arrangement of chemical bonds in the model. One might represent atoms by small spheres, linked by spokes—the *ball and stick* approach. For more complex topologies, one might be more interested in the bonded *framework* than the precise locations of individual atoms, and a *wireframe* model is a clearer representation.

An alternative approach is to *simplify* the bonding picture by defining coordination *polyhedra*, usually the arrangements of anions around a central cation. This approach is particularly useful for understanding complex framework silicate minerals (including zeolites), constructed from a single, basic structural element (e.g., the $SiO_4$ tetrahedron).

Seamlessly switching between different representations—from conventional (and often complex) models, to stylized models such as polyhedral representations—helps identify structural motifs: an underlying shorthand for the detailed structure. This becomes the *visual vocabulary* for describing complex structures.

Simply put, one learns to "*see the wood for the trees*".

## A Tool For Exploration and Discovery

Although a static view of a structure can be represented by different structural models, it is not always easy to appreciate its three-dimensional nature. We overcome the limitations of such "snapshot" images by using the mouse, trackpad or Leap Motion Controller to rotate the structure—with the option of red/blue 3D stereo for an "out-of-the-screen" experience.

The emphasis of the program is firmly on user *interaction*. You can easily measure the structure using the screen tools, or manipulate its orientation and scale. You can change atom colours and styles. Crystal engineering tools let you create space in the lattice, insert atoms or place whole molecules. You can move atoms, and design new structures. Similarly, you can create new molecules by pointing and clicking, then optimize their geometries using the Relax Molecule command.

## A Means of Empowerment

Crystallography emerged as a discipline in its own right, during the first half of the twentieth century. At first it was a very specialist science, but as interest in solid-state structures grows, new ways are being sought to present crystallographic data more easily, and to apply them to the frontiers of modern scientific research—often in new, interdisciplinary areas such as Materials Science and Earth Sciences.

Now, as we progress through the twenty-first century, we hope that CrystalMaker will help to stimulate the *New Crystallography*: unlocking the secrets of our crystalline world, and making crystal structures accessible to all.

Chapter 1

# Introducing CrystalMaker X

This chapter explains what CrystalMaker is designed for, its key features, and the major changes from earlier versions of the software.

## CrystalMaker Key Features

CrystalMaker X is a brand new design, combining the very-best 3D graphics with interactive measurement, energy modelling, crystal engineering, animation and video—and all presented within a beautifully-designed professional user interface.

### Build Crystals & Molecules Fast

With CrystalMaker you can build any kind of crystal or molecular structure quickly and easily. Built-in symmetry handling and the elegant spacegroup explorer takes the slog out of crystallography, and the program will automatically generate all your bonds and polyhedra. Molecule building is even easier: point-and-click to add atoms and bonds (hydrogens can be added automatically); use the **Relax** command to minimize energy and optimize your structure.

### Comprehensive Data Import & Export

Building structures is fun, but you can also import data from one of the 42 or so formats supported by CrystalMaker X. These include the ubiquitous CIF, Protein Data Bank (PDB), SHELX and VASP. A range of output options is available for saving structural data, bond distances, coordination environments or web pages.

### Outstanding 3D Graphics

Enjoy photo-realistic graphics with depth fading and perspective plus spectacular 3D stereo. Benefit from high-resolution printing and save your graphics at user-defined sizes to a wide range of formats, including 3D files for printing or viewing on other devices such as in iBooks on macOS or iOS.

Work with massive structures, using depth profiling and measurement. Bonds and polyhedra are automatically generated, with full error propagation, plus cluster shell and coordination network visualization and powerful output options.

## Real-Time Manipulation

Click-and-drag with the mouse, use the keyboard, or toolbar. View parallel to a vector or plane normal. Take advantage of multi-touch rotation and scaling with a trackpad, the Touch Bar (MacBook Pro models)—or use simple hand gestures in space, using a Leap Motion Controller.

## Powerful Measurement

Preview coordination environments, clusters and shells; visualize bond distances and histograms on screen or save to disc. Measure distances, angles, torsion angles on screen. Calculate angles between planes and vectors.

## Transformation & Crystal Engineering

CrystalMaker lets you transform the unit cell, changing the lattice type, building a supercell, moving the origin, or applying an arbitrary matrix transformation. You can also project the unit cell onto a chosen lattice plane, to create a "surface cell".

Even if you don't want to change your structure, you can make it easier to understand: use CrystalMaker's selection tools to quickly isolate areas of interest and "see the wood for the trees".

CrystalMaker's real-time crystal engineering tools let you insert space within your crystal lattice, place new atoms or entire molecules in the crystal—and design new crystal lattices.

**Freedom to explore:** CrystalMaker provides multiple **undo** levels—so you can safely make changes without worrying about how to get back.

## Animation

CrystalMaker goes beyond static structures, letting you explore structural behaviour, molecular dynamics, vibrational modes, or visualize the trajectory of a computer simulation.

The key to this is that each document window can hold multiple structures: these can serve as the "frames" of a movie or animation. Simply drag-and-drop separate files into the same window (or open a single, multi-structure file), then rearrange the resulting structure thumbnails to build assemble the frames of your animation.

You can make changes to one structure and then synchronize the rest of the structures to match. You can view your animation on screen, adjusting the frame rate using a slider control. You can even change model parameters, rotate and scale structures, all during the animation: a great way to understand dynamical behaviour in 3D! Finally, you can record the entire sequence as a movie, with a single menu command.

### Integration with Diffraction Software

CrystalMaker X is designed to work seamlessly with our award-winning SingleCrystal and CrystalDiffract programs. You can share data directly from CrystalMaker, via a single menu command. In addition, you can synchronize orientations with SingleCrystal in real time: rotate a crystal structure in CrystalMaker and see its diffraction pattern rotate in SingleCrystal (or vice versa).

**Compatibility Note:** CrystalMaker X requires SingleCrystal 3.0 or later, and CrystalDiffract 6.7 or later.

## What's New in CrystalMaker X?

CrystalMaker X is an entirely-new program, developed from scratch for the latest Mac and Windows operating systems. Every line of code has been rewritten, with an entirely-new, object-oriented architecture, brand-new OpenGL-based graphics engine, new interface design, and incomparable new features. The program also features an integrated structures library with some 1200 structures, packaged in an elegant Library interface with browser, viewer and search capabilities—and which can be extended to include all of your structures.

### State-of-the-art design

CrystalMaker X is a workstation-class 64-bit, multi-processor, multi-touch, multi-structure application.

- Object-oriented design using native "Cocoa" (Mac) and ".NET" (Windows) code. This gives the software a "hotline" to the operating system and provides full access to the system's performance as well as an elegant system-specific user interface.
- 64-bit precision for all calculations and storage: taking advantage of modern memory and processor architectures.
- Multi-processor design for faster performance. CrystalMaker is optimized to perform multiple calculations in parallel, giving massive speed improvements in areas such as bond searches, porosity and electron density calculation.
- Multi-touch rotation, zooming and scrolling with a trackpad. Use familiar "pinch-to-zoom", swipe and rotate gestures to control your structure's orientation.
- Drag-and-drop structures between windows. The multi-structure design lets you share structures between windows, duplicate them and rearrange their sequences.

## Built for Mac

CrystalMaker has always been a *native* Mac program. The results speak for themselves:-

- **Retina display**: gorgeous high-resolution graphics on the latest Macs.
- **Dark Mode** for macOS 10.14 "Mojave".
- **Full-screen mode** including "Spaces" support.
- **Multi-touch** rotation and scaling.
- **Force-touch** control.
- **Haptic feedback**: feel the structure you are measuring! (requires a force-touch mouse or trackpad with haptic feedback enabled).
- **Document tabs** (requires macOS 10.12 or later).
- Dedicated **Touch Bar** interface (MacBook Pro) with powerful controls for rotation, scaling, animation, structure building and measurement.
- **Quick Look** thumbnails and previews, so you can keep track of your files (and preview multi-structure file content) directly from the Finder.
- Security-compliant **sandboxed application**: works with "Gatekeeper" to help keep your Mac safe from malware and viruses.

It is worth emphasizing these points because so much scientific software is designed for other platforms and "ported" to the Mac as an afterthought. Any hapless users then have to endure poor designs, ungainly workflows and lethargic performance—and must wonder why they chose a Mac in the first place…

We believe Mac users deserve better! That's why we focus on design, workflow and performance. We build genuine *native* applications: delivering a *real* Mac experience—and thereby justifying your valuable hardware investment.

Examples of different Touch Bars available in CrystalMaker X (MacBook Pro with Touch Bar).

## Built for Windows

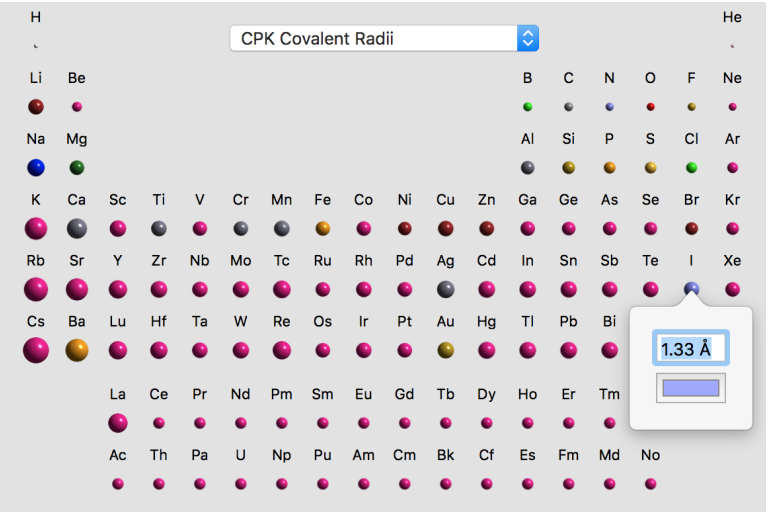
CrystalMaker is also available as a true *native* Windows program. This isn't a "port" of the Mac version, but was written, from scratch, for the latest Windows operating systems. CrystalMaker X for Windows provides:-

- Native Windows interface and system performance.
- High-resolution screen display (e.g., Microsoft Surface Pro).
- Multi-touch rotation and scaling (e.g., Microsoft Surface Pro).
- Code-signed application for extra security.

## Beautiful new interface

The program was designed to maximize your productivity, by placing controls at your fingertips, without crowding the interface. The Structures List, Output Log and Inspectors are all available in the main document window (and can be toggled open or closed). In addition, much functionality is available via popover windows, including plot range, cluster control, rotation angles, animation settings.

- Integrated document window with Structures List, Inspector, Output Log and toolbar—now with spring-loaded sidebars.
- Integrated structures library with searchable browser plus built-in viewer.
- Symmetry Explorer.
- Packing Explorer: design molecular crystals in real time.
- Vibrations Explorer: animate vibrational modes & IR spectrum.
- Preferences window with elements editor and Periodic Table display.

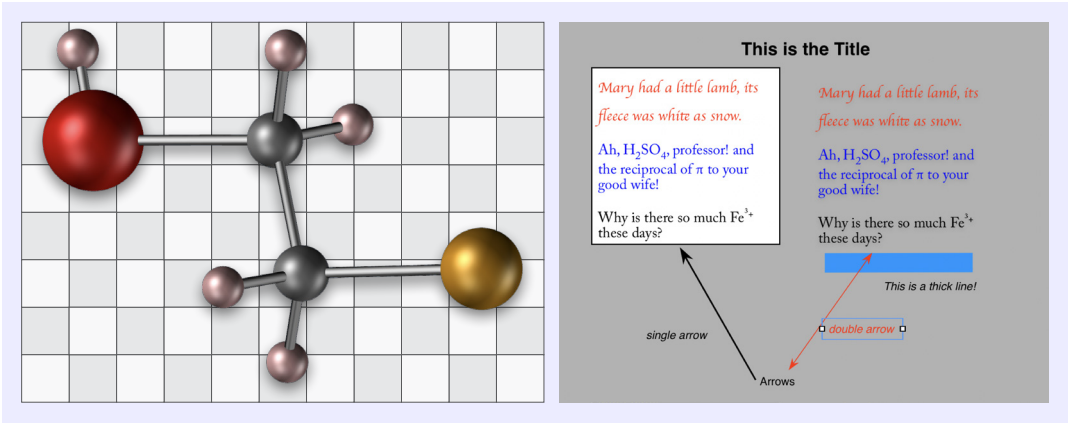



Editing element radii using the Periodic Table editor in the new Preferences panel.

## Stunning Graphics

CrystalMaker X uses an advanced new graphics engine, based on *OpenGL* but optimized to deliver class-leading rendering with unsurpassed transparency effects. Both Mac and Windows versions support high-resolution ("Retina") displays and offer flexible output options.

- **Pixel-perfect OpenGL graphics**. Complex intersections between multiple objects (e.g., spheres and planes or polyhedra) are accurately rendered.
- **Transparency done properly**. CrystalMaker X uses powerful algorithms to accurately show complex transparency and overlaps.
- **High-performance**. Take advantage of graphics acceleration on your computer's graphics card to speed rendering.
- **Customizable reflectivity** and 5 light sources. Adjust your lighting and object properties in real time, with easy slider and angle controls.
- **Rich-text annotations** with subscripts and superscripts.
- **Vector graphics output** using PDF and EPS (Mac) or WMF (Windows).
- **High-resolution output** with transparent backgrounds.




Multiple light sources create more vibrant images, which can be exported with transparent backgrounds (left). Rich-text annotation objects let you prepare figures for publication (right).

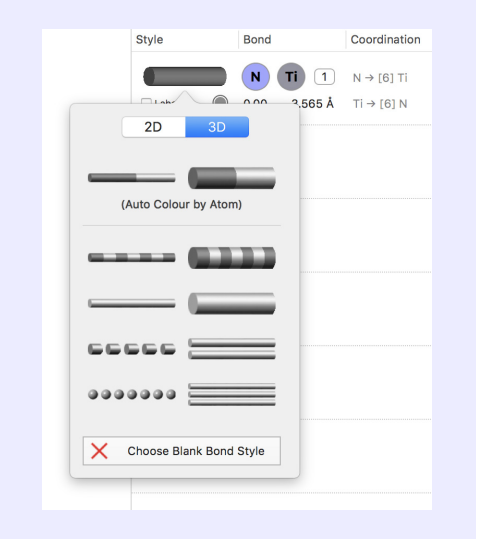
## Real-Time Editing

CrystalMaker X's integrated inspectors make structure editing a breeze.

- **Info** pane with rich-text notes plus structure info (chemical formula, symmetry, density, etc.) automatically updated as the structure is edited.
- **Atoms** inspector displays all of the atoms or structural sites, grouped by chemical element or molecule. Atom, ellipsoid or polyhedral previews are all editable and changes can be applied to multiple rows. More commands,

including auto colouring and atomic radii selection, are available from a contextual menu.

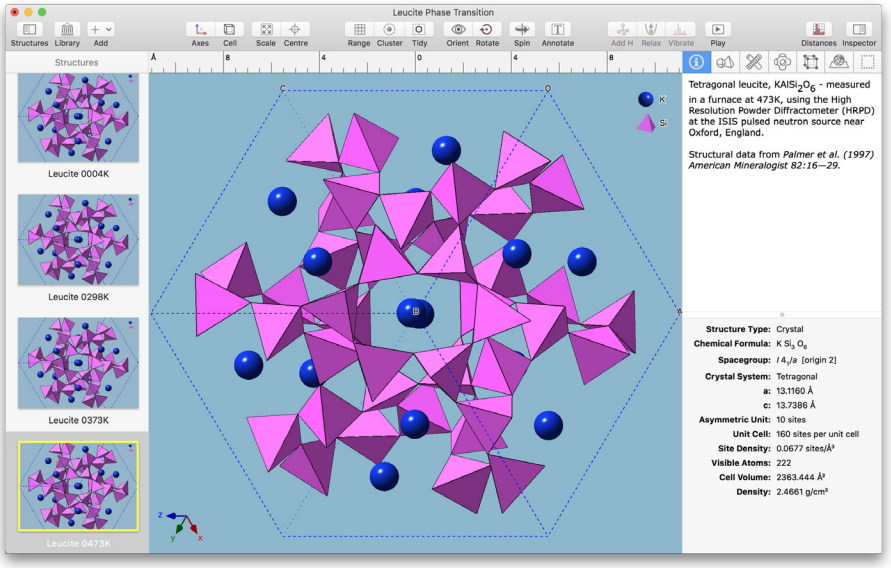
- **Bonds** Inspector combining bond specification requests with style and labelling controls, plus coordination previews.
- **Volume** Inspector lets you manage multiple sets of lattice planes (including symmetry-related planes) and volumetric datasets.
- **Model** & **Rendering** inspectors for all other aspects of a structure's display. Contextual menus in each control group let you customize your preferences, reset styles, or apply the current settings to all structures in the document.
- **Selection** inspector is displayed whenever one or more objects are selected. You can simply point and click on an object, then use the Inspector to edit the object's settings. The Inspector changes, depending on what is selected. Powerful "Actions" popup menus allow you to propagate your changes to symmetry-related atoms or bonds, isolate your selection, and much more.
- Interactive **Cluster** display. A new toolbar button provides real-time control over spherical "nanocluster" display.




Editing a bond style "on the fly" using the Bonds Inspector

## Multi-Structure Visualization

CrystalMaker X is a multi-structure application, allowing you to display unlimited numbers of structures in the same window, at the same time. The structures are listed in the Structures List: the visible structure(s) are shown with a list highlight; to make more than one structure visible, shift- or command-click on the thumbnails.



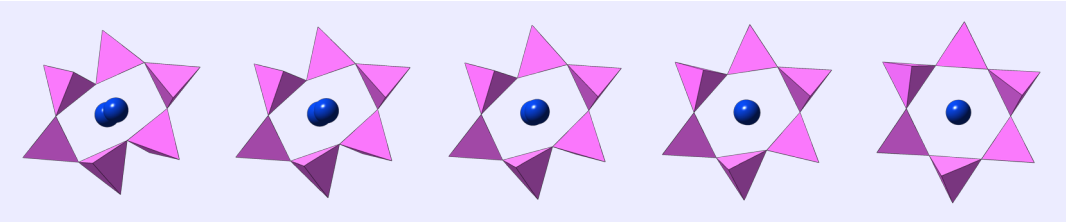

CrystalMaker X document window showing multiple structures loaded.

### Drag-and-Drop Structures Between Windows

Simply drag a thumbnail from one Structures List and drag it into the Structures List of another document.

### Synchronization with Atom-Level Control

CrystalMaker X lets you take an arbitrary selection in one structure, isolate it, and then reveal the corresponding atoms in all the other structures in your document's Structures List. This is ideal for showing how rings or channels distort with changing temperature or pressure.



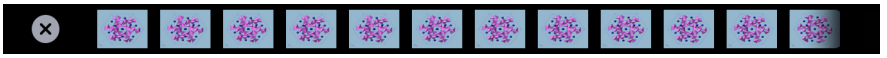
Atom-level synchronization lets you map the visible atoms in one structure (such as an arbitrary cluster) to atoms in all the other structures, thereby letting you animate the results, without having to individually hide atoms in each structure.

This is a major improvement on the old **Synchronize** command in previous versions of CrystalMaker, which could only apply the same range of fractional coordinates, and which ignored individual atom visibilities.

## Fast Animations You can Save

Unlike earlier versions of the software, CrystalMaker keeps your structures in memory, rather than having to read and write to disc. This makes it possible to use very-fast (up to 30 fps) animations. All structures are saved in the same document, together with your animation settings, letting you animate whenever you wish.

Touch Bar Animation control.



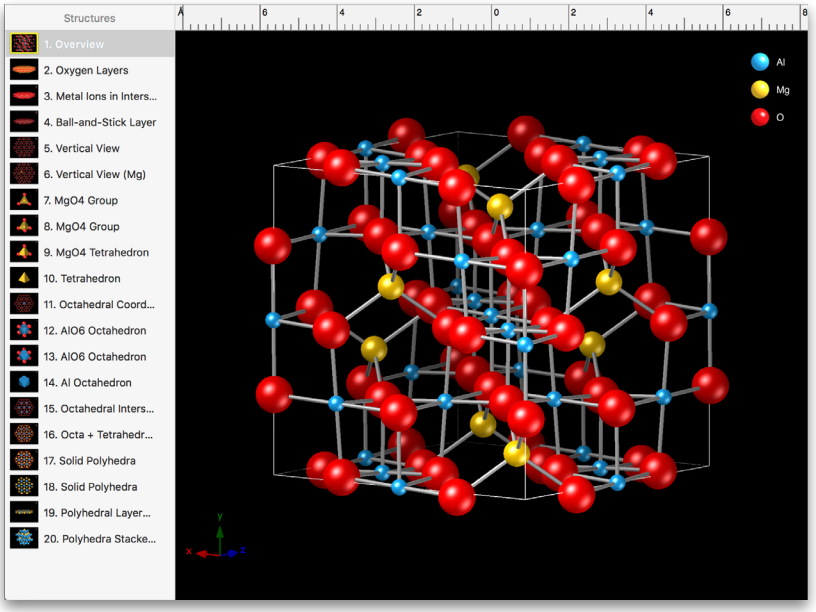
## Rotate and Scale Animations

Visualize structural changes from any direction; rescale; change your model type—all whilst animating! This is an incredibly-powerful way of understanding structural behaviour.

## Create Self-Contained Teaching Resources

Create insightful teaching resources, illustrating the building blocks for a complex structure via a sequence of related structures. These can tell a story, letting students assemble a structure from a sequence of individual units. Your job is made easier by the fact that you can select a structure thumbnail in the Structures List and duplicate it; you can then make changes to the copy, whilst preserving the original.

Including multiple structures in the same document lets you provide a self-contained teaching resource.



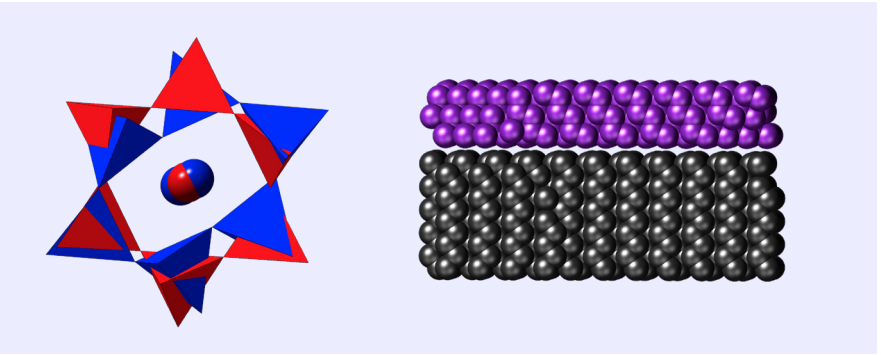

**Structural Architecture:** We include some powerful teaching resources in our Library Browser. These include guided tours of the crystal structures of an YBCO superconductor, the oxide phase spinel and the mineral quartz. Please see the folder path: Reference Library > Teaching Collection > Structural Architecture.

### Compare Structures Directly

Compare differences between two or more structures simultaeously. You can superimpose structures, then rotate the result to quickly identify differences.

### Create Interfaces

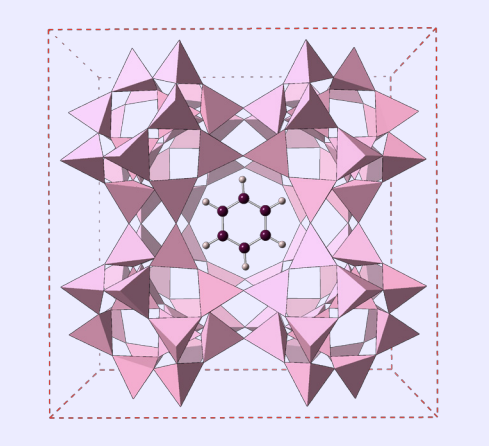
Create multi-structure *crystal* interfaces without having to merge them. Keep structures separate, so you can easily change their orientations, adjust the number of atoms, and reposition them relative to the other structures (you can lock or unlock structures to control the actions of the Rotate and Move tools).



Multi-structure displays. Left: high-(red) and low-temperature (blue) phases of leucite. Right: interface between silicon (111) in purple and (110) in grey.

### Merge Multiple Structures into a Single Molecule or Crystal

CrystalMaker X builds on the old "Place Molecule" command, but allows you to combine more than two structures, and lets you choose which of the structures will be the host. So, for example, you could place a molecule into a crystal and then have the merged result as a crystal, or a molecule.



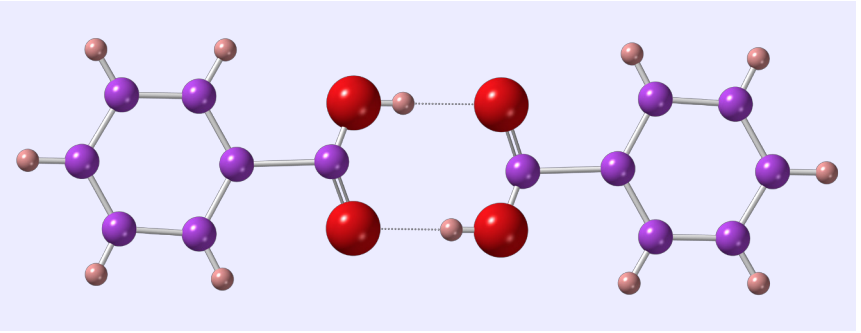
A new crystal containing a molecule, which was merged into a host crystal.

## Flexible Bonding

CrystalMaker X introduces a wider range of bond styles including double-, triple-segmented- and dotted- bonds, as well new "thin" bond styles. Bonds can also be labelled with their length—and the labels rotate with the model.

A new concept of "Secondary bonds" lets you show *inter-molecular* interactions, with primary bonds for *intra-molecular* bonding. This combination allows you to show long-range bonding, without ending up with a fully-interconnected "framework" structure; CrystalMaker ignores secondary bonds for the purposes of defining a "molecule". You can also use secondary bonds to show rotatable distance measurements.

Benzoic acid dimer showing C=O double bonds and O…H hydrogen bonds.

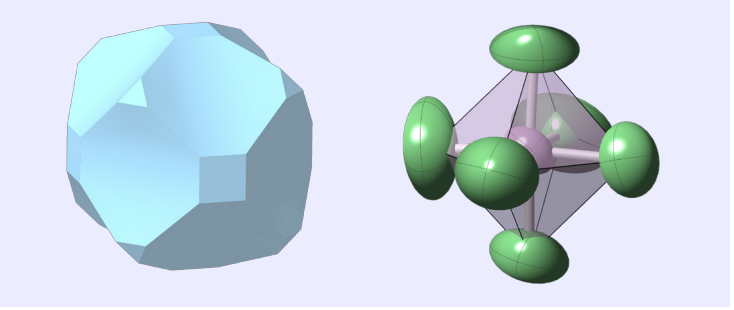


## Powerful Polyhedra

New options include concave polyhedra (with or without curved faces), displaying ellipsoids-as-vertices, opacity control and edge control. Different styles can now, for the first time, be applied to different atoms of the same site, allowing you to combine, say, ball-and-stick and rendered polyhedral representations of the same structure.

CrystalMaker offers control over polyhedral frame widths and face opacity (translucent styles). You can tweak which vertices appear in which faces, by adjusting the out-of-plane tolerance (this allows larger faces with more vertices).

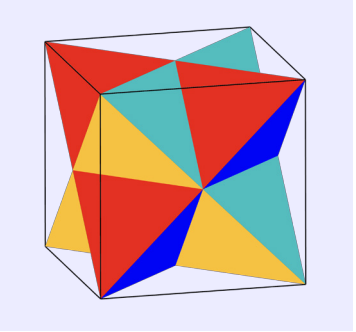
New polyhedral display options. Left: a concave polyhedron with smoothly-rendered faces. Right: A polyhedron with thick edges and vertex ellipsoids.



## Multiple Lattice Planes

CrystalMaker X allows unlimited display of multiple lattice planes in the same window. These can be separate planes, or multiple *sets* of parallel planes. Symmetry-related planes can be shown with a single menu command and you can use a pair of planes to generate a slab of crystal (which is faster than having to use the **Slice Crystal** command twice).

Multiple planes of the form {111} in a cubic crystal.



## New File Formats

CrystalMaker X can read from 15 new file formats, some of which comprise a range of flavours and may include multiple structures and/or volumetric data:-

- 3ED Volumetric
- CASTEP `Cell`
- CASTEP Volumetric (`chdiff_fmt`, `den_fmt`, `elf_fmt` formats)
- CASTEP Output (includes all frames in the trajectory)
- Gaussian CUBE Volumetric
- DEN Volumetric
- DL_POLY `Config` and `Revcon` formats (plus existing `History` import)
- GRD Volumetric
- GULP (loads input, output structures plus any volumetric data)
- RMCprofile
- SYSTRE
- VASP Volumetric (`ELK`, `CHK`, `CHGCAR`)
- VASP Trajectory (`XDATCAR`)
- Voxel file (volumetric data)
- XCrySDen (XSF) Structure File (including animated files)

CrystalMaker X can export data to 6 new file formats:-

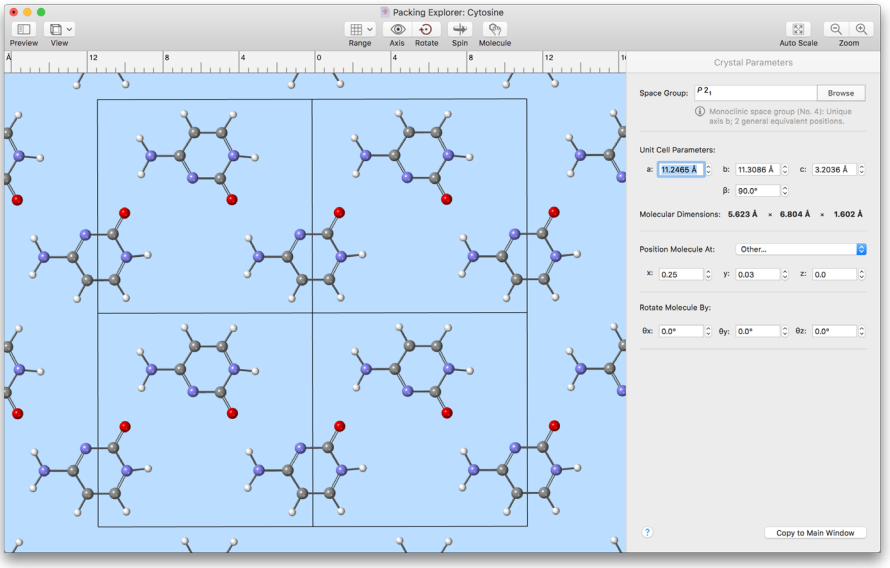
- CASTEP `Cell`
- DL_POLY `Config`
- GRD Volumetric
- RMCprofile
- VASP
- Voxel file (volumetric data)

*Note: CrystalMaker X no longer supports the obsolete MacMolecule 1.x file format.*

## Packing Explorer

Turn any molecule into a molecular crystal with the new Packing Explorer window. This interactive interface lets you explore the best way to pack your molecule or crystal fragment, with the ability to move and rotate the molecule, change its symmetry and adjust the proposed cell parameters.

- Rotatable preview: visualize packing in different orientations.
- Change model type: e.g., space-filling for packing; ball-and-stick for clarity.
- Rotate the molecule relative to the proposed unit cell.
- Edit molecular placement: move the molecule within the unit cell.
- Edit symmetry live: use the Space Group popover to browse different symmetries.

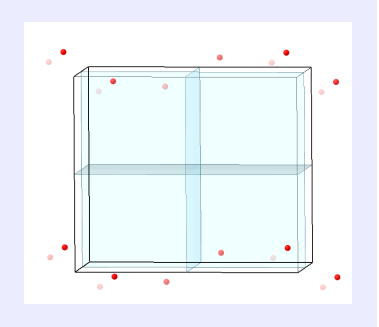



Experimenting with molecular packing using the Packing Explorer.

## Symmetry Explorer

Browse symmetry relationships in 3D: You can choose any spacegroup, or define your own symmetry elements and visualize their relationships.

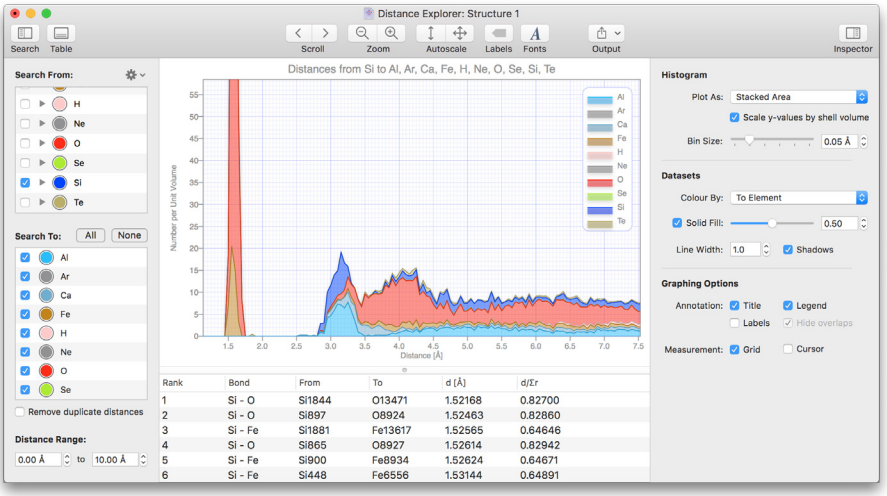
- Space group popover, with info display.
- Rotatable preview of general-equivalent positions.
- Slider controls to edit the general-equivalent position.



Visualizing a monoclinic space group with the Symmetry Explorer.

## Distance Explorer

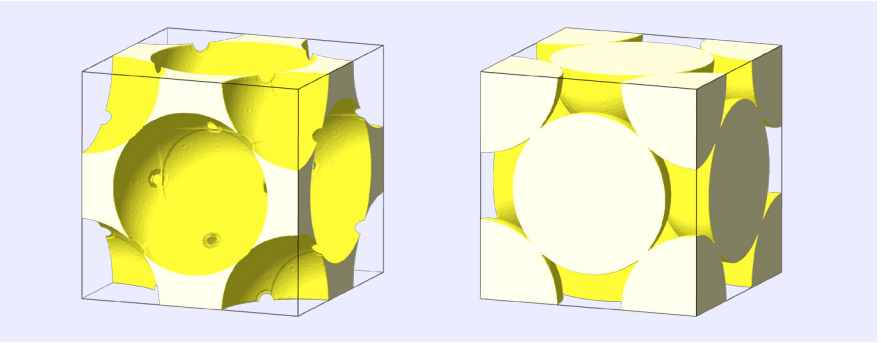
CrystalMaker lets you calculate pair-distribution relationships and visualize them in a dedicated "Distance Explorer" window. This has been given a radical overhaul in CrystalMaker X, adding multi-touch control, different graph types, and the ability to customize the display to better understand local coordination environments.



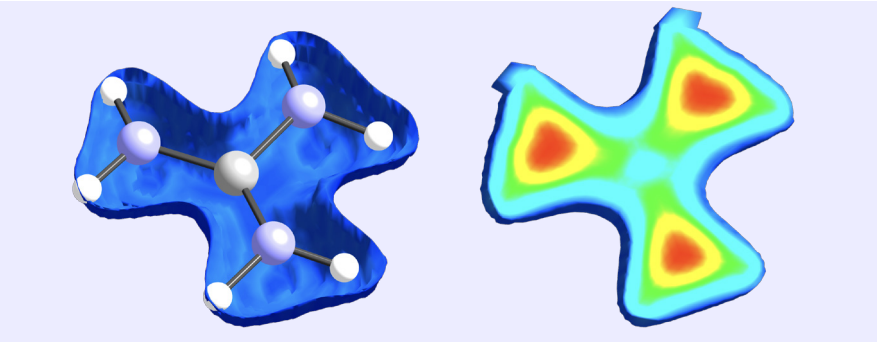

Visualizing coordination environments for silicon in a disordered material, using the Distance Explorer. The graph is coloured according to the neighbour species.

## Volumetric Data

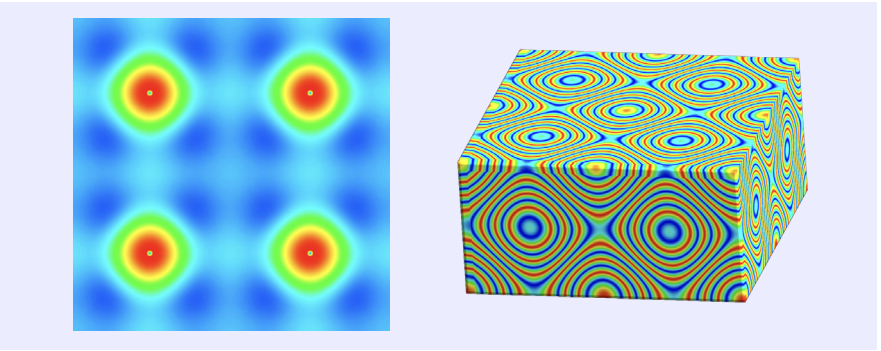
CrystalMaker lets you visualize volumetric data imported from a wide range of text data formats, or generated within the program in porosity, surface or electron density calculations. You can have multiple datasets for the same structure and combine these. Powerful visualization controls let you adjust volumetric display in real time.



Negative (void) and positive (filled) space in one unit cell of copper.



Charge density for an organic molecule: an envelope (left) and a gradient-filled volume (right).

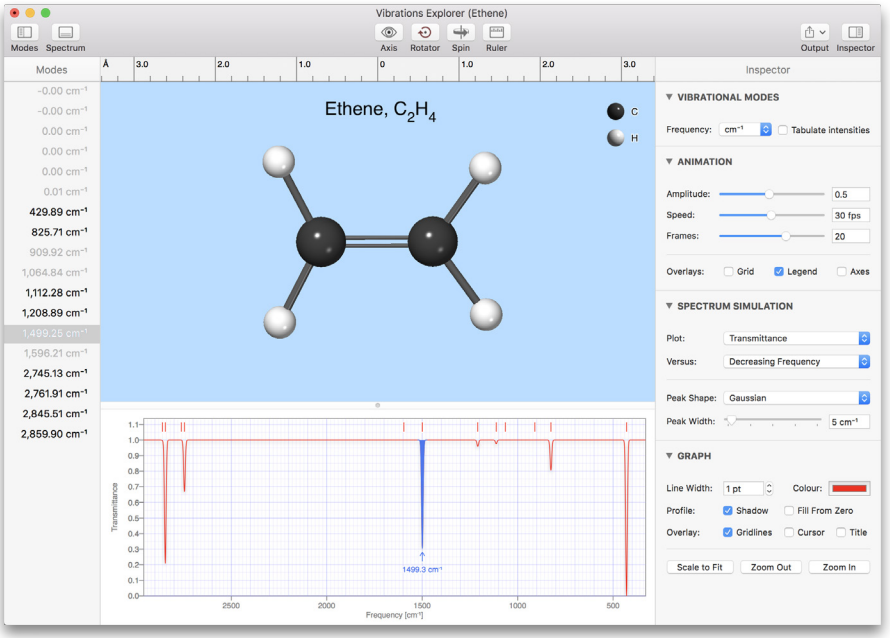


Electron density projection (left) and an isosurface (right) showing intersections with the plot range.

## New Simulation Engine

CrystalMaker X has a redesigned simulation engine for faster and more-accurate output, letting you build and relax molecular structures *and* calculate their vibrational properties.

- True energy-minimization algorithm (not just structure optimization).
- Calculate energy for any molecular structure.
- Extensive new potentials library for a wide range of bonding configurations.
- Two-stage process: Monte Carlo followed by Least Squares for greater finesse.
- Simulates vibrational modes (eigenvectors) and their frequences.
- Infra Red spectrum display.
- Visualize vibrational modes with real-time rotation and scaling.




Visualizing vibrational modes for ethene.

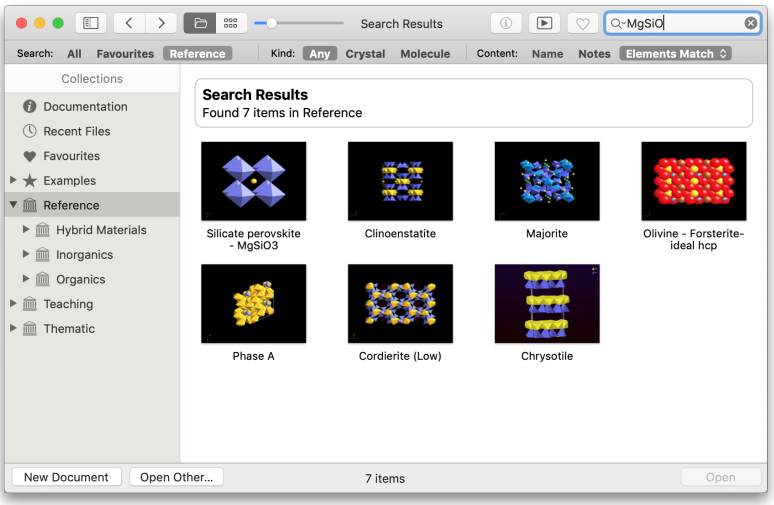
Touch Bar interface: clicking the "film strip" displays a scrubber control (bottom)

## Integrated Library

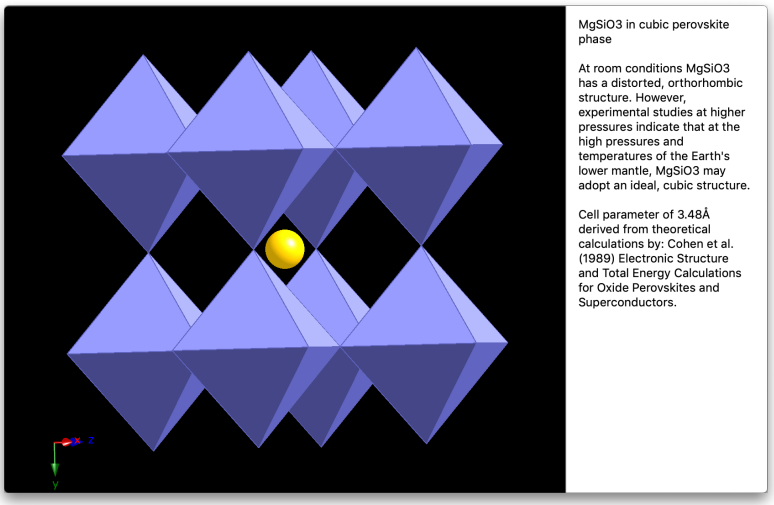
The integrated Library window lets you find structures quickly and easily, providing a single location for your recent files, favourite items, program examples—and our very-extensive reference library (approximately 1200 structures, with over 400 minerals). A powerful search command lets you quickly locate structures by title, notes or chemical formula.

Additional Teaching and Thematic collections plus an integrated "CrystalViewer" with rotatable previews and animations, make this suitable for student use or general teaching.

The Library is available as both a standalone window (via the View menu) or as a sheet window, via the toolbar's Add popup.




Searching for magnesium silicates using the Library's browser interface.




Previewing a structure using the Library's viewer mode.

## Other New Features

CrystalMaker X has many more enhancements which will become clear as soon as you start using the program. However, here are just a few to whet your appetite.

### Graphics

- **Legend.** A key to the atoms in your structure, the Legend displays all the visible sites or atoms in your structure. The Legend can have a frame and/or a translucent background. It can be dragged to different parts of the window or hidden entirely.
- **New atom styles** including "pie-chart" spheres, defect symbols & emoji styles.
- **Labelled Bond Distances**. Bond distances can now be preserved as "Distance Measurements" (which are secondary bonds, displayed with a dotted line style) with the bond distance shown alongside.
- **Colour-by-Molecule** command: in a molecular crystal, this command will apply different colours to unrelated molecules in the structure (symmetry-related molecules will have the same colour).
- **Emphasize front cell edges**. Sometimes it is difficult to infer which unit cell edges are the *front* edges, and which are the *back*. With the **Emphasize Front Edges** option in the Model Inspector, the front edges are emphasized with thicker lines than the back edges, thereby making the cell orientation clearer.
- **Coloured unit cell faces**. Whilst the unit cell is generally represented by its edges, you have the option of displaying its faces in any colour and transparency.
- **Powerful Surface Overlay**. Wrap your structure in a Space-Filling, Van-der-Waals or Solvent-Excluded surface. Adjust your "probe sphere" radius in real time and observe how the shape changes.
- **Perspective grid**. When perspective is in effect, the grid changes to show the walls of a bounding box, emphasizing how scale varies with depth.
- **Customizable Axial vectors.** The axial vectors can be repositioned in any of the screen corners, or placed in the centre of the structure. The distance from the corner of the screen to the centre (the "axial inset") can be changed and a new, "snug fit" option allows for tighter positioning within a chosen corner. The axes can be made larger, and their cones and/or labels hidden. Use the **Axes** group in the Model Inspector to choose the position. A new set of Reflectance controls also lets you change the reflectivity of the axes—for example, you can apply different material properties (China, Metal, Plastic, Rubber…) to them, or opt for a "flat" 2D appearance.

### Calculations

- **Cavity Finder.** CrystalMaker X can now calculate the positions and sizes of cavities in your structure—with the option of visualizing these using

appropriately-sized translucent spheres.

- **Distance Map.** Visualize channels and their connectivity via a colour-coded distance map. Using theVolumetric Dataset histogram/range slider, you can emphasize voids or cavities above a minimum size.
- **Calculate Molecular Centroids** command generates dummy atoms at the centres of each molecule. You can use these as proxies for the molecules in a complex molecular crystal, hiding the actual molecules and focusing on how their positions (centroids) change during the course of an animation.
- **Least-squares best-fit plane through points.** This improves on previous versions of the program and gives consistent, accurate results.
- **Best-fit line through points**. This allows you to calculate the orientation of a selected group of atoms.
- **Interpolate Structures.** Generate smooth animations by adding one or more interpolated structures to an existing sequence.
- **Rings Through Atom.** CrystalMaker can summarize all of the rings through a single, selected atom.
- **Smart "Bend Selection" command** for nanotube generation. Unlike earlier versions of the program, the bend algorithm now removes overlapping atoms where the opposite sides of the structure come together to make a cylinder.
- **Twinning.** Generate a mirror-image of the current structure—useful when trying to mimic common forms of twinning.
- **Energy**. Calculates the energy for the displayed molecule. Allows you to compare different structures.
- **Powder Diffraction Interface.** Seamlessly transfer structural information to CrystalDiffract with the option of adding new diffraction patterns to an existing window, replacing the current pattern, or working in "Live Diffraction Mode", with real-time structure/diffraction updates.

### Measurement

- **Separate Bond Angle & Torsion Angle** tools. Owing to public demand, we have reinstated the Torsion Angle Tool as a separate tool in its own right. (In CrystalMaker 9 this tool had been merged with the Bond Angle tool.)
- **Rotatable Distance & Angle Measurements.** You can now rotate and scale your structure without losing your Bond Distance, Bond Angle or Torsion Angle measurements.
- **Rollover Distance and Angle Measurements.** The Bond Distance and Bond Angle tools both now feature rollover modes, so you can take measurements simply by moving the mouse: no clicking required.
- **Width and Height of Rectangular Selection** is displayed when you click-and-

drag with the Arrow tool.

- **Atom Search**. You can search for an atom or site label in the current structure; whereupon the corresponding row of the Atoms Inspector is selected. You can also search for an individual *atom* by entering its atom number in the search field. If the atom is visible, it will be marked selected, and its properties displayed in the Selection Inspector.

### Selection

- **Ring Selection.** If one atom in a ring is selected, the remaining atoms in the ring can also be selected using the new **Extend Selection > Ring** command on the Graphics Pane's contextual menu.
- **Fragment Selection.** Similar to molecular selection, the new **Extend Selection > Fragment** command lets you select all atoms that are bonded directly or indirectly to the current selection. Unlike molecular selection, this command does not select an entire framework: selection stops at hidden atoms, thereby letting you isolate visible chunks of material without inadvertantly selecting everything on screen.
- **Selectable bonds**. Simply click on any bond with the Arrow tool and it will appear selected. The bond properties are then displayed in the Selection Inspector, for easy editing.
- **Selectable atom rows in the Atoms Inspector**. One or more rows can be selected (command-click to make a discontinous selection) in the list; you can then use the contextual menu to select the corresponding atoms on the screen.
- **Select Symmetry-Related Bonds**. The Selection Inspector lets you take any selected bond and offers the option of selecting all *symmetry-related* bonds.

### Usability

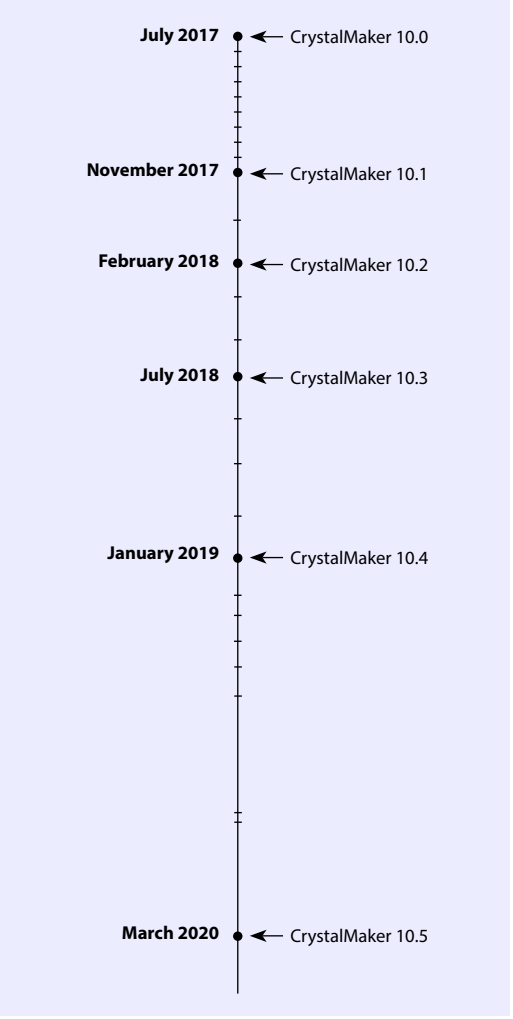
- **Hide Minimally-Bonded Atoms.** This new command on the **Transform > Atom Range** submenu lets you quickly tidy up a complex structure by hiding all atoms with fewer than 2 bonds. This should be ideal for molecular-organic frameworks.
- **Trim to Selection.** This new command on the **Transform > Atom Range** submenu helps speed up the program by reducing the physical atom range—atoms which are carried in memory regardless of their visibility—to a block that just encompasses the current selection.
- **Add Title command:** You can have a structure's name automatically displayed as a new annotation object, using this command from the **Model** menu. The title is displayed in one of six positions in the graphics pane (which you can customize using the Preferences panel). Holding down the **shift** key adds titles to add structures in the Structures List: invaluable when working with many frames from a simulation or strucure sequence.

- **Add Atom Tool with Live Distance Display.** Holding down the **shift** key when using the Add Atom tool displays a labelled preview of the bond to be inserted between the last-clicked atom to the current mouse position.
- **Flexible Range Generation**: specify whatever range limits you require, without them being reset (earlier versions of the software required all range limits to start at the origin, resetting negative values; the new program has no such limitations).
- **Preserve Molecular Coordinates as you Rotate**. CrystalMaker provides both screen coordinates *and* your original (orthogonal) molecular coordinates.
- **Edit Position and Size of Annotations** by entering numeric values in the Selection Inspector.
- **Create Bonds with the Distance Tool.** When measuring bond distances, a popup window allows creation of a bond using the Distance Tool; holding down the shift key allows a new bond *specification* to be generated, allowing automatic generation of similar bonds throughout the structure.
- **Edit Atom or Site Labels** directly in the Atoms Inspector, without having to use the Crystal or Molecule editors.
- **Edit Bond Specifications from a Selected Bond**. You can edit the properties of any selected bond (in the Selection Inspector) and then apply your changes to all bonds which share the same bond specification. Alternatively, you can select a bond and use the Selection Inspector's **Show in Bonds Inspector** command to go directly to the corresponding bond specification.
- **Specify default anion and cation polyhedral styles.** Unlike earlier versions of the program, you can now specify separate preferred polyhedral styles for both anions and cations. This avoids difficulties with dense structures, such as orthosilicates, where oxygen is highly coordinated and a default polyhedral display might show inter-penetrating oxygen-centred *and* metal-centred polyhedra.

## CrystalMaker X Updates

CrystalMaker X was released in July 2017. Since that date there have been numerous incremental updates, plus a number of major releases, with significant functionality, as summarized in a timeline below:-

CrystalMaker version timeline. Minor updates are indicated by the tickmarks.




These major "*.y*" updates as well as the minor "*.y.z*" updates were provided as free updates to licensed CrystalMaker X customers.

Chapter 2

# Getting Started

CrystalMaker is a professional application available for Mac and Windows computers, with extensive support options and examples files. This chapter provides a brief introduction to the software, including system requirements, installation, and licensing.

> **A Note about the Demo Version**
>
> This User's Guide is designed for the *Full-Feature* version of CrystalMaker.
>
> If you are using the free, *Demonstration Version*, some features may not be available: this version is designed to give you a *flavour* of the full program, but you cannot save files, record program settings, or specify preferences.

## Using this Guide

This User's Guide should provide a very comprehensive outline of the major program features. We don't expect you to read it from cover-to-cover, but would recommend the following key sections:

- **All users** should browse *Chapter 4: Document Window*. This is designed to provide a quick orientation to the program; the interface changes from version to version, and will certainly be different to other programs you may have used, so it's important to get your bearings earlier, rather than later!
- **If you are a new user**, we *strongly* recommend that you watch the **Quick Tour** video (and ideally the **Video Tutorials**), then complete the **Self-Guided Tutorials** (all available from the program's **Help** menu, and also from the Library's **Documentation** collection). These are designed to get you up-to-speed very quickly, so you can *maximise your productivity*. They should address most of the queries that you might have when using the software.

The User's Guide describes the program interface, followed by sections on how to build crystal and molecular structures, then describing display and manipulation, before finishing with how to get data *out* of the program: exporting data, graphics and video.

### Searching for Topics

We have tried to provide a comprehensive yet logically-structured guide. If you need to find specific information, here are some suggestions:

- This guide includes a *Table of Contents* (at the beginning) and an *Index* (at the end).
- If you are viewing the guide electronically, you can click on the *Contents* or *Index* page entries to go directly to the corresponding pages.
- If you need to search for a keyword or phrase, you should be able to use the **Search** command in a PDF viewer such as Adobe (Acrobat) Reader or Apple Preview.

**Use the Tips:** Throughout this guide you will find little yellow boxes, like this one. These are designed to offer advice, to help you use the program more effectively.

**More Depth**

You will also find blue boxes, like this one. These offer greater depth and insight into using the program. You can skip these if you're only looking for quick answers, but they may be useful for understanding a bit more about the background behind certain topics and design choices.

## Interface Reference Convention

In the following chapters we refer to elements of the program's interface (such as button names, menu commands and keys on your keyboard) using **this font**.

You will also encounter many references to menu commands written in an abbreviated manner, such as "**Edit > Copy**", which means "from the **Edit** menu choose the **Copy** command".

### Mac & Windows Shortcut Keys

Mac and Windows operating systems use different key combinations for menu shortcuts ("accelerator keys"). In this guide we make repeated reference to **command** and **option** keys, which are included on the standard Mac keyboard Windows users should use the following translation:

| Mac | Windows |
|---|---|
| **command** | **control** |
| **option** | **alt** |

## System Requirements

CrystalMaker is a modern 64-bit object-orientated application, designed to take full advantage of modern operating systems and hardware. The Mac and Windows versions are *separate applications*, written from scratch, for their respective operating systems, using only the official development frameworks from Apple and Microsoft. This guarantees optimum performance and the best-possible user experience.

### Mac

CrystalMaker for Mac is a state-of-the-art 64-bit multi-processor *native* application, written in Objective-C and using Apple's own "Cocoa" framework. It is designed to take full advantage of recent Mac hardware and supports key Mac technologies including:-

- Retina graphics
- Multi-touch (rotation and zooming)
- Force-touch (previews)
- Haptic feedback ("feel your structure as you measure it")
- Dark Mode
- Touch Bar interface (MacBook Pro)
- Full-screen mode and "Spaces"
- Quick-Look previews
- Finder thumbnails
- QuickTime video
- Apple Help (with search)
- Code-signed, sandboxed application (to keep your Mac safe)

To run CrystalMaker for Mac you will require:-

- 64-bit Intel-based Mac
- MacOS X 10.10 "Yosemite" (not recommended), 10.11 "El Capitan" , 10.12 "Sierra", macOS 10.13 "High Sierra", 10.14 "Mojave" or 10.15 "Catalina".

We strongly recommend using the very-latest operating system, as this offers major enhancements—including system-level bug fixes—as well as support for the latest hardware. Note that CrystalMaker for Mac is a workstation-class application, so for best results your hardware should be commensurate with this; in particular, we recommend having a discrete video card (although this is not essential).

## Windows

CrystalMaker for Windows is a native 64-bit program, written in C# and using Microsoft's `.NET` framework. It is designed for modern operating systems and features:-

- Microsoft installer
- Native Windows interface
- High-DPI graphics (e.g., Surface Pro)
- Multi-touch rotation and scaling (e.g., touch-sensitive displays)

The program requires:-

- 64-bit system.
- Video card with OpenGL 3.3 for later
- Windows 7 (Service Pack 1), Windows 8 or **Windows 10** (recommended).
- **.NET** Framework 4.6 for later

We *strongly recommend* that you keep your computer operating system up-to-date (i.e., Mac users should be using macOS *Mojave* or later; Windows users should be using 64-bit Windows 10). We reserve the right to remove support for older operating systems as time progresses.

**Please Update Your Graphics Card Drivers!**

CrystalMaker X for Windows features very-high performance 3D graphics which are designed to take full advantage of the advanced video acceleration capabilities of modern graphics cards. Following the release of Windows 10, it is imperative that you update your graphics card driver to ensure full compatibility!

We are aware of numerous bugs in older graphics drivers, which result in serious display issues. These are NOT CrystalMaker bugs, but are caused by outdated graphics drivers that are incompatible with Windows 10.

Please note that your graphics card drivers will NOT be automatically updated as part of the standard Windows Update mechanism, as they are from third parties, not Microsoft.

Even if your computer claims to have up-to-date drivers, this is unlikely to be the case. Please visit your graphics card vendor's website to download and install the latest drivers.

# Installation

Mac and Windows versions have different installation procedures: Mac users can simply drag-and-drop files, whereas Windows users will need to run an installer program.

## Mac Installation

This a simple matter of dragging-and-dropping the downloaded CrystalMaker application to your *Applications* folder. As a modern Mac application, CrystalMaker includes all its resources (including examples and library files, online help and this User's Guide), neatly packaged within the application "bundle".

## Windows Installation

Windows users will need to run the installer program. This gives the option of installing the essential program files (application, online help, user's guide), plus supporting resources (examples files).

### Licensing your Installation

The first time you launch CrystalMaker you are prompted to personalize your copy of the program. This process also creates a preferences file.

**Do not forget to updated your graphics card drivers** (as per the warning on the previous page).

### Registering Your Licence

It is very important that your licence is registered as we can only provide technical support (and upgrades) to registered users. You can register when you install the software, by clicking the **Register** button in the reminder dialog that appears following your installation. Alternatively, you can register later, by choosing the **Help > Register CrystalDiffract** command.

> **Multi-User Licence Registration**
>
> We only require one registration per licence. So, if you have a multi-user licence, such as a Group or Site Licence, only the official "keeper" of the licence needs to register with us. Once we have received that registration, the other users are entitled to receive technical support, within the terms of the specific licence.

## Diffraction Support

CrystalMaker X is designed to work seamlessly with **SingleCrystal 3** or later: an award-winning program for simulating X-ray, neutron and electron diffraction patterns from single crystals. The program includes synchronized structure/diffraction rotation with CrystalMaker, as well as auto-indexing of observed patterns (e.g., transmission electron diffraction patterns).

CrystalMaker X is also designed to work seamlessly with **CrystalDiffract 6.8** with a "Live Diffraction Mode" where you can edit your structure in CrystalMaker (e.g., moving or rotating groups of atoms) and see the corresponding powder pattern update in near real time. You can also add, update or replace existing powder patterns directly from CrystalMaker.

CrystalDiffract can perform multi-structure powder diffraction simulations with real-time parameter control, lets you visualize and measure observed data, in comparison with ideal, simulated data.

For more information, please visit http://crystalmaker.com, where you can download free Demo versions of these two programs.

**Warning:** CrystalMaker X requires SingleCrystal version 3.0 or later and CrystalDiffract 6.8 or later. Earlier versions of the programs will not work as they do not understand the new 64-bit CMDX document file format.

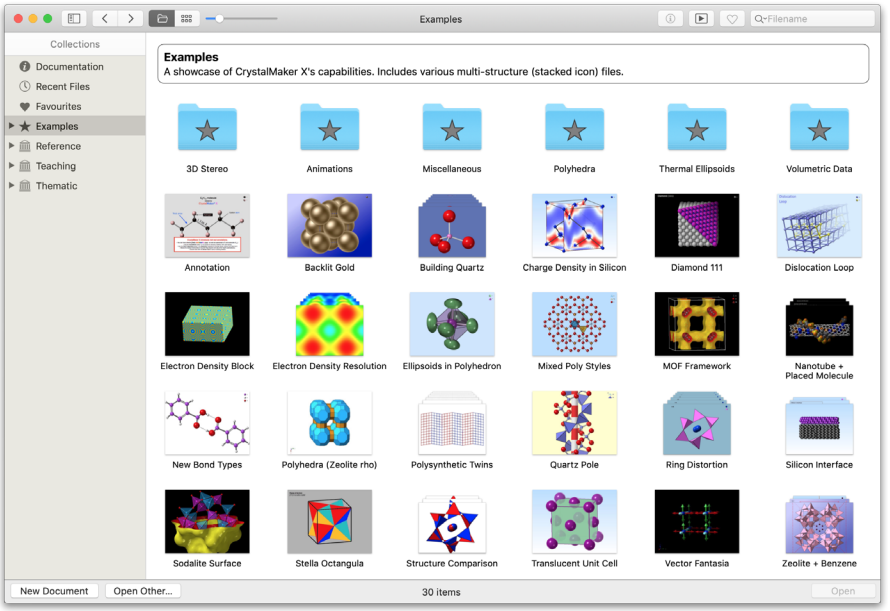
Chapter 3

# Structures Library

Whilst you can build or visualize any of your own structures in CrystalMaker, the program also includes structures of its own: presented in an integrated Library window. This is shown the first time you launch the program, and can be used as a "springboard" to let you rapidly open structures without having to search for them via your operating system.

## Library Organisation

In its default, "browser" state, the Library window is divided into two vertical panes: a Collections list, on the left, which lets you explore a hierarchy of folders; and an "icon view" on the right which shows the contents of the selected folder.




The Library window, showing a browser interface with a selection of Examples files.

## Library Collections

It is important to emphasize that the Library is not just another "database". Instead, it combines the best aspects of a "photo album"—letting you add your own "Favourite" structures, catalogue and search them—with a curated exhibition of carefully-chosen (and generally high-quality) structures, ready for instant display. By combining reference, teaching, thematic—and your own structures—in the same interface, you have a convenient portal for browsing a wide range of materials for use in both teaching and research.

The Library is subdivided into seven major groups, or (to pursue a bibliographical analogy) "collections" :-

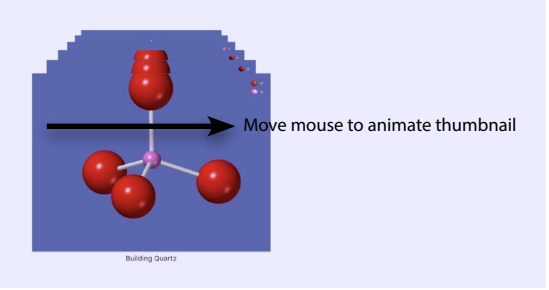
- **Documentation:** quick links to the PDF versions of the user's guide and tutorial, the online help system, our extensive online video tours and tutorials, software updates and help request form.
- **Recent Files:** includes recently-opened documents (as registered by your operating system).
- **Favourites:** this is your part of the library, where you can add your own documents and organise these into folders.
- **Examples:** a showcase designed to illustrate features of the program.
- **Reference:** a complete set of structures designed for searching and browsing. Some 1,200 files are found here, including over 400 minerals—many being multi-structure documents with different views or models of the same material, designed to improve understanding.
- **Teaching:** a collection of structures designed for use in teaching, including:
  - Atomic Radii (periodic tables with atomic, ionic, covalent radii);
  - Basic Structure Types (crystal-chemical "type structures");
  - Crystalline Elements (crystal structures of the elements);
  - Lattice Types;
  - Structural Architecture (animations of important structures);
  - Polyhedra.
- **Thematic:** structures related to specific themes, such as "Battery Materials", "Food Chemistry" and "Medicines".

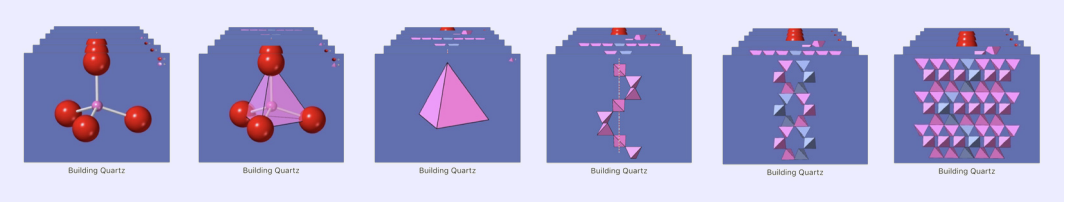
Note that the Thematic and Teaching collections essentially duplicate structures from the Reference collection. Therefore, when searching for a structure, you generally only need to search the Reference collection.

## Icon View

The icon view on the right is just like a Mac Finder window, or a Windows document explorer window: it contains thumbnails to represent files (documents) and folders. Notice that two sorts of thumbnail are shown: a single-picture thumbnail, and an "image stack". The latter relates to a multi-structure document. You can animate an image stack by moving the mouse pointer from left to right across the stack; the individual "frames" in the stack will then be shown.

A multi-structure document thumbnail, shown as an "image stack".




Animating the "Building Quartz" thumbnail, showing the individual structures within this multi-structure document.

### To Change Thumbnail Size:

Do one of the following:

- Use an "expand" or "pinch" gesture on your multi-touch trackpad.
- Click-and-drag the slider control in the window toolbar.

### To open a file from the Library

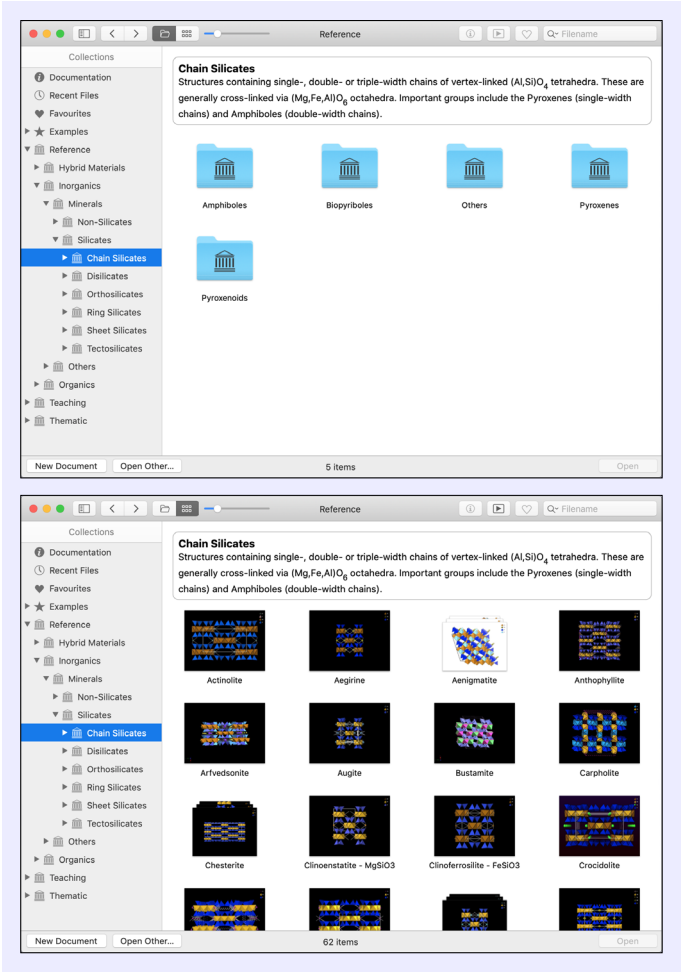
Do one of the following:

- Double-click a file thumbnail.
- Select one or more thumbnails (shift- or command-click for a multiple selection), then click the **Open Selection** button on the bottom right-hand corner of the window.

**Rotatable Previews:** The Library includes rotatable previews for all structures files, which can be animated and zoomed to full-screen size. The dedicated "CrystalViewer" mode is described later in this chapter.

### Displaying a Flat View

You have the option of displaying either a folder view (i.e., all folders and files in a given directory) *or* a "flat" view, showing all contents of all folders *and* their sub-folders, that are contained within the current directory (which saves having to traverse the folder hierarchy). To toggle between the views, click the selector button ( ) in the window toolbar.



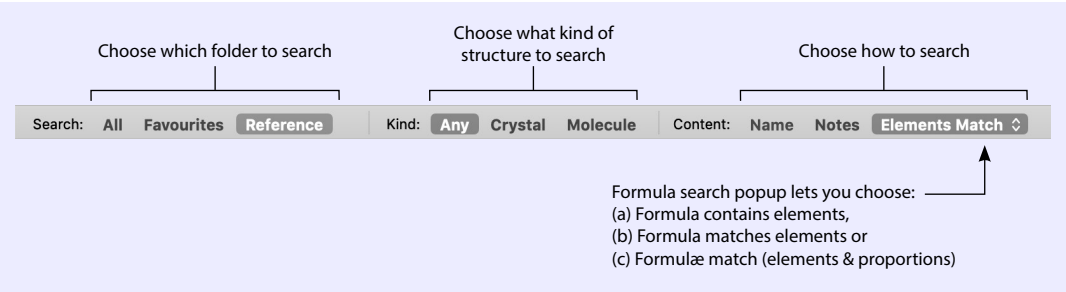

The Library window in "Folder View" (top) and "Flat View" (bottom).

## Auto Show and Hide

By default, the Library window is set to hide itself whenever a document window is opened in CrystalMaker; closing the last document window causes the Library window to reappear, so you can resume browsing. You can use the program's **Preferences** panel to customize this behaviour.

## Searching for a Structure

CrystalMaker X provides a handy search command for quickly locating documents that match your search criteria. A search *Scope Bar*, lets you customize your search location, search kind and exact content to be searched. The default search location is the *Reference* collection, but you can change this by specifying the current folder, your Favourites folder, or all folders. You can opt to search for just crystals, molecules or both.



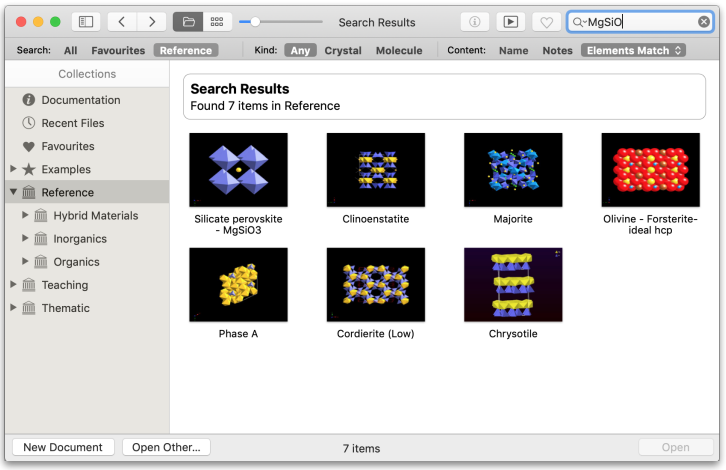

The Search Scope Bar, requesting an elements-match search for any crystals or molecules in the "Reference" collection.

You can use the Scope Bar to specify one of the five different search types:

- By filename
- By notes
- Formula *contains* elements (e.g., "SiO" would yield $SiO_2$ *and* $KAlSi_2O_6$)
- Formula *matches* elements (e.g., "SiO" would yield $SiO_2$ but *not* $KAlSi_2O_6$)
- Exact formula match (e.g., "Fe2O3" would yield hæmatite but *not* magnetite, which has a different element ratio, $Fe_3O_4$)

Placeholder text in the **Search** field indicates which search method is active.

Searching for all magnesium silicate phases in the Reference collection. The search type here is "Formula Matches Elements".



### To perform a search:

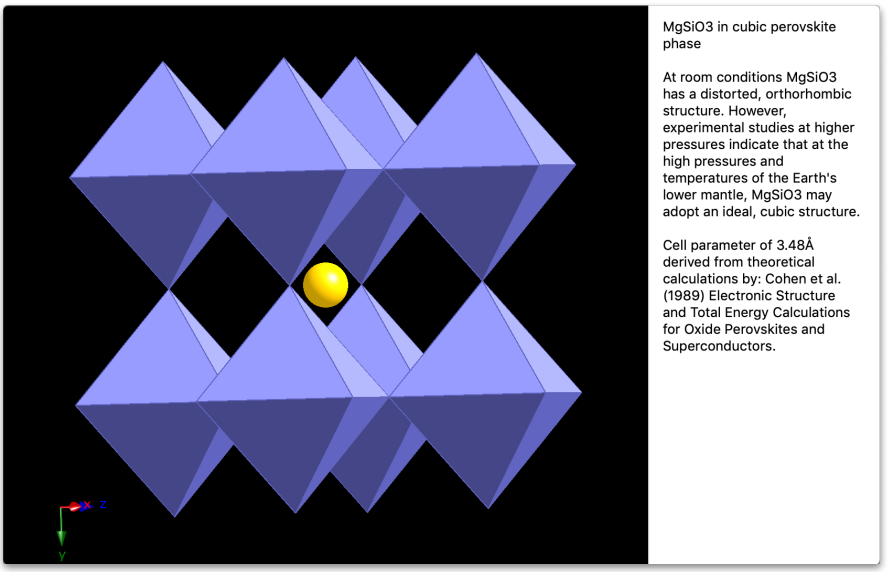
1. Type your search text in the search field (if searching by formula, use correct capitalization, or leave spaces between symbols, i.e., "`Al2O3`" or "`al2 o3`").
2. If necessary, use the Scope Bar to modify your search requirements.

### To clear search results:

- Click the close box (grey circle with a white "X") on the right-hand side of the **Search** field.

## CrystalViewer

To find out more about a file—without actually opening it in the main program—you can preview its structure(s) and notes, using an integrated Viewer mode. This lets you view a rotatable structure, without the complexity of the usual CrystalMaker interface, and might be useful for introductory teaching.




Previewing a structure in the Library's Viewer mode. The browser interface is replaced by a rotatable structural model and its notes.

### To show the viewer:

Do one of the following:

- To temporarily show the Viewer whilst the mouse or trackpad is held down, Mac users can **Force-Click** a thumbnail (N.B., requires a Force-Touch trackpad with the "Force Click and Haptic Feedback" options enabled). On releasing the pressure, the viewer is hidden and one returns to the browser interface.
- Move the mouse pointer over a thumbnail so that an Info button ( ⓘ ) appears in its top right-hand corner; click this button to enter Viewer mode.

- Select a thumbnail by clicking on it with the mouse, then click the Info button in the window's toolbar.

### To exit the Viewer:

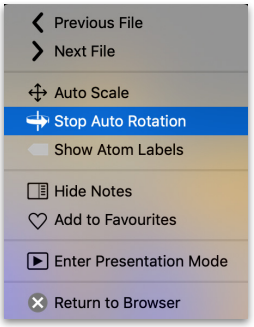
Do one of the following:

- Press the **escape** key on your keyboard.
- Move the mouse to the top of the Viewer, so that the close box (grey "X" icon) appears, and click this.
- Right-click to display the contextual menu, then choose: **Return to Browser**.

### Working with the Viewer

If the selected file is a multi-structure file, it will be animated using its saved settings; otherwise the structure will be auto rotated (you can disable auto-rotation using the **Stop Auto Rotation** command on the viewer's contextual menu, as illustrated below).

The Viewer's contextual menu.

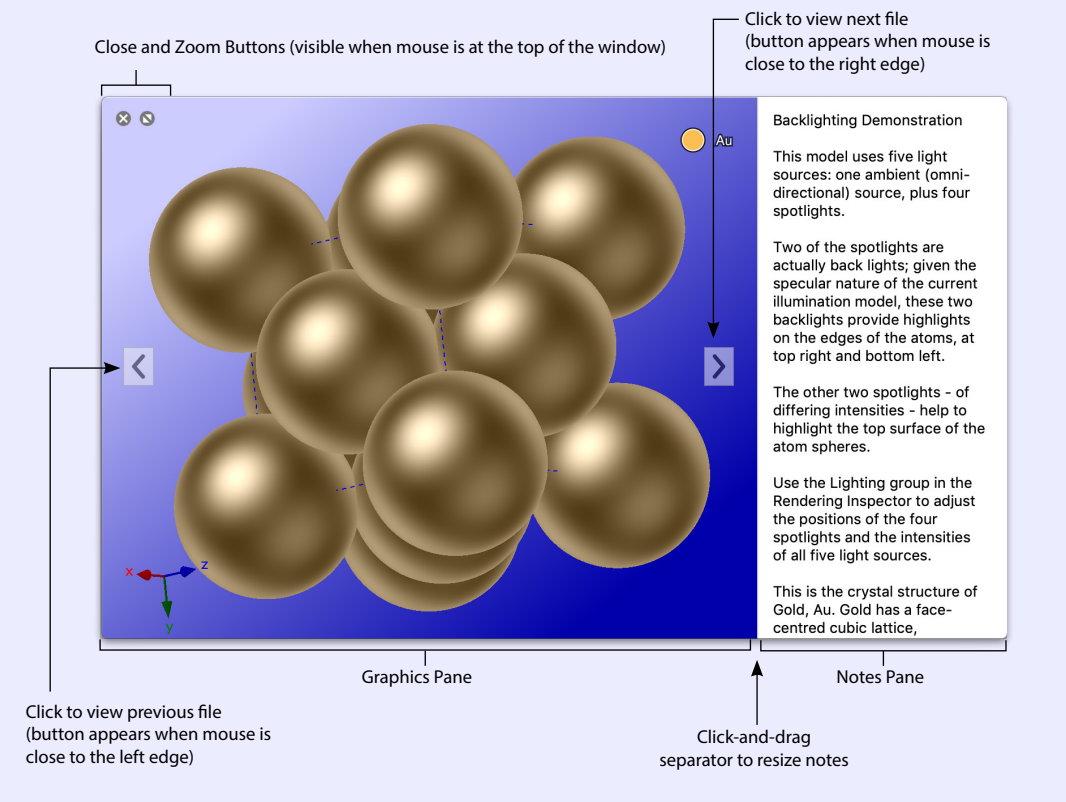



You can manipulate a structure in the Viewer using CrystalMaker's standard operations:-

- Click-and-drag with the mouse to rotate (hold down the **shift** key down to rotate about an axis out of the screen—or use a trackpad rotate gesture).
- Use pinch or expand gestures to change the scale (use the contextual menu to auto scale).

You can also use the Viewer to browse through all structures in the browser's icon view. The easiest way to do this is to move the mouse to the left- or right-hand sides of the Graphics area, whence an arrow button will appear; clicking the arrow moves onto the next or previous files.

The Viewer can be resized (this also resizes the Library's browser interface) and zoomed to full-screen, using the (normally-hidden) zoom button towards the top-left corner of the window. Note that, for clarity, the window's close and zoom buttons are hidden until the mouse is moved towards the top of the window.

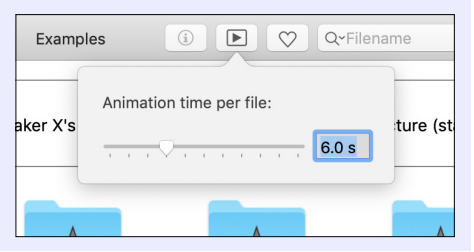



Anatomy of the CrystalViewer interface. For clarity, the Previous/Next buttons and the close/zoom buttons are hidden until the mouse moves into the appropriate part of the window.

## Presentation Mode

The **Play** button in the browser's toolbar lets you enter a special, full-screen, "Presentation Mode". Here, each file (whose thumbnail appears in the browser's icon view) is shown in turn; multi-structure files are animated; single-structure files are simply rotated.

You can customize the presentation options by clicking-and-holding down the mouse on the Play button, which causes a popover to appear, with a slider to adjust the presentation time per file.




Customizing the Presentation Mode by clicking-and-holding the Play button until the popover appears.

## Cataloguing Your Structures

The Library Browser isn't just about reference materials (useful though that may be). Any recently-opened documents can be browsed in the Recent Files collection). You can also add your own structures directly to the Library, using the Favourites collection.

### To Add Structures to the Library:

1. Click the **Favourites** collection, in the library's Sidebar ("Collections" list). If the Sidebar isn't visible, click the Sidebar icon in the Library window's toolbar.
2. Drag-and-drop any structures files and/or folders into the Favourites' icon view pane. Thumbnails will now appear as CrystalMaker starts to catalogue your structures. They will then become searchable.

**Favourites Button.** You can add any file in the Library to your Favourites: simply select the thumbnail and click the Favourite button in the window toolbar.

### To Rearrange Favourites:

You can rearrange your "Favourites" simply by dragging icons into folders (or into different locations in the Sidebar). Note that all your files *must* be located within the *Favourites* collection; you cannot move files into, say, the Reference collection.

### To organise documents into a folder:

1. Shift-click on the documents you wish to select.
2. Right-click and choose: **New Folder with Selection** from the contextual menu.

### To Remove Favourites:

Do one of the following:

- Drag the items from the Favourites' icon view, out of the Library window.
- Right-click and choose: **Remove Selected Items**.

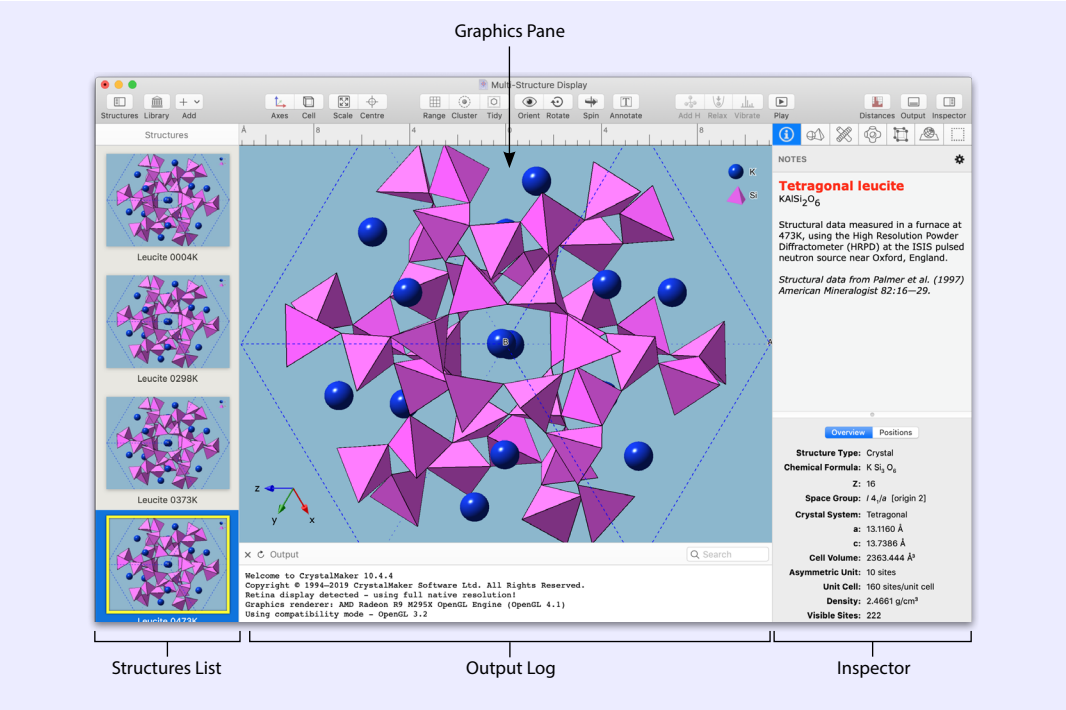
Chapter 4

# Document Window

CrystalMaker X has a very-rich user interface with most of the controls you will need to use located right around your structure, in the same document window. This chapter describes the layout and design of this window and how you can use sidebars to work with multiple structures, design interfaces and create animations.

## Document Overview

The document window is divided into four panes: a Structures List on the left, a Graphics Pane with an Output Log underneath (by default), and a tabbed Inspector pane on the right-hand side.

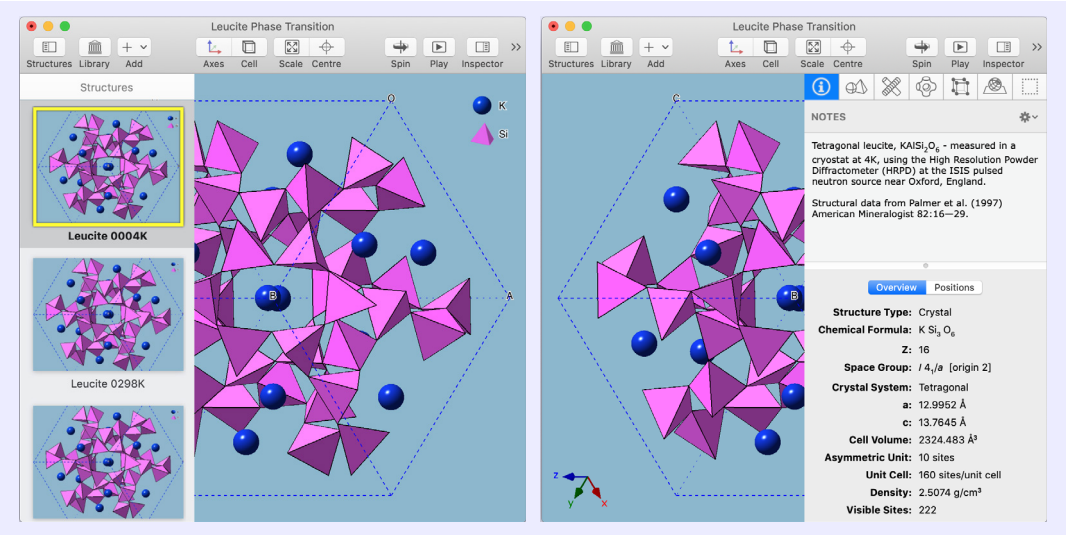



Document window, in "horizontal layout", showing the Structures List, Graphics Pane, Log and Inspector.

Unless a document has been saved with multiple structures, the Structures List will normally be hidden, as is usually the Output Log. You can open and close all the various "Utility" panes (Structures List, Output Log, Inspector) and your settings will be saved with the document, together with the window size and position. The document window also includes a toolbar, which can be customized in the usual way (e.g., right-click in the toolbar and choose: **Customize Toolbar…**).

## Sliding Sidebars

As an alternative to keeping the various sidebars open, you can instead have them slide into view only when required: simply move the mouse towards the appropriate edge of the window and pause until the sidebar slides into view.




Sliding Sidebars in Action: Users with small screens can opt to work without any sidebars visible; moving the mouse towards the left of the window causes the Structures List to slide into view (left); moving the mouse towards the right of the window causes the Inspector to slide into view (right). Moving the mouse outside a sliding sidebar and back over the structure causes the sidebar to slide back out of view.

**Haptic Feedback.** Mac users with force-touch trackpads (and with "Haptic Feedback" enabled in the Trackpad pane of their System Preferences panel) will feel a slight vibration or "buzz" as they pass over the "trigger point".

For example, to show the Structures List you would move the mouse towards the left-hand side of the Graphics window and hover; beyond a certain "trigger point" (about 15 pixels from the edge) the Structures List will then slide into view, over the Graphics pane. Moving the mouse back over the structure (and outside the sidebar) will cause the sidebar to slide back, out of view.

### Organising Document Windows

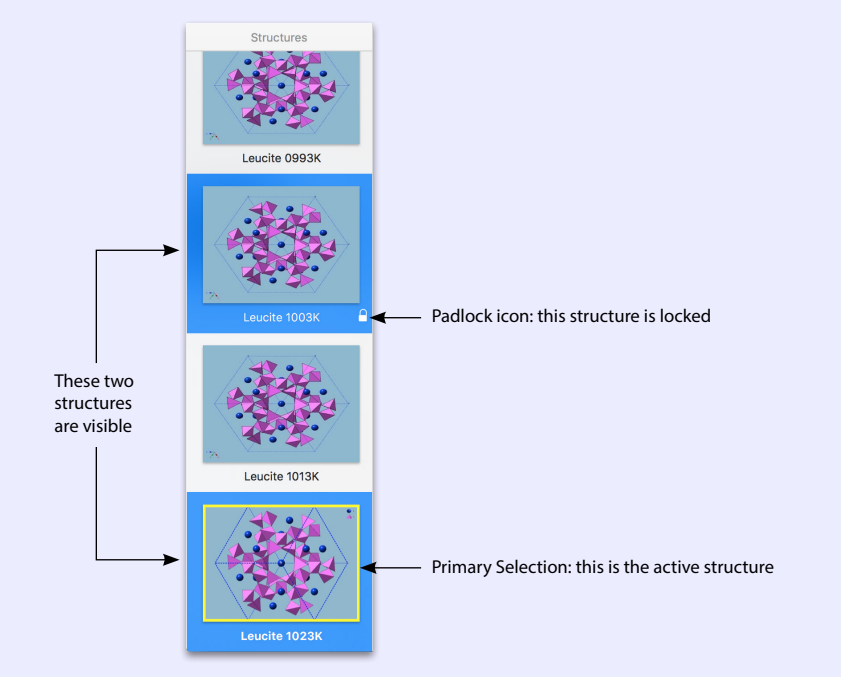
CrystalMaker's Window menu includes commands to neatly **Tile** or **Stack** multiple windows on the same screen (on the Mac, these commands relate to the *active space*).

Mac users running macOS 10.12 "Sierra" and later can collapse multiple document windows into a single, tabbed window ("document tabs"). This can be useful for reducing clutter, although having separate windows allows you to compare their contents and drag structures from one window to another.

## Structures List

The Structures List shows all structures that are saved with the document, each with its own thumbnail image which is updated as the structure is changed. You can use the list to switch between the different structure(s) to be displayed, to rearrange their order, lock one or more structures (to prevent it from being rotated) or to copy a structure into a different window.

Structures List in "thumbnail mode", showing two visible structures, one of which is locked.




### Primary Selection

CrystalMaker lets you select multiple thumbnails to display their structures simultaneously, but there is only one *primary selection*: this is the thumbnail highlighted in yellow. The primary selection is the *active* structure, whose

properties are displayed in the Inspector, on the right-hand side of the screen. You can only ever have one *primary selection*, but you can still rotate and zoom all structures.

## Using the Structures List

Generally you will only need to use the Structures List if you want to work with multiple structures in the same document. However, you can also use the Structures List to load new structures, or to copy a structure from one window to another.

### To display the structures list:

Do one of the following:

- Click the **Structures** button in the toolbar.
- Right-click in the Graphics Pane and choose: **Show Structures List**.
- Choose: **View** > **Structures List** > **Thumbnail View** or **List View** (concise layout).

### To display a structure:

Do one of the following:

- Click the structure's thumbnail in the Structures List.
- Use the up/down arrow keys on your keyboard to move up or down in the list.

### To display multiple structures simultaneously:

Do one of the following:

- **Shift**-click thumbnails for a contiguous selection (e.g., A, B, C)
- **Command**-click thumbnails for a discontiguous selection (e.g., A, C, E).

### To change the primary selection in a multi-structure display:

- Cick on another selected list row (its thumbnail will become highlighted in yellow, and the scale and background colour may change, depending on that structure's settings.)

### To lock a structure:

Do one of the following:

- Move the mouse pointer to the structure's thumbnail in the Structures List and hover the mouse just to the right of the structure name so that a padlock ( 🔒 ) icon appears. Click the padlock to lock the structure ( 🔒 ).
- Right-click on the structure's thumbnail in the Structures List and choose: **Lock**.

### To copy a structure to another window:

Do one of the following:

- With the thumbnail selected, choose: **File > New Window with Structure**.
- Right-click on the thumbnail and choose: **New Window with Selection**.
- Drag a thumbnail into the Structures List of the other window.

### To remove thumbnails:

Do one of the following:

- Select the thumbnails you wish to remove and press the **Delete** key on your keyboard.
- Right-click on the thumbnail you wish to *retain* and choose: **Delete Others** from the contextual menu.
- Select the thumbnail(s) you wish to *retain*, then right-click on one of them and choose: **Delete Hidden Structures**.

### To save all structures as separate documents:

Do one of the following:

- Choose: **File > Export Structures**.
- Right-click in the Structures List and choose: **Export Structures**.

In both cases you will be prompted to specify a destination for the new document files.

**Mac Sandbox Limitations.** As a modern, 100% native, macOS application, CrystalMaker for Mac fully complies with Apple's "Sandboxing" requirements. As a result, the application is forbidden to write multiple files to certain areas of your computer. For this reason, the "Downloads" folder is used; you can create folders within this—but the application is not authorised to generate files outside this folder. (This limitation does not apply to saving a regular document; it only applies to batch output.)

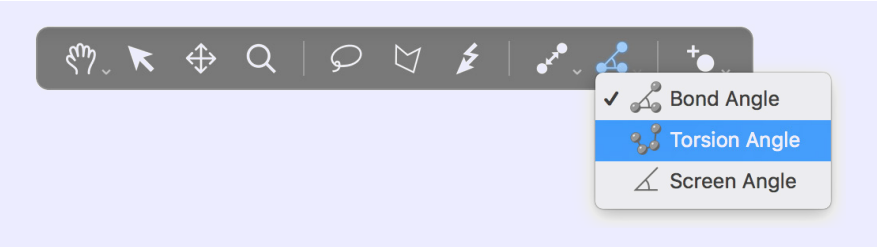
## Graphics Pane

The portion of the window where structures are displayed is called the Graphics pane. A ruler can be displayed along the top and can be hidden, if required.

### Tool Strip

When the mouse is inside the Graphics Pane a floating tools palette is displayed. You can click and drag this to other parts of the window, or hide it entirely.

The Tool Strip, in horizontal orientation, showing a tool selection menu.



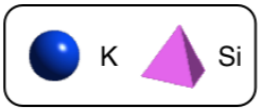

The active tool is shown highlighted in blue. Notice that some of the tools have small inverted chevrons next to them, indicating the presence of popup menus with alternative tools. For example, you can replace the **Bond Distance** tool with the (screen) **Distance** tool or the **Add/Delete Bond** tool. Similarly, you can replace the **Bond Angle** tool with the (screen) **Angle** tool or the **Torsion Angle** tool.

**Tool Strip Reference.** For more information about the individual tools in the Tool Strip, please see: Appendix A: Tools Reference.

## Legend

By default, a Legend is displayed on the top right-hand corner of the Graphics pane. As with the Tools Palette, the Legend can be dragged to different parts of the window or hidden entirely.

The Legend, shown in horizontal mode, with a border.




### To customize the legend display:

- Right-click in the Legend to display a contextual menu.

## Ruler and Grid

By default, a ruler is displayed along the top of the Graphics pane. This provides a reference to the current length scale, and is graduated in Ångstrøm units (1 Å = 0.1 nm). A grid can also be displayed, graduated in the same units as the ruler, and displayed behind the current structure.

### Why Å and not nm?

Because Å units are the perfect size for crystal structures! An "average" atom is about 1 Å in size, and interatomic distances are on the order of just a few Å. By contrast, nanometres are exactly 10× too large, requiring use of fractions, which becomes annoying after a while. Note: the Å is an officially-recognised S.I. distance unit, so there's no reason not to use it.

### To show or hide the ruler:

Do one of the following:

- Choose: **View > Show/Hide Ruler**
- Right-click in the Graphics pane and choose: **Show/Hide Ruler**

### To show or hide the grid:

Do one of the following:

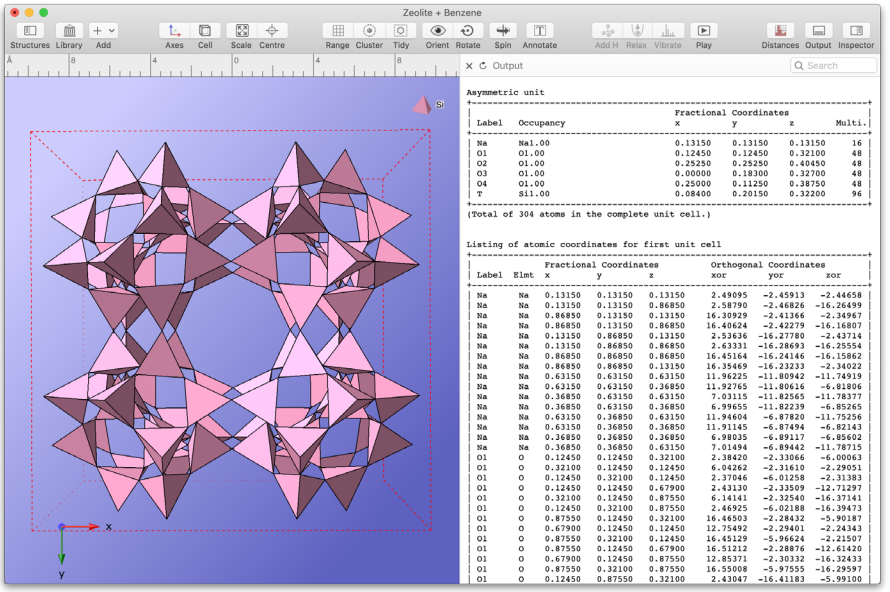
- Click in the ruler to toggle the grid on or off
- Choose: **View > Show/Hide Grid**
- Right-click in the Graphics pane and choose **Show/Hide Grid**

## Output Log

The Output Log is a resizable pane that displays status information and the results of screen tool operations, bond searches, modelling calculations, etc. You can copy text from the Output Log to other programs. Alternatively, a contextual menu provides commands for saving output as a text file, or printing.

The Output Log can be displayed in horizontal or vertical layouts—the latter is useful for displaying extended output, as illustrated below.

A document window in "vertical layout", showing the Output Log on the right-hand side.



### To display the Output Log:

Do one of the following:

- Click the **Output** button in the toolbar (if visible).
- Right-click in the Graphics Pane and choose: **Show Output Log**.
- Choose: **View** > **Output Log** > **Horizontal Layout** (or **Vertical Layout**).

### To switch to a Vertical layout:

Do one of the following:

- Click the **Rotate Layout** button ( ↻ ) in the Output Log's header bar.
- Right-click in the Output Log and choose: **Vertical Layout**.
- Choose: **View** > **Output Log** > **Vertical Layout**.

### Searching for Text

The Output Log's header bar includes a **Search** field, where you can enter a search term. Press the **return** key on your keyboard to start a (case-*insensitive*) search. The first occurrrence of your search term will then be highlighted. To search for a second occurrence, press the **return** key again; the output will be scrolled to show the next occurrence, and you can continue pressing the return key until the search resumes from the beginning.

### To save output:

Do one of the following:

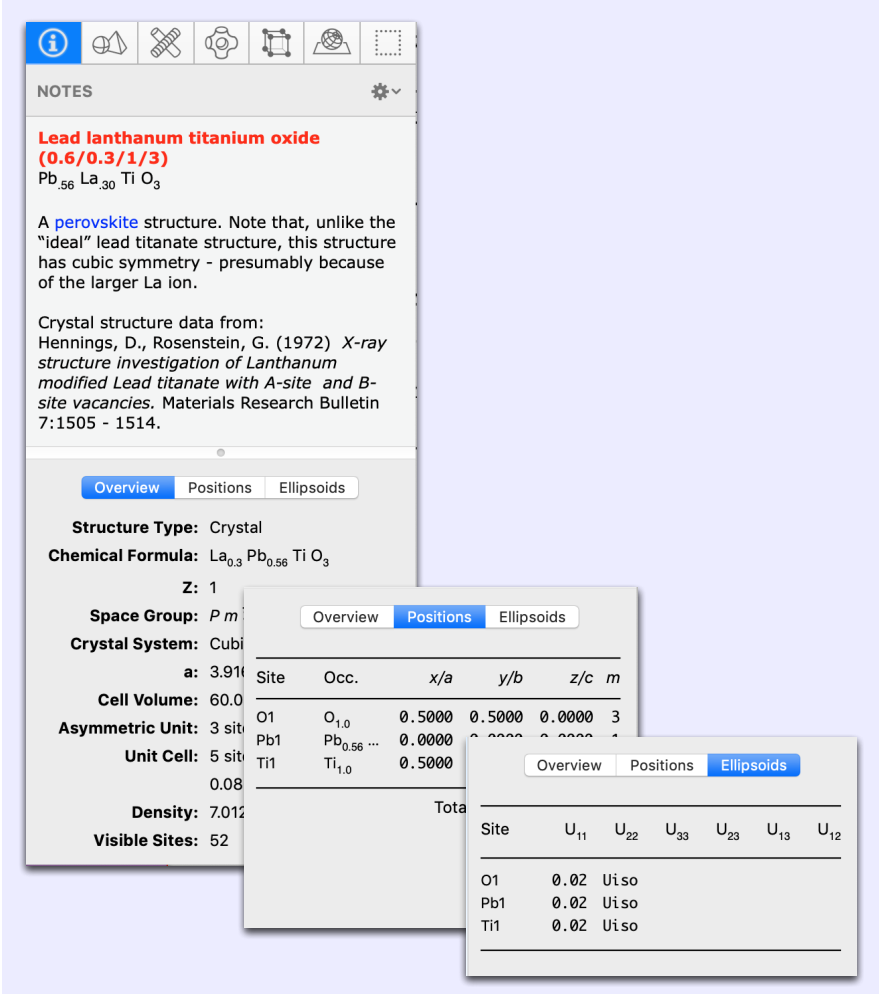
- Right-click in the Output Log and choose: **Print** or: **Save Text**.
- Select the text you wish to save, then drag-and-drop it into another program.

# Inspector

CrystalMaker X's Inspector pane provides a series of tabbed panes for displaying information about the structure, its selection, or editing Model and Rendering attributes. The icons at the top of the Inspector let you navigate the various panes, described in more detail below.

## Info Inspector

This, default pane, is split into a rich-text Notes pane (top) where you can enter or review information about the structure; and an Info pane (bottom) where structural data such as chemical formula, spacegroup, cell parameters, density and number of atoms are automatically displayed.




The Info Inspector, showing rich-text notes plus auto-generated structural information, divided amongst three tabbed panes.

### Notes Pane

The information that you enter into the Notes pane can be searched, via the Library Browser, if the "**Notes Contains**" search option is selected.

The Notes pane can display rich text; you can use the contextual menu, or the Actions menu (cog icon) on the top right-hand side of the Notes pane, to change text styles, apply superscripts or subscripts, and edit colours.

### Info Pane

The Info pane's **Overview** tab includes useful structural information, which is updated as you edit your structure, e.g., the "Display Formula" shows numbers of each species of atom (scaled by their site occupancies).

The **Positions** tab gives an abbreviated listing of sites, their occupancies, and fractional coordinates (structural coordinates for molecules). This is designed for quick reference; for more-detailed information, you can customize the Atoms Inspector, or refer to the full structural data presented in the crystal or molecular editors (**Edit > Structure**).

Finally, the **Ellipsoids** tab is only shown if a structure includes *atomic displacement parameters*. These might be isotropic (Uiso) or anisotropic (Uij).

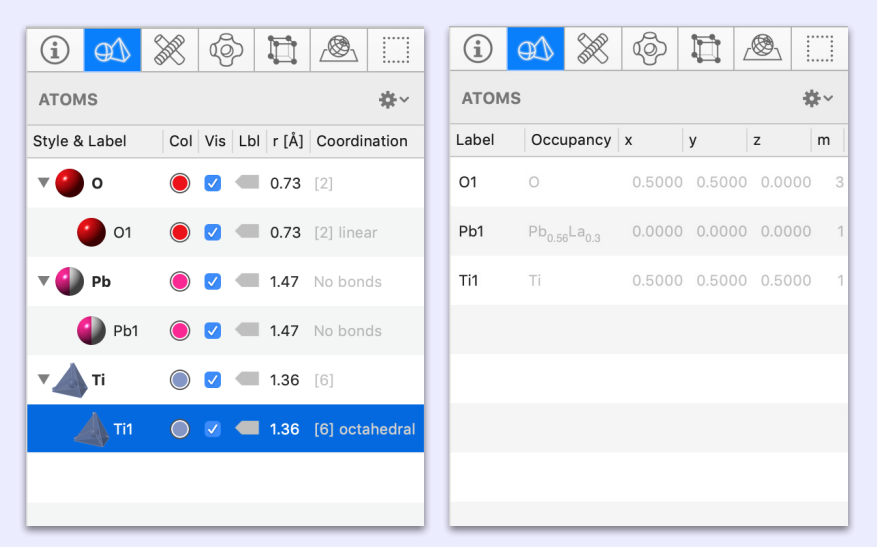
## Atoms Inspector

This resembles the "Site Browser" in earlier versions of CrystalMaker, but is far more powerful. Atoms can be grouped by chemical element or by molecule; groups are represented by a disclosure triangle, which lets you collapse the individual atoms or sites within the group.

The "Standard" list columns are, from left to right:-

- Preview icon for Atom, Ellipsoid or Polyhedral style. Click to change the style.
- Element or site label. Double-click to edit the text. (If editing element text, all associated atoms or sites will have their site occupancies changed.)
- Colour button.
- Visibility checkbox: toggle all corresponding atoms on or off.
- Label checkbox.
- Radius field. Double-click to edit the radius of all corresponding atoms.
- Coordination field. This is for information only, and is auto-generated.

You can select one or more rows in the list and have any changes applied to the selection: useful if you need to edit many sites in one go. An **Actions** menu (cog icon, top right) and a contextual menu provide additional functionality.




The Atoms Inspector in its "Standard" (left) and "Coordinates" view (right).

## Customizing the Atoms Inspector

CrystalMaker 10.4 introduced a customizable Atoms Inspector, where you can switch between one of two preset layouts: Standard or Coordinates. In addition to these two presets, you can explicitly set column visibilities using the **Show Columns** submenu in the Inspector's Actions menu.

## Colouring Options

The Actions menu has a **Colour** submenu which lets you colour atoms by element, by coordination number, by molecular or by site.

Colouring by element is the default option. CrystalMaker takes its colours (and atomic radii) from your default "Element Table" (which you can browse in the Preferences panel). You can of course customize colours using the colour buttons for individual elements or sites—and there are additional options to apply the "CPK" model colours, CrystalMaker's preferred colours (taken from the "Shannon & Prewitt" element table), or your chosen default colours.

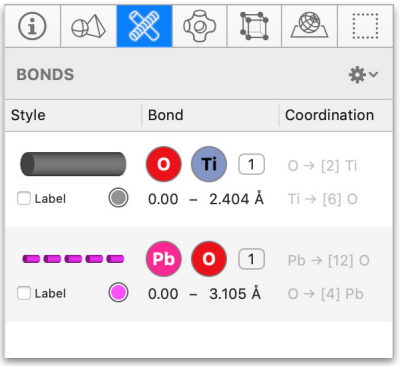
Users working with Red/Blue Stereo plots may find the new **Optimize for Red/Blue Stereo** option useful. This shifts any colours in the red/cyan "danger zone" towards safer hues.

## Atomic Radii

As with colouring, CrystalMaker loads a default set of atomic radii from your default "Element Table". You can reset radii using the Radius field, but you also have the option of applying a specific element able (e.g., Covalent Radii or Van-der-Waals radii) to the current structure, using the **Actions > Radii** submenu.

## Bonds Inspector

This Inspector lets you edit all of the bonding specifications for the current structure, as well as providing a coordination preview. It effectively combines the old "Edit Bonding" dialog in CrystalMaker 9, with the same program's "Bonds List".



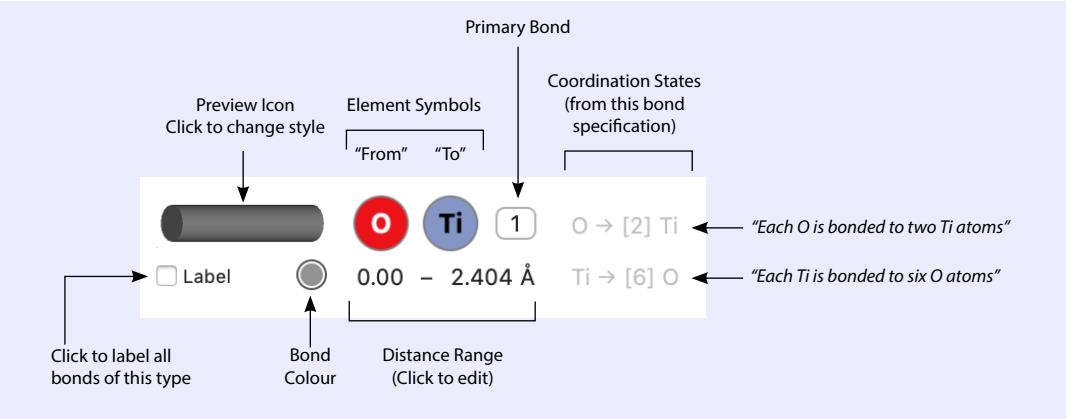

The Bonds Inspector, showing two bond specifications, each with a preview.

### To add a new bond:

Do one of the following:

- Double-click on an empty row.
- Click the Actions button (cog icon, top right) and from its drop-down menu choose: **Add Bond Specification**.
- Right-click anywhere in the Bonds Inspector and choose: **Add Bond Specification**.

You can then use the row controls to edit the bond specification.




Anatomy of the Bonds Inspector: each list row provides a full definition of an individual bond specification, including element pair, distance range, bond style and colour.

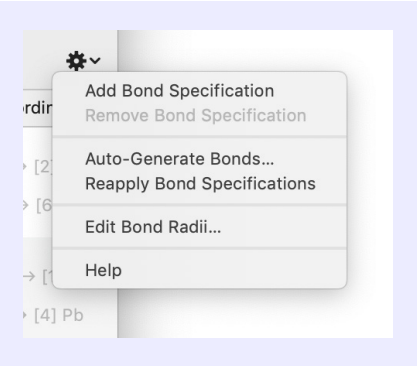
## Primary and Secondary Bonds

A new feature introduced by CrystalMaker X is the ability to specify certain bonds as being "secondary" bonds—as indicated by a number "2" button in the Bond column. Secondary bonds are designed to show *inter-molecular* bonding, and are ignored by the program when trying to determine what is, and what isn't, part of a molecule. By contrast, primary bonds—designated by the number "1" button in the Bond column—indicate internal, or "intra-molecular" bonding.

**Distance Measurements.** You can also use secondary bonds as a way of preserving arbitrary distance measurements in a structure.

## Bond Actions

The Bonds Inspector's Actions menu includes commands to auto-generate bonds (using the sum of atomic radii to determine appropriate distance ranges), to reapply existing bond specifications to the structure, or to let you edit the radii of bond cylinders (this is a shortcut to the appropriate control in the Model Inspector).

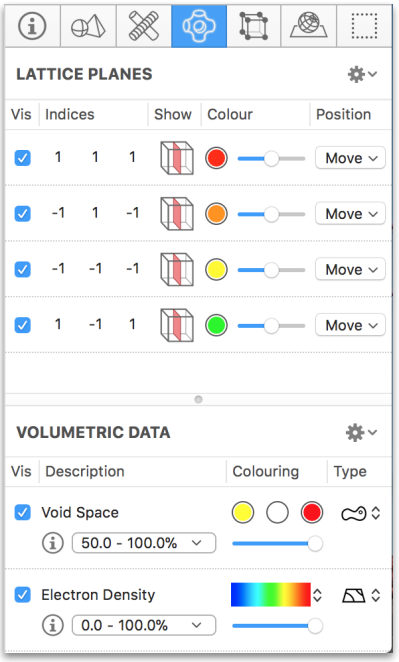



The Bonds Inspector's Actions menu.

**Editing Custom Bonds.** The Bonds Inspector only lists bond specifications: requests for bonds to be generated. You may, in addition, define custom bonds, between specific atoms in your model. To edit the properties of such bonds you will need to select the bonds to be edited, and then use the Selection Inspector (as described later in this chapter).

## Volume Inspector

The Volume Inspector (crystals only) lets you add or manipulate lattice planes and volumetric data. These two types of model objects both extend throughout the the volume of your plot—and it is possible to display volumetric information superimposed onto any visible lattice planes (hence the combination of these two in the same Inspector).




The Volume Inspector, showing the Lattice Planes and Volumetric Data lists.

### To add a new lattice plane:

Do one of the following:

- Double-click on an empty row in the **Lattice Planes** table.
- Click the Actions button (cog icon, top right) and from its drop-down menu choose: **Add New Plane**.

### To add a new volumetric dataset:

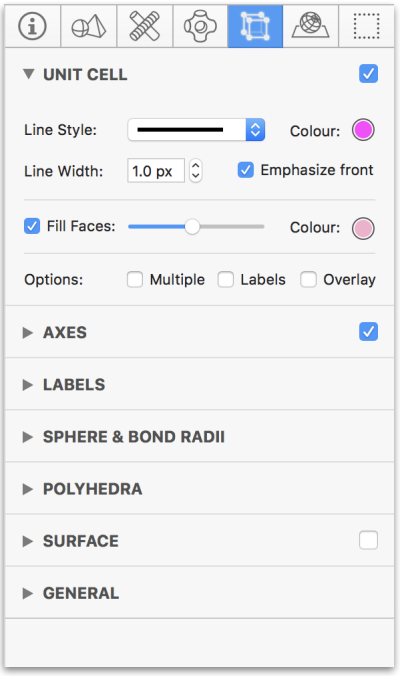
Do one of the following:

- Double-click on an empty row in the **Volumetric Data** table, then choose what type of dataset to add using the popup menu that appears.
- Click the Volumetric Data Actions button (cog icon) to display a drop-down menu, then use its **Add Volumetric Data** submenu to specify what type of dataset to add.

## Model Inspector

Most of the settings that control your model's appearance are included here—apart from the atoms and bonds, which you've already met in their dedicated inspectors. The Model Inspector lets you control the unit cell display, axial vectors, add one or more lattice planes (and change their positions), manage volumetric datasets, overlay a solvent-excluded surface "envelope", and apply labels.

The Model Inspector also lets you control general settings for how atom spheres, bond cylinders, and polyhedra are drawn on screen. For example, you can define minimum radii for spheres and cylinders, customize polyhedral edge styles and frame widths, and choose whether to show ellipsoids or atom spheres at the vertices of your polyhedra.




The Model Inspector, showing unit cell controls. Other controls are accessed by clicking the disclosure triangles for Axes, Lattice Planes, etc.

**Manage Your Defaults.** Both the Model Inspector and Rendering Inspector include contextual menus for each control group. These menus let you record the current settings as your default (preference) settings, or reset the group to the defaults, or reset to the factory defaults. Alternatively, if you right-click on the selected Model or Rendering tab icon, you can set defaults for *all* groups at the same time.

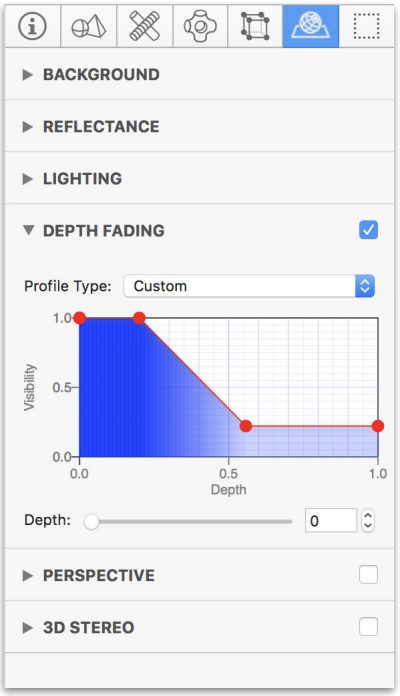
By managing your defaults, you can improve your workflow: recording your favourite model and rendering settings so that these can be applied for all new structures.

## Rendering Inspector

For any structural model, you can change the way it is rendered on screen by editing the background colouring, lighting, material reflectivity, degree of perspective and depth fading. You can use up to four light sources: one ambient (omni-directional) plus up to three spotlights. Interactive controls let you adjust their directions and intensities.

The reflectivity of different types of objects can be changed. For example, you might want your atoms to look bright and shiny, your bonds metallic, and your polyhedra softly rendered without harsh contrasts as the model is rotated.

Finally, this inspector lets you enable or disable 3D display, with a choice of red/blue stereo or stereo-pair display.

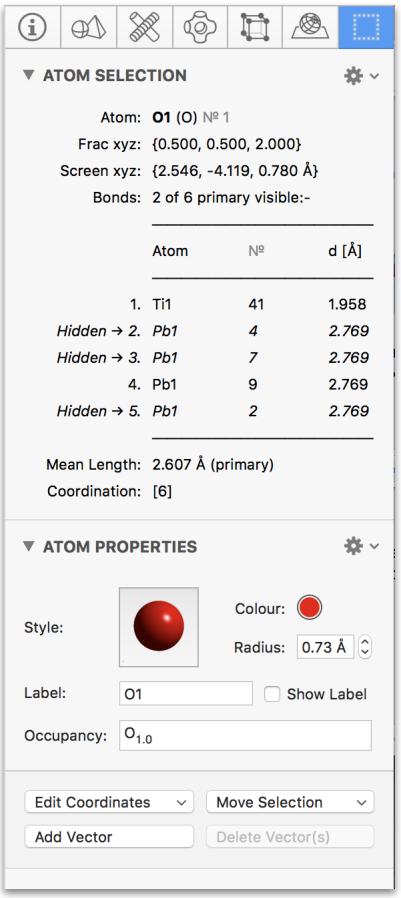



The Renderng Inspector, showing depth-fading controls.

## Selection Inspector

CrystalMaker lets you select one or more atoms, bonds, polyhedra, vectors or annotation objects (lines, arrows, textboxes). Once selected, their properties are displayed in the Selection Inspector. For example, this allows you to change the colours of a group of selected atoms, compared to the rest of the structure; or you might want to display one group of atoms as a rendered-solid polyhedron, whilst the rest of the structure appears like a "ball-and-stick" model.

The Selection Inspector also displays handy information about the selection, such as the number of bonded atoms. Action menus (cog icons) provide additional commands, such as showing the corresponding entry in the Atoms Inspector, calculating a list of bond distances or angles and so on.




The Selection Inspector, sshowing information about one selected oxygen atom.

## Adding Structures to the Empty Document

Your document is a container for one or more structures. You can add existing structures to the document using drag-and-drop, or via a file menu. If one of the dropped documents is itself a multi-structure container, its individual structures will be added to the Structures List. New structures can be added by entering their details into an editor window—or you can click with the Add Atom tool to draw a new molecule.

### To add existing structures to the document:

Do one of the following:

- Drag-and-drop file icons into the Graphics Pane or Structures List
- Drag-and-drop a Structures List icon from another window into the current window's Graphics Pane or Structures List.
- Choose: **File > Add to Window** and choose **Structure from Library** or **Other Structure**
- Click the **Add** (+) toolbar button and choose: **Structure from Library** or **Other Structure.**

### To add a new crystal to the document:

Do one of the following:

- Choose: **File > Add to Window > New Crystal**, or
- Click the **Add** (+) toolbar button and choose: **New Crystal**.

### To add a new molecule to the document:

Do one of the following:

- (If no other structures are visible) choose the **Add Atom** tool from the toolstrip and click to draw your new molecule.
- Click the **Add** (+) toolbar button and choose: **New Empty Molecule**. (You can then use the **Add Atom** tool to draw your molecule.)
- Choose: **File > Add to Window > New Molecule**. (You can then type in the coordinates of atoms in your molecule.)
- Click the **Add** (+) toolbar button and choose: **New Molecule**.

**Readable File Formats.** CrystalMaker supports over 40 different file formats. For details of the types of files that can be read into the program, please see: *Chapter 13: Data Import/Export*.

## Multi-Structure Animation

A powerful feature in CrystalMaker X is the ability to animate multiple structures in the same window. You can rotate and scale structures during the course of the animation and change the model type and other settings such as Stereo 3D. This allows you to explore structural behaviour more effectively.

### To start or stop an animation:

Do one of the following:

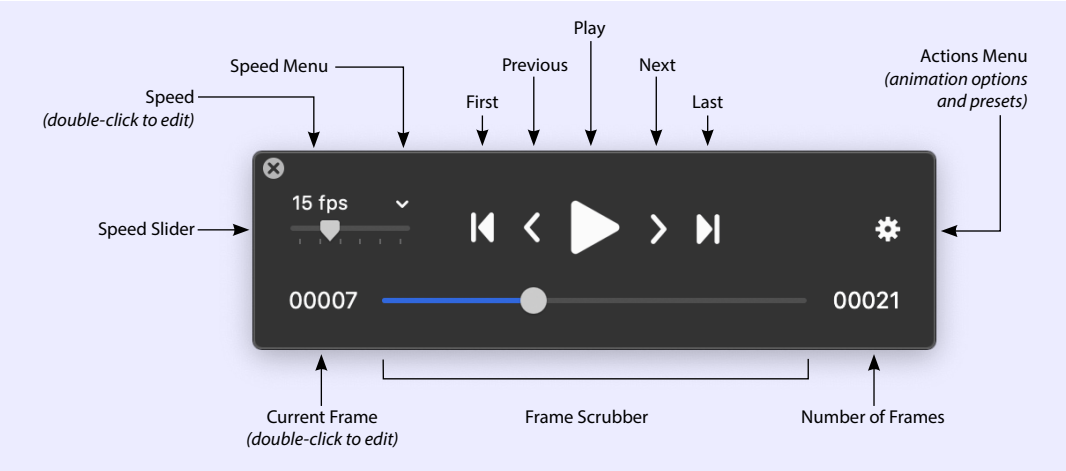
- Click the **Play** button ( ▶ ) in the toolbar.
- Click the **Play** button in the Playback Controls window.
- Choose: **Transform** > **Play** (or **Transform** > **Stop Playing**).

### Animation Settings

Use the Playback Controls window (**View** > **Playback Controls**) to change the animation speed (frames-per-second), whether to loop back-and-forth, auto-rotate, synchronize scales and rotation.

You can also use the prominent "Frame Scrubber" control to rapidly scan ("scrub") through a structure sequence.

**Playback Controls Shortcut.** You can quickly show the Playback Controls by clicking-and-holding down the toolbar's **Play** button.




Anatomy of the Playback Controls window.

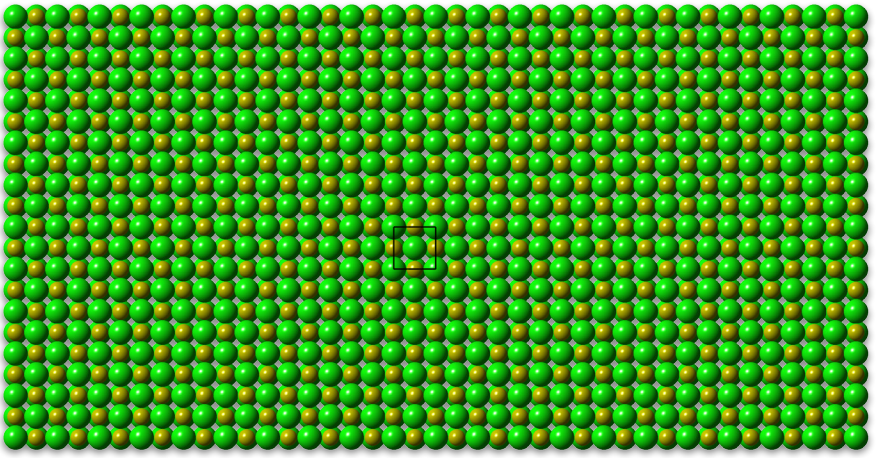
**Save Your Animation.** Your animation settings are saved with the rest of your document, so you can replay your animation at any time. You can also export your animation as a movie, as described further in Chapter 13: Graphics & Video.

Chapter 5

# Building Crystals

This chapter describes how to create new crystals, display them, and edit them, within CrystalMaker. We start by examining what kind of data are required to specify a crystal. Next we introduce the crystal editor, how to specify bonds and polyhedra and specify atom colours and their radii.

**Building Molecules:** If you need to build non-periodic objects such as molecules, please see Chapter 6: Building Molecules. If you wish to import crystallographic or molecular data from a text file, then you should also refer to *Chapter 14: Data Import/Export*.



A crystal is a soild material with a regular arrangement of atoms: represented by a unit cell (black square), which can be repeated ad infinitum.

## Techniques for Building a New Crystal

You can create a new crystal in one of three ways:-

- By adding a new crystal to an existing document. To do this, click the toolbar's Add button (+) and choosing: **New Crystal** from its popup menu (or choose: **File > Add to Window > New Crystal**).
- By tiling an existing molecule, using the **Transform > Molecule to Crystal** command. A "Packing Explorer" window will appear, letting you experiment

with *symmetry*, *lattice parameters*, etc. for your new crystal.

- By entering data in a text file. Use a word-processor or text editor to create a plain text (ASCII) file with crystallographic data. Open the file in CrystalMaker using the **File > Open** command. (See *Chapter 13: Data Import/ Export* for more details about the formatting required.)

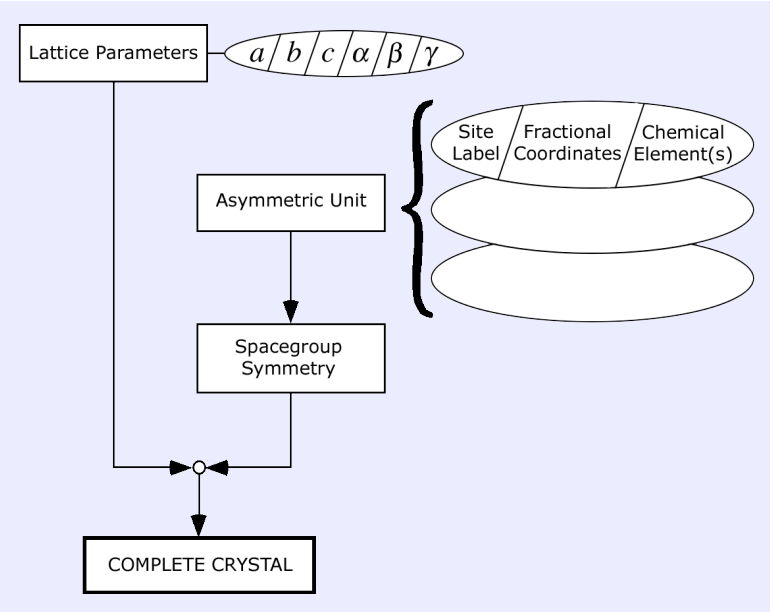
## Elements, Atoms and Sites

To create and edit crystals you need to understand the way in which CrystalMaker distinguishes atoms, elements, and crystallographic sites.

To construct a crystal we require three main ingredients: the lattice parameters (the repeat distances parallel to *x*, *y*, and *z*; plus the inter-axial angles), the spacegroup symmetry, and the asymmetric unit (the smallest group of atoms which, when combined with the spacegroup symmetry, generates all the atoms in the unit cell).

For each atom in the asymmetric unit CrystalMaker requires a site label, at least one chemical element symbol and occupancy fraction, plus the fractional coordinates (i.e., fractions of the unit cell dimensions *a*, *b*, *c*).

A crystal structure is defined by its lattice parameters, asymmetric unit and symmetry.




### Site Label

This label is used to *uniquely* identify a site in the asymmetric unit. You can have any number of characters, but please ensure that you:-

- Choose a **unique label** for each site in your structure. This is good practice—and is required if you wish to use the program's **Synchronize** command: the site label is the only way to relate sites between different structures.
- **Avoid using spaces** (e.g., use "Si1" or "Si_1" intead of "Si 1"). This is to prevent problems exporting your data to other programs (e.g., most crystallographic file formats require that an atom or site label should not include any white space).

## Site Occupancy

CrystalMaker needs to know what kinds of atoms reside on a particular site—and in what proportions. Atoms are identified by their chemical element symbols, e.g., "Al", "Si". Alternatively, you can use custom symbols (which must not contain spaces), such as "Zz" (for a dummy site, perhaps) or "Fe3+".

In an ideal crystal, each site would be associated with one, and only one, type of atom; its *site occupancy* would be set to 1. You would therefore enter the site occupancy as either:

```
Si 1.0
```

or

```
Si
```

(in the latter case, CrystalMaker will *infer* an occupancy of 1.0).

However, real crystals may well show *partial occupancy* of certain sites (e.g., there are many vacancies in the crystal), or even *multiple occupancy* associated with disordered atom distributions. CrystalMaker therefore allows you to define a site's occupancy in terms of any number of element symbols, each with a fractional occupancy value, as illustrated in the following examples.

### Example 1

A high-temperature superionic conductor is known to contain a disordered arrangement of Ag ions. The crystal structure was refined assuming *partial occupancy* of Ag ions over many different, but *symmetrically-related* sites, labelled "M1". Each site has a 10% probability of containing an Ag atom. The site occupancy would therefore be written as:-

```
M1:  Ag 0.1
```

### Example 2

A mineral shows a disordered arrangement of Al and Si atoms over its two tetrahedral (T) sites. A crystal structure refinement gives the T1 site a 75% probability of containing Si and 25% probability of Al; the T2 site has 25% Si and 75% Al. The site occupancies are therefore:-

```
T1:  Si 0.75   Al 0.25
T2:  Si 0.25   Al 0.75
```

CrystalMaker uses the *most abundant* (or "major") element on each site as a tag to group atoms by chemical composition (so in example 2, the T1 site is treated as "Si" and the T2 site as "Al").

Using their (major) element symbols, atoms can be assigned different colours, radii, and bonds. CrystalMaker recognises the element symbols in your currently-active **elements table** (visible in the **Elements** pane of the Preferences panel) and automatically sets the colour and atomic radii for such atoms.

## Site Occupancies and "Grey" Atoms

CrystalMaker respects any partial- (e.g., $Si_{0.75}$) or mixed- (e.g., $Si_{0.75}Al_{0.25}$) occupancies you enter: you will see the results in any calculated formula, the density—or indeed, in any diffraction calculations. What you won't see is any change to the display: each atom is still represented by a sphere, not a vacancy. Some users find this confusing, but actually, this is the only correct and consistent way of depicting the structure.

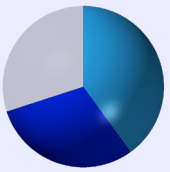
Firstly, one must consider symmetry, which maps all atoms of the same site onto each other, thereby "merging" them into "grey" atoms.

Secondly, one needs to understand that partial- or mixed-occupancy reflects *disorder* in a system: differences in occupancy that vary with regard to position in the lattice and time. Since structure determination involves summing up the contributions from billions of unit cells over many hours of time, each atom is necessarily an average, "grey" atom, with a statistical probability of being occupied by one or more different elements.

We can't, for instance, say that one atom in the unit cell is 100% Si, whereas another is 0% Si; instead we have to settle for the average occupancy: since this is the only information we can glean from the structure refinement.

Now, if you wish to make a model that shows atom spheres in some parts of the unit cell and not others (or, for a chemically-disordered system, say "Si" in one position and "Al" in another), then you will need to edit your structure by hand—perhaps discarding any symmetry and editing site occupancies, or otherwise selecting atoms and changing their colours and/or occupancies.

A better solution is probably to choose a distinctive display style for disordered sites, e.g., the "two-tone" or "beach-ball" sphere styles. CrystalMaker X also offers a new "Pie-Chart" sphere type, which can show differently-coloured sectors, depending on the atom's fractional occupancy.



A "Pie-Chart" sphere corresponding to a fractional occupancy of $Al_{0.4}Si_{0.3}$. Here, Al corresponds to cyan, Si to blue and the unoccupied fraction is translucent.

## Fractional Coordinates

For a crystal structure, the atomic coordinates are specified in terms of fractions of the unit cell edge lengths, *a*, *b*, and *c*. Why fractions? It makes symmetry relationships easier to understand, e.g., so-called "special positions" such as (½, ½, ½) or the origin (0, 0, 0)—and means that the cell parameters can be adjusted (e.g., to allow for thermal expansion) without necessarily needing to edit all the atomic positions.

You can enter your coordinates using decimals or fractions, e.g.,

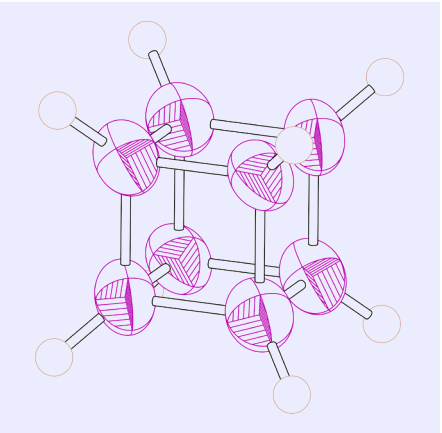
```
0.5    0.25   0.125
```

or

```
1/2    1/4    1/8
```

## Atomic Displacement Parameters

Atomic displacement parameters (also known as temperature factors) can be used to define "thermal ellipsoids": showing the uncertainties in atomic positions, caused by temperature, disorder, errors in the refinement, and other statistical anomalies.



Atomic displacement parameters displayed for an organic molecule.

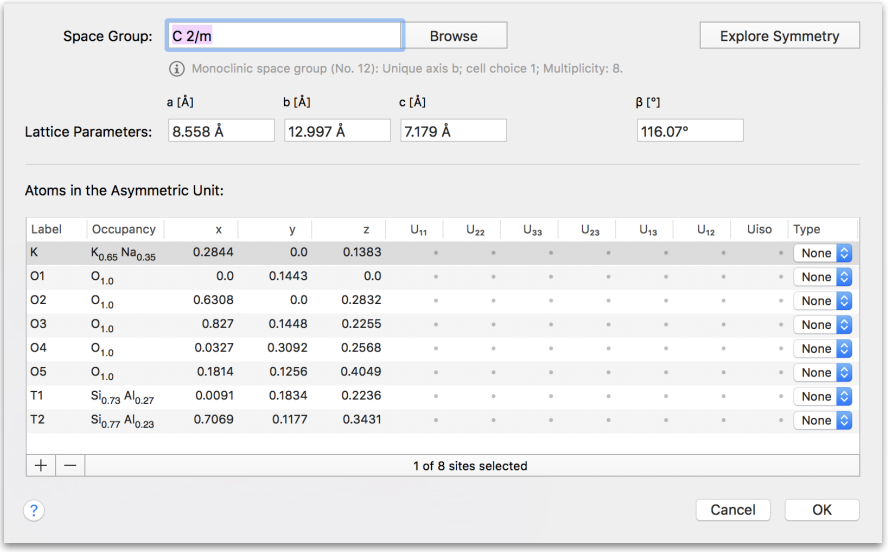
CrystalMaker can read atomic displacement parameters from text files (e.g., CIF, GSAS, PDB, SHELX or CrystalMaker text format), or you can add values using the Crystal Editor. CrystalMaker supports either *isotropic* (spherical) displacement parameters, denoted *Uiso*, or *anisotropic* (ellipsoidal) displacement parameters, which should be entered as *Uij* values.

You can customize sizes of the ellipsoids by entering a probability factor, using the **Sphere & Bond Radii** group in the Model Inspector. Ellipsoid styles—including the option of plotting some atoms (e.g., H) as small spheres—can be set (for the Ellipsoids model) using the Atoms Inspector.

# The Crystal Editor

If you are creating a new crystal, ensure a document window is open (**File > New Window**) then choose **File > Add to Window > New Crystal**. Alternatively, to edit an existing crystal, choose:**Edit > Structure**. The Crystal Editor appears:

The Crystal Editor (shown here as a sheet window on macOS).




This window is organised into three sections:

- Space group symmetry
- Lattice parameters
- Atoms in the asymmetric unit.

## Defining Symmetry

The first step in editing a crystal is to specify its symmetry, in the form of a space group symbol, or by entering general equivalent positions.

### Space Group Symbol

You can either enter a space group directly into the **Space Group** field, or you can click the **Browse** button and select a symbol from the Space Group popover (as described later in this chapter). Space group symbols can be entered in one of three formats:

- **International Notation**. You must use the correct form, with spaces between the various operators (e.g., *C2/c* entered as: "**C 2/c**"). You can use the *short* international symbol (e.g., "**C 2/c**"), or the less ambiguous *full* international symbol (e.g., "**C 1 2/c 1**"). The full symbol lets you specify unconventional symmetry settings.

- **Schoenflies Symbol**. You must use parentheses, and enter the symbol without any spaces, e.g., $C_{2h}^{6}$ entered as: **C2h(6)**.
- **Space Group Number**. As listed in the *International Tables for Crystallography (Vol. A: Space-group symmetry)*. CrystalMaker will assume the standard setting for the space group.

The 230 conventional *crystallographic* space groups are all handled, as are a number of unconventional settings. If your entry isn't recognized by CrystalMaker, a warning triangle will appear next to the **Space Group** prompt.

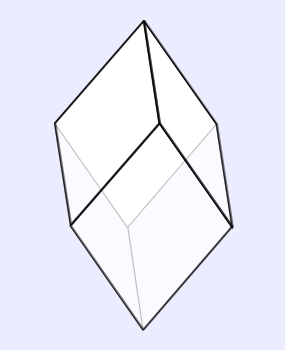
Examples of different space group formats recognised by CrystalMaker.

| Space Group Symbol | CrystalMaker Space Group Format | | |
|---|---|---|---|
| | International | Schoenflies | Number |
| $P\,\bar{1}$ | P -1 | C1(1) | 1 |
| $P\,m$ | P m | Cs(1) | 6 |
| $P\,a\,\bar{3}$ | P a -3 | Th(6) | 205 |
| $P\,2\,2\,2_1$ | P 2 2 21 | D2(2) | 17 |
| $P\,n\,m\,a$ | P n m a | D2h(16) | 62 |
| $R\,\bar{1}\,c$ | R -3 c | D3d(6) | 167 |
| $C\,2/c$ | C 2/c | C2h(6) | 16 |
| $I\,4_1/a$ | I 41/a | C4h(6) | 88 |
| $P\,4_1\,2_1\,2$ | P 41 21 2 | D4(3) | 92 |
| $P\,4_2/m\,n\,m$ | P 42/m n m | D4h(14) | 136 |
| $I\,a\,\bar{3}\,d$ | I a -3 d | Oh(10) | 230 |

## Rhombohedral Space Groups

Traditionally, some crystals with trigonal symmetry were represented using a *rhombohedral* unit cell. This has the shape of a cube stretched (or compressed) along its body diagonal, resulting in cell parameters $a = b = c$ and $\alpha = \beta = \gamma \neq 90°$.

A rhombohedral unit cell. The *xyz* axes are parallel to the cell edges, with a three-fold symmetry axis passing along the body diagonal from bottom to top.



Rhombohedral cells are rarely used today, as hexagonal axes ($a = b \neq c$ and $\alpha = \beta = 90°$; $\gamma = 120°$) are preferred for trigonal crystals. However, CrystalMaker still allows the choice of either axis setting. When you enter a Rhombohedral (R) spacegroup, your interaxial angles are used to select the appropriate unit cell.

**Rhombohedral as Hexagonal:** If you regularly use *hexagonal* axes for plotting rhombohedral spacegroups, remember to set the interaxial angles to $\alpha = \beta = 90°$ and $\gamma = 120°$, before entering your *R* spacegroup symbol.

### Origin Setting

When you type a spacegroup symbol into CrystalMaker, it is converted into a set of "general equivalent positions", relative to the unit cell origin. Unfortunately, in some cases there may be an offset between the positions CrystalMaker uses, and the positions implied by a particular setting of a spacegroup:

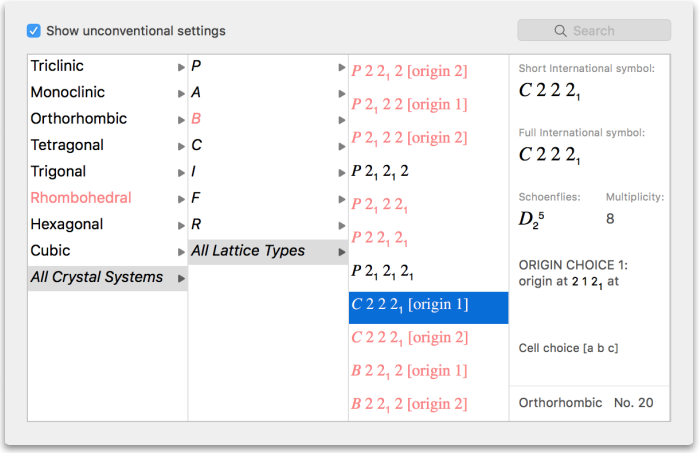
- Some structures are published with their origins deliberately displaced, perhaps to highlight a unit cell relationship between two phases with different symmetries;
- Certain space groups can have more than one "origin choice". These are listed in the *International Tables for Crystallography* and in the Space Group popover. Unless instructed otherwise, CrystalMaker will choose the first origin choice listed in the International Tables.

For these ambiguous cases, you may need to explicitly state the origin choice you wish to use. There are three ways of doing this:

- By typing the origin choice into the **Space Group** field. Use square brackets to enclose the word "**origin**", followed by "1" or "2", e.g., "**F d 3 m [origin 2]**".
- By choosing your origin choice from the Space Group popover (see below).
- By defining an *origin offset* using the Symmetry Explorer (see "Advanced Symmetry Options" later in this chapter).

## Space Group Popover

The Space Group popover lets you choose a space group from a list. You can display the popover by clicking the **Browse** button in the Crystal Editor.




The Space Group popover, showing an orthorhombic space group selected. Unconventional settings are shown in red.

The popover includes a search field and an option to display unconventional settings (e.g., different origin settings or unusual cell choices such as Orthorhombic *B* and *I* lattices). Below this is a browser interface, letting you choose a space group in terms of its crystal system, and lattice type (or to browse all space groups for all lattice types and/or all crystal systems). The fourth column of the browser is a preview, showing information about the selected space group.

### To choose a space group:

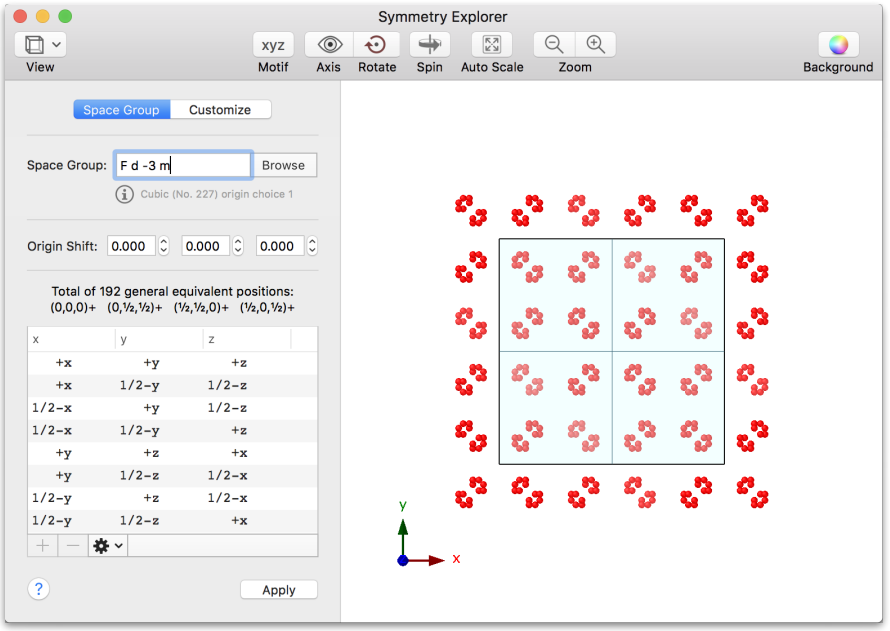
1. Select a crystal system from the first (left-hand) list. (The **Rhombohedral** entry allows you to plot a trigonal crystal using rhombohedral axes.)
2. Select a lattice type from the second list (only lattice types that are consistent with your choice of crystal system are shown).
3. Select a space group symbol from the third list. When you make a selection, the corresponding space group symbol is copied into the Crystal Editor's **Space Group** field.

### To search for a space group:

1. Type your space group symbol (short or international notation, Schoenflies symbol, or space group number) into the **Search** field at the top of the popover.
2. Press the **return** key on your keyboard. If the space group symbol is found, its entries in the crystal system, lattice type, and symbol lists will appear highlighted, and the preview column displays more information about this space group.

## Advanced Symmetry Options

Sometimes you may need more flexibility when defining symmetry: maybe you are using a non-conventional spacegroup setting, or you would like to enter symmetry positions manually. In these cases, you can use the Crystal Editor's **Explore Symmetry** button to display the Symmetry Explorer: a self-contained window that lets you experiment with symmetry in a highly-interactive way.




The Symmetry Options dialog, with general equivalent positions displayed for a cubic spacegroup.

The window is divided into two halves. On the left are controls for entering a space group symbol and browsing its general equivalent positions (GEP). On the right is a rotatable preview, showing the GEPs.

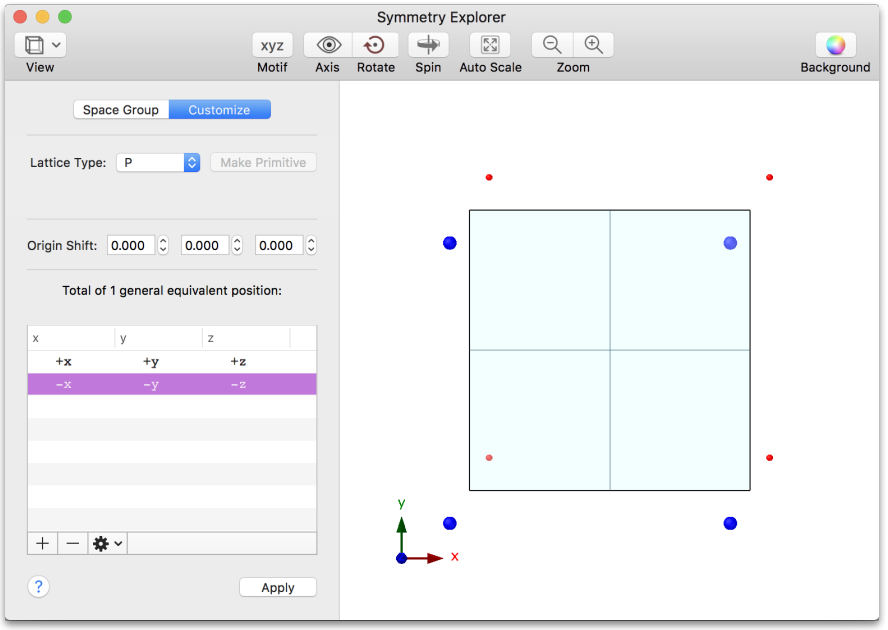
**Resizable:** This window can be resized to let you display more GEPs and see a larger preview.

### Constrained Lattice Parameters

CrystalMaker will automatically set any lattice parameters which are constrained by symmetry. This would mean, for example, that you would only need to enter the *a* lattice parameter for a cubic crystal ($a = b = c$; $\alpha = \beta = \gamma = 90°$).

### Defining Symmetry Operators Manually

To enter general equivalent positions yourself, click the **Customize** tab. The **Space Group** field is hidden and in its place is a popup menu letting you choose a lattice type.




Editing a general equivalent position in the Symmetry Explorer. The blue spheres in the preview on the right correspond to the selected row in the GEPs list on the left.

To add a new GEP, click the + button at the bottom of the GEPs list. A new GEP is added to the list and you can edit its components. These should be of the form:

```
    +x        -y     +z
  1/2+x     1/2-y     +z
```

(you may enter translations as fractions "`1/2`" or decimals "`0.5`"). Press the tab key to move between columns. To delete one or more GEPs, select their rows, then click the – button.

## Origin Shift

You can use the **Origin Offset** fields to tell CrystalMaker that there's an offset between your data and CrystalMaker's symmetry. (Please note that this is not the same as simply moving the origin to a different atom in the structure. If you do simply want to move the origin to, say, a specific atom in the structure, you can do that using the Transform > Unit Cell > Move Origin command—as detailed in *Chapter 10: Transformation*.)

Enter your offset values as fractional coordinates; you can use fractions "`1/2`" or decimals "`0.5`".

**Choose Space Groups from the Popover:** When in doubt, use the Space Group popover: it gives a choice of origin settings for some spacegroups and a choice of rhombohedral or hexagonal axes for trigonal "R" spacegroups.

### Applying Changes

Clicking the **Apply** button with apply any changes you have made to the frontmost Crystal Editor window.

## Fun with Symmetry

The Symmetry Explorer isn't just for editing an existing structure's symmetry. You can use this window at any time (**View > Show Symmetry Explorer**) and experiment with different symmetry relationships.

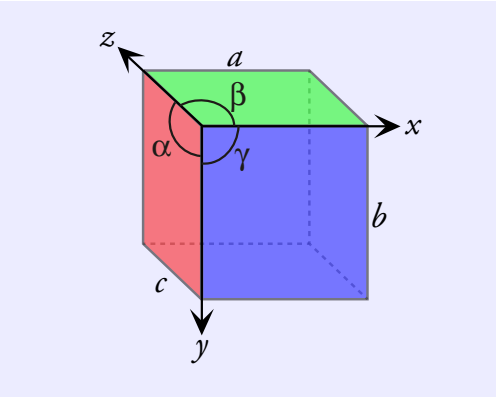
Use the Symmetry Explorer to:

- Visualize *multiplicity* and spatial relationships in any orientation.
- Identify individual GEPs by selecting them from the list and seeing their corresponding "atoms" light up in the Graph View.
- Specify a view direction (**Orient** toolbar button) so you can view symmetry in a specific orientation.
- **Zoom** and **Auto Scale** using toolbar buttons.
- Auto-rotate (**Spin**), or **Rotate** through a fixed angle.
- Visualize *special positions* by editing the **Motif** and seeing multiplicity changes.

Note that you can rapidly browse spacegroups by keeping the Space Groups Popover open and visualizing the different GEPs as you change your space group selection.

## Lattice Parameters

Lattice parameters define the shape and size of the unit cell:




Unit cell geometry. The axes, *x y z*, edge lengths, *a b c*, and angles, α β γ.

In general, dimensions *a*, *b* and *c* (in Ångstrøm units) and inter-axial angles α, β and γ (in degrees) would be required, but for most space groups, only the *unconstrained* lattice parameter fields can be edited. For example, a cubic unit cell requires just the *a* parameter). The constraints are summarized below:

Crystal systems and their lattice constraints.

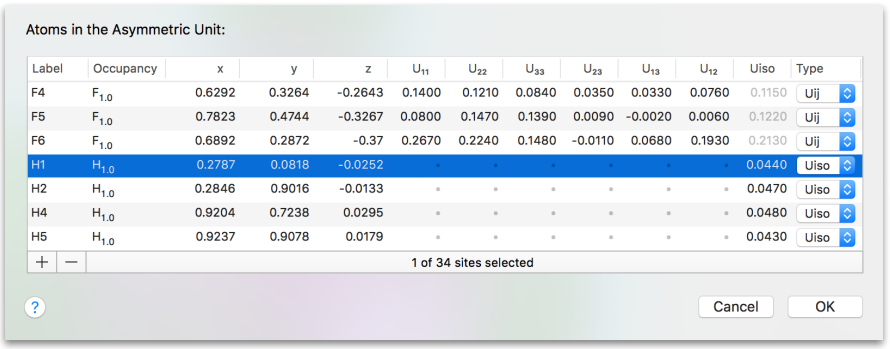
| Crystal System | Unit Cell | Essential Symmetry |
|---|---|---|
| Triclinic | $a \neq b \neq c$<br>$\alpha \neq \beta \neq \gamma$ | none |
| Monoclinic | $a \neq b \neq c$<br>$\alpha = \beta = 90° \neq \gamma$ | one two-fold axis |
| Orthorhombic | $a \neq b \neq c$<br>$\alpha = \beta = \gamma = 90°$ | three orthogonal two-fold axes |
| Tetragonal | $a = b \neq c$<br>$\alpha = \beta = \gamma = 90°$ | one four-fold axis |
| Cubic | $a = b = c$<br>$\alpha = \beta = \gamma = 90°$ | four three-fold axes |
| Trigonal | *Rhombohedral Setting:*<br>$a = b = c$<br>$\alpha = \beta = \gamma \neq 90°$ | one three-fold axis |
| | *Hexagonal Setting*<br>$a = b \neq c$<br>$\alpha = \beta = 90°; \gamma = 120°$ | |
| Hexagonal | $a = b \neq c$<br>$\alpha = \beta = 90°; \gamma = 120°$ | one six-fold axis |

## Asymmetric Unit

The Crystal Editor includes a list of sites in the asymmetric unit. CrystalMaker uses their coordinates, in conjunction with any symmetry, to generate the full unit cell. The list also includes the site label, its occupancy, and atomic displacement parameters (U11…U12 and Uiso).

**Customizing the Editor:** You can resize the Crystal Editor to make more atoms visible. Click a column heading to sort the list; drag a column to change its position (Mac).

Editing a site row in the Crystal Editor.




| Label | Occupancy | x | y | z | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{23}$ | $U_{13}$ | $U_{12}$ | Uiso | Type |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| F4 | $F_{1.0}$ | 0.6292 | 0.3264 | -0.2643 | 0.1400 | 0.1210 | 0.0840 | 0.0350 | 0.0330 | 0.0760 | 0.1150 | Uij |
| F5 | $F_{1.0}$ | 0.7823 | 0.4744 | -0.3267 | 0.0800 | 0.1470 | 0.1390 | 0.0090 | -0.0020 | 0.0060 | 0.1220 | Uij |
| F6 | $F_{1.0}$ | 0.6892 | 0.2872 | -0.37 | 0.2670 | 0.2240 | 0.1480 | -0.0110 | 0.0680 | 0.1930 | 0.2130 | Uij |
| H1 | $H_{1.0}$ | 0.2787 | 0.0818 | -0.0252 | • | • | • | • | • | • | 0.0440 | Uiso |
| H2 | $H_{1.0}$ | 0.2846 | 0.9016 | -0.0133 | • | • | • | • | • | • | 0.0470 | Uiso |
| H4 | $H_{1.0}$ | 0.9204 | 0.7238 | 0.0295 | • | • | • | • | • | • | 0.0480 | Uiso |
| H5 | $H_{1.0}$ | 0.9237 | 0.9078 | 0.0179 | • | • | • | • | • | • | 0.0430 | Uiso |

### To add a new site to the list:

1. Either:
   - Double-click on an empty row, *or*
   - Click the + button.

   A new row appears with its first field highlighted.
2. Type a label (no spaces please) in the **Label** field, to identify your site. We strongly recommend that you choose a unique label for each site.
3. Tab to the **Occupancy field** and enter the chemical occupancy for this site:
   - If this site is fully-ordered, just type the element symbol, e.g., "Si".
   - If this site is disordered, you can enter a chemical formula, e.g., "**Si 0.7 Al 0.2 Ge 0.1**". You can have as many occupants as you like, but the total occupancy must not exceed 1 (please see the box for important information about disordered sites).
4. Press the **tab** key to move the next field and enter a fractional *x* coordinate for the site. Repeat for the *y* and *z* coordinates.
5. If required, tab to the atomic displacement parameter fields and enter the appropriate data. Use the **Type** popup menu to specify what type of displacement parameter is required.
6. Press the **return** key or click outside the row to finish editing.

### To edit an existing site:

1. Click on the item you wish to edit so that it appears highlighted.
2. Enter a new value, then press the **return** key, or **tab** to the next field.

### To delete a site:

1. Select the site row.
2. Press the – button to delete the site.

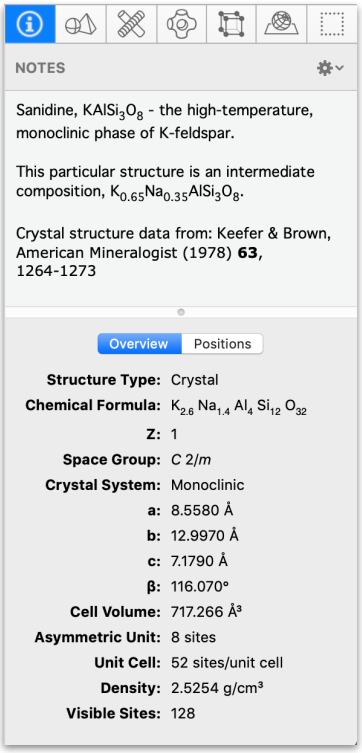
## Generating a Crystal Structure

Once you have defined symmetry, entered lattice parameters and added atoms to the asymmetric unit you simply need to click the **OK** button to generate a crystal structure with these parameters. CrystalMaker will generate one unit cell for you—but without any bonds or polyhedra. These are discussed later in this chapter.

## Structure Info

The Info Inspector includes two panes: the Notes pane is a rich-text editing field shown at the top of the Inspector; at the bottom is an information pane with data about the current structure (in the case of a multi-structure display, the information shown is for the *primary selection*).

The Info Inspector, showing its tab bar at the top with the Notes pane below, and the automatically-generated Info pane on the bottom.




### To show the Info Inspector:

Do one of the following:

- Click the Info icon ⓘ in the Inspector's tab bar.
- Choose **View > Inspector > Info**.

### Notes Pane

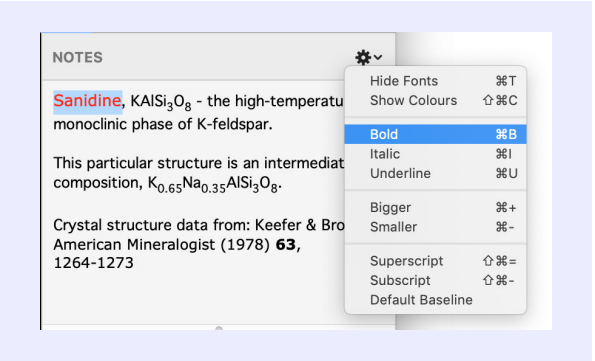
At the top of the Info Inspector is a rich-text editing field where you can add general information about your structure.

> **Searchable Notes:** Your notes can be searched in the Library window. It is therefore useful to include as much information about your structure as possible, e.g., author and structure names and any other descriptions that you may find helpful in future searches.

CrystalMaker supports multi-byte (unicode) script systems such as Japanese and Korean. You can also use styled text, with different fonts, styles, colours, superscripts and subscripts. Drag-and-drop editing is possible and there is an undo command.

To edit selected text, use the Actions menu (or right click to display a contextual menu):-

Editing Notes using the Actions menu.




Formatted notebook text is saved in a CrystalMaker binary file, together with a plain text alternative for use in older versions of the program. Please note, however, that most of the notebook text will be lost if you *export* the structural data to a non-CrystalMaker file format such as CIF or PDB.

## Info Pane

The Info pane, shown at the bottom of the Info Inspector, provides two or three tabs with automatically-generated information about your structure.

The **Overview** tab includes the bulk formula of your crystal (or molecule) and the display formula (which corresponds to the *visible* atoms on screen at any one time). For crystals, the spacegroup, crystal system and lattice parameters are shown, plus cell volume, density and site density (numbers of atoms per cubic Å).

Two additional tabbed panes are provided to list atomic **Positions** and (where relevant) atomic displacement parameters—or "(Thermal) **Ellipsoids**".

# Atom Colours & Radii

When you define a new structure, CrystalMaker attempts to match your element symbols with those in its current elements table. For each successful match, element radius and colour values are retrieved. This saves you from having to manually define atom colours and radii each time you edit a new structure.

CrystalMaker relies on atomic radii for bond and polyhedra generation. However, atomic radii vary from structure to structure, depending on the type of bonding (ionic, covalent) and the degree of coordination involved. CrystalMaker provides default element tables for atomic-, covalent-, Van-der-Waals- and ionic radii.

The element tables also specify default colours. Some tables use the "CPK" colour scheme, which is widely used by organic chemists. Unfortunately the range of standard CPK colours is rather limited (many "exotic" elements have the default "light pink" colour). For more vibrant and diverse colour sets, try exploring the range of non-CPK tables provided.

## Choosing an Element Table

Atomic radii are more than just about aesthetics. CrystalMaker uses the sum of atomic radii (plus 15%) as a guide for deciding which bonds to generate. This means that if your atomic radii are inappropriate for your current structure type, automatic bond generation may fail. It is therefore crucial to apply the correct element table before you start working with new structures.

### For inorganic structures we recommend:

- **Shannon & Prewitt Ionic "Crystal" Radii** (This is pre-installed as the default element table.) These radius values correspond to the Shannon & Prewitt "crystal radii" (Shannon & Prewitt, 1969; Shannon, 1976) and are suitable for general purpose work with inorganic structures which do not show strong covalent bonding.

### For organic structures choose one of the following:

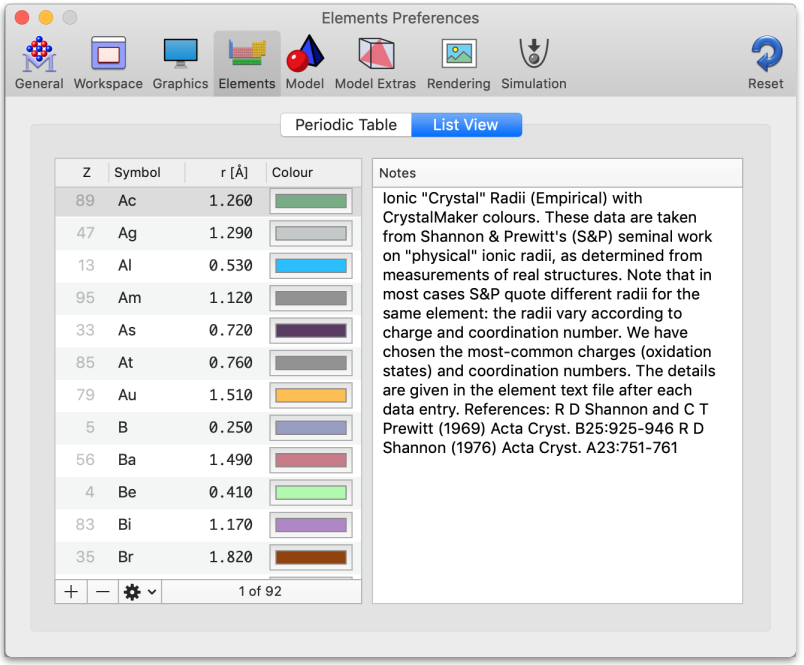
- **CSD CrystalMaker Covalent Radii** (these data are designed to work with CrystalMaker's bond search algorithms).
- **CPK Covalent Radii** ("CPK" colour scheme)
- **CPK Van-der-Waals Radii** (good for space-filling models)

## Editing Global Colours & Radii

You can view and edit the contents of CrystalMaker's current elements table using the **Elements** pane in the Preferences panel. (To display the elements panel, choose: **CrystalMaker > Preferences** on Mac, or **Edit > Preferences** on Windows).

The Elements pane offers a choice of two tabbed views: a list view, or a table view. The List View includes buttons for adding or removing elements from an existing table. An Actions button (cog icon) includes a popup menu with commands to switch between different preset element tables. You can also import another element table, saved as a text file, into the program.

The Elements Preferences pane in "List View".




### To load a different element table:

1. Click the Actions button to display its popup menu.
2. Select **Load Preset** and choose an element table from its submenu.

### To save a custom element table:

1. Click the Actions button to display its popup menu.
2. Choose: **Export Data**.
3. Specify a filename and location in the file dialog that appears. A text file will be generated containing your element definitions.

Please refer to *Chapter 14: Data Import/Export* for the Elements File format.

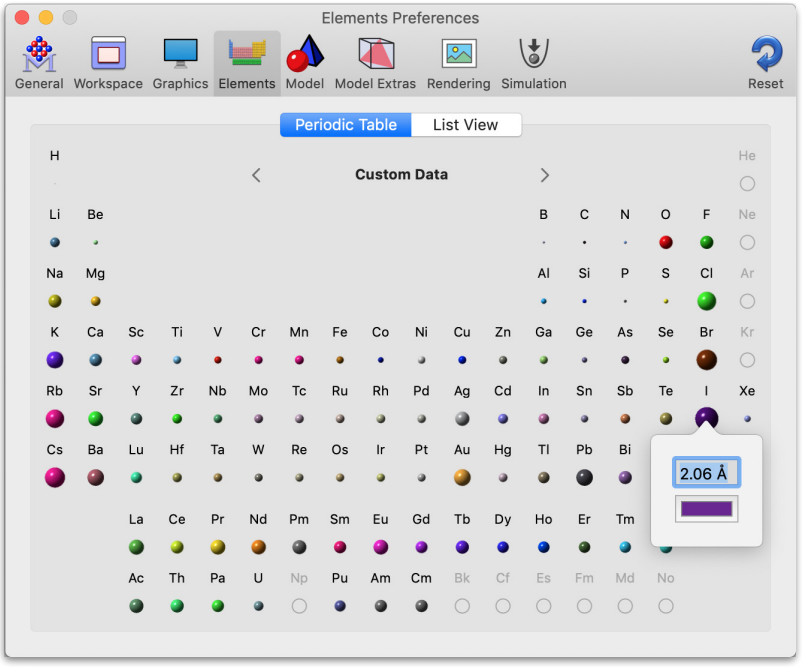
### To edit an existing element definition:

1. Locate the element row to be edited.
2. Click on the **Radius** field, enter a new value, then press the **return** key.

3 Click on the **Colour** button and choose a new colour from the Colour Picker that appears.

> **Apply Element Tables Directly:** You can use the Atoms Inspector's contextual menu to reset a structure's colours and radii to those of the current element table. You can also apply other element tables—all without affecting your default settings.

The **Periodic Table** view allows you to quickly browse through different preset tables, using the popup menu provided. You can also edit individual element colours and radii by clicking on an atom sphere and choosing a new colour or radius from the popover that appears:



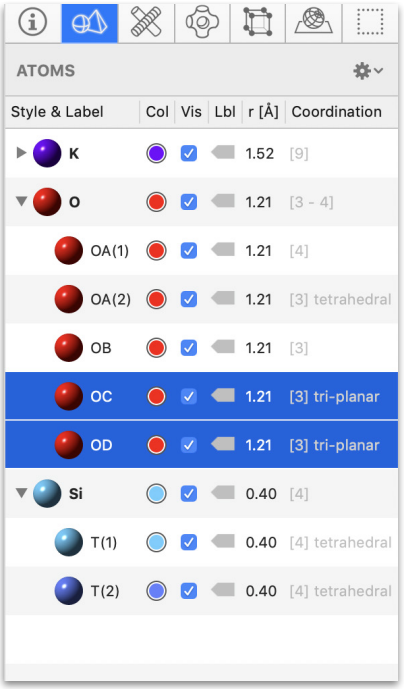

The Elements Preferences pane in "Periodic Table" view, with an element being edited.

Periodic table of the elements showing covalent radii and CPK colours.

The Shannon & Prewitt (S&P) ionic crystal radii, using CrystalMaker colours.

## Using the Atoms Inspector

The Atoms Inspector displays atom style, colour, visibility, labelling, radius and coordination information for all sites, grouped by chemical element.




The Atoms Inspector showing sites in the orthoclase structure, grouped by chemical element. The "O" and "Si" element rows have been opened to reveal their corresponding sites. Two oxygen sites, O4 and O5, have been selected.

You can use the Atoms Inspector to edit information in one of three ways:

- For an individual site row;
- For an element row (any changes that you make are automatically applied to *all* sites with that element type);
- For one or more *selected* site rows. You can select a row by clicking on it; **shift**-click to extend the selection, or **command**-click to make a discontiguous selection.

**Streamlined Interface:** Users upgrading from an earlier version of CrystalMaker may be interested to know that the Atoms Inspector combines the old "Site Browser" with the "Atoms" pane of the former Model Inspector.

### To display the Atoms Inspector:

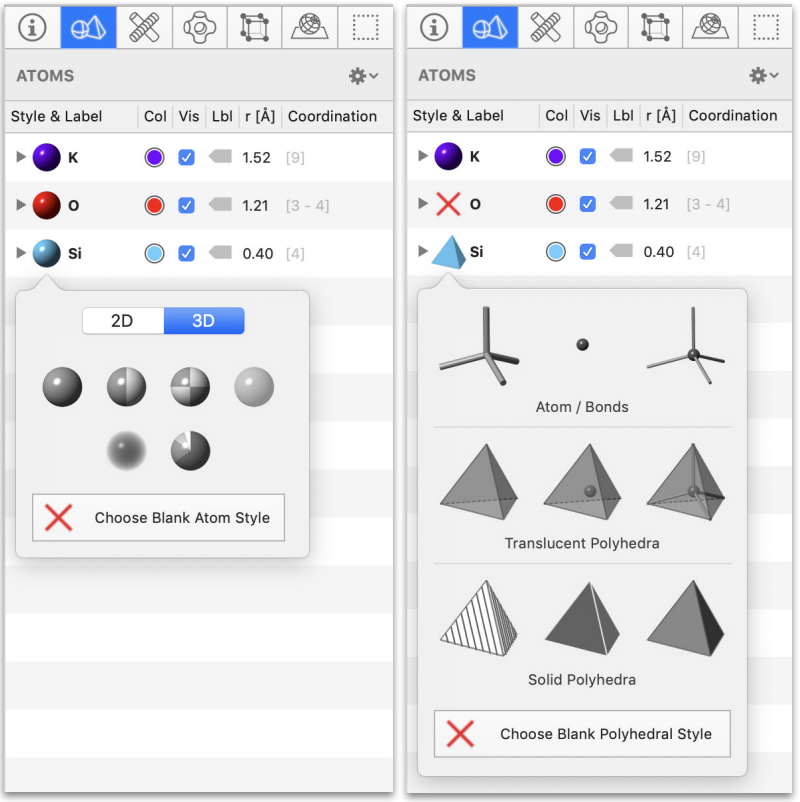
Do one of the following:

- Choose: **View** > **Inspector** > **Atoms**.
- Click the **Inspector** button in the toolbar, then select the Atoms icon ( ) in the Inspector tab bar.

## Changing Atom Styles

You can change the atom sphere, ellipsoid or polyhedral style by clicking the preview icon on the left-hand side of the list row. (Again, any changes made to an *element* row are automatically applied to all atoms with this element type.)

The preview icon depends on the current model type. So, to change an atom sphere style, you would need to be viewing a Ball-and-Stick or Space-Filling model; to change an ellipsoid style, you would need to be viewing an Ellipsoids model; and to change a *polyhedral* style, you would need to be viewing a Polyhedral model. (Use the Model menu to switch between different model types, or use one of the handy keyboard shortcuts provided.)




Editing atom styles for all Si atoms in the orthoclase structure. Left: sphere styles shown for a Ball-and-stick model; right: polyhedral styles shown for a Polyhedral model.

## Column Settings

In addition to changing atom styles, you can change element types, labels, colours, visiblity status, labelling visibility and radii:

- Double-click a **site label** to edit its text. If the row is an *element row*, you can change the **element symbol**; this will then change the occupancy for any atoms associated with that element symbol.

- Use the **Col** column to change the element and/or site colour.
- Click the **Vis** checkbox to toggle the visibility of a particular site or all atoms with that element. (Note that, for a crystal structure, atoms will be made visible within the current plot range.)
- Click the luggage-tag icons in the **Lbl** column to show or hide atom labels. These are text strings that appear next to the atoms and which move with the atoms as the structure is rotated or scaled. (You can edit the label positioning and content using the **Labels** group in the Model Inspector.)
- Use the "**r [Å]**" column to edit atomic radii (this overrides any settings from the current element table). Note that the radii being edited are the space-filling radii.

**Custom Columns:** CrystalMaker provides two default column layouts: Standard (as illustrated on the previous page) and Coordinates (which summarizes site labels, their occupancies, fractional or structural coordinates, and multiplicities). You can use the Actions menu's Show Columns submenu to customize the column display. Note that rows can still be selected and you can then use a contextual menu to toggle visibility or atom labels—even when the "Vis" or "Lbl" columns themselves are hidden.

### Applying a Different Element Table

The Atoms Inspector's **Actions > Radii** submenu has commands to load a preset element able and apply its radii to any matching elements in the current structure. This is useful, for example, if you wish to switch to, say a Van-der-Waals model (where atom spheres are depicted larger than their usual covalent radii).

## Automatic Colouring Options

The Atoms Inspector's contextual menu includes commands to automatically apply a spectrum of colours to different sites. You can colour by:

- Element
- Coordination Number
- Molecule
- Site

Colouring by element simply applies the current element row colour to all atoms or sites associated with that element. Colouring by *coordination number* applies a range of colours from blue to red, with red corresponding to the most-highly-coordinated sites or atoms. This is a good way to visualize disordered structures, making the variations in bonding readily apparent.

If you have a *molecular crystal*, CrystalMaker can differentiate different molecules in the structure using different colours. Finally, colouring by *site* applies unique colours to each site in the structure.

**To reset all colours to the current element table colours:**

1. Click the Actions popup menu button to display its menu.
2. Choose the **Colour > Use Default Colours** command.

### Synchronizing Colours and Radii

If you are working with a multi-structure document, you can use the Actions menu to apply colours and atomic radii to all structures in the document. The following commands are available:-

- **Colour > Apply to All Structures**
- **Colour > Apply Defaults to All Structures**
- **Radii > Apply to All Structures**
- **Radii > Apply Defaults to All Structures**

These commands will be useful if you wish to reset all structures to the default colour or radii values—or if you wish to use the currently-visible structure as a "template", and have its colours and radii applied to the remaining structures in the document.

## Defining Bonds

You can request bonds to be generated between specific atom types (elements) in your structure, and within a specific distance range. CrystalMaker allows unlimited numbers of bonds per site, although it is best to ensure that your bonding is at least physically reasonable!

### Primary vs Secondary Bonds

Unlike earlier versions of the program, CrystalMaker X has two classes of bonds: Primary and Secondary:

- Primary bonds are "first class" bonds, used to indicate strong bonds (e.g., within a molecule). These are used when generating coordination polyhedra and when searching for individual molecules in an extended structure.
- Secondary bonds are designed for depicting inter-molecular interactions, and are ignored by the program when determining what constitutes a molecule, or when generating coordination polyhedra.

### Coordination Polyhedra

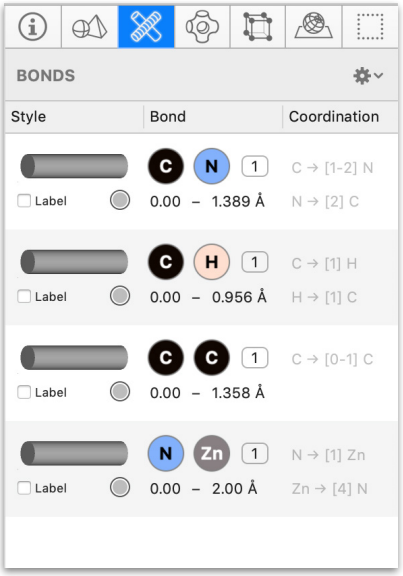
When CrystalMaker generates bonds, it also searches for, and generates coordination polyhedra. All you have to do is to use the Atoms Inspector to choose what sort of polyhedron should be displayed for each site for a "Polyhedral" model.

## Using the Bonds Inspector

CrystalMaker's Bonds Inspector (one of the panes available in the Inspector) provides a key to the bond *specifications* in your structure: these are requests for specific bonds to be generated automatically. (Note that you can also define bonds on a per-atom-pair basis, but these are "on offs", and so will not be shown in the Bonds Inspector.)

Navigate to the Bonds Inspector by clicking its icon in the Inspector tab bar ( ), or by choosing: **View > Inspector > Bonds**.

Each row in the Bonds Inspector is a separate *Bond Specification*. You specify a distance range within which bonds should be generated between the "from" and "to" element symbols. You can also specify bond *styles*, colours and whether the bond should be treated as a *Primary* bond (e.g., an intra-molecular bond) or a *secondary* bond (e.g., an inter-molecular bond, or simply a distance measurement, used for 3D annotation purposes). You can edit any existing bond specifications by clicking and editing their values.



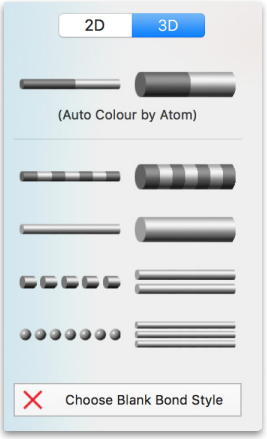

The Bonds Inspector, showing a series of bond specifications for an organic structure.

### To add a new bond specification:

1 Add a blank bond specification by doing one of the following:-

- Double-click on a blank list row *or*
- Click the Actions button (cog icon, top right) and from its drop-down menu, choose: **Add Bond Specification**.
- Right-click in the list and choose: **Add Bond Specification** from the contextual menu.

2 Click the **Style** preview and choose a new bond style from the Bond Style popover that appears. A range of 2D ("line art") and 3D (rendered) styles are available, including thick or thin bonds, double-, triple bonds plus dotted and dashed cylinder styles.




The Bond Style popover, showing a range of 3D (rendered) bond cylinder styles.

3 Depending on your choice of bond style, either one or two colour buttons will be displayed beneath the bond style preview, letting you customize the colouring.

4 Use the pair of element popup menu buttons to choose "**From**" and "**To**" element symbols. Notice that CrystalMaker will choose a default maximum distance value, calculated as the sum of radii plus 15%—but this is something you can edit…

5 Edit the distance range by clicking on the pair of distance values below the coloured element popup menu buttons. Press the return or enter keys to replot the structure with your new values.

Notice that the Bonds Inspector provides coordination previews for atoms with the "From" and "To" element symbols.

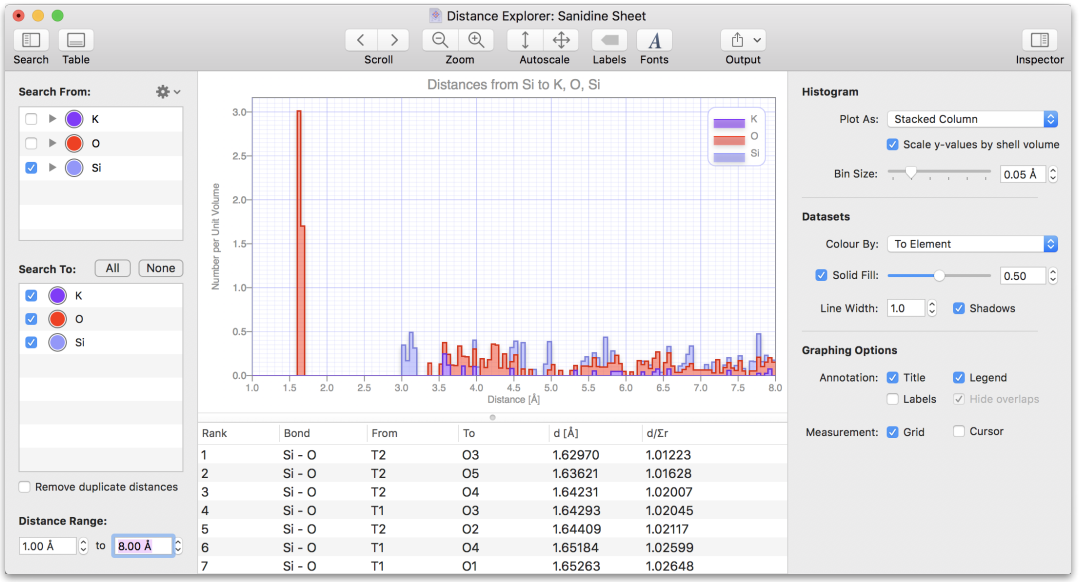
### To delete a bond specification:

1 Select the appropriate row by clicking on its row number.

2 Press the **delete** key on your keyboard, or right-click and choose: **Remove Bond Specification**.

## Exploring Distances

It can be difficult to decide what is the most-appropriate distance range to use for particular bonds. Whilst the coordination previews in the Bonds Inspector can help, the *Distance Explorer* is a better starting point, showing the number of *neighbours* as a function of distance in the structure.




A Distance Explorer window for a silicate structure, showing bonds from Si to all other elements in the structure.

The Explorer window is divided into three parts: controls for specifying the search parameters (in the lists, on the left), a display area (with histogram at the top and a list view at the bottom) and an Inspector on the right, with controls to customize the graph.

**Multi-Touch:** The graph supports standard multi touch gestures for zooming and scrolling.

### To display the Distance Explorer:

Do one of the following:

- Click the **Distances** button in the toolbar.
- Choose: **Calculate > Explore Distances**.

### To start a distance search:

1. Locate the element or site you wish to search *from* in the **Search From** list. Ensure that the checkbox is set. (If you wish to search from a specific site, rather than all sites for the same element, click the disclosure triangle to the left of the element symbol to reveal all sites containing that element.)

2. Select the elements you wish to search *to* in the **Search To** list.
3. If necessary, adjust the **Distance Range** fields, then press the return or enter keys to start a search.

### Manipulating the graph

Use standard multi-touch gestures to scroll and zoom the graph (or use the toolbar's scroll, zoom and scaling buttons). Click in the graph to display cursor, which you can drag anywhere to measure the graph.

### Graphing options

CrystalMaker lets you change the graph type (e.g., histogram vs. area graph; stacked vs. unstacked) and specify whether y-values (numbers of neighbours as a function of distance) should be scaled according to the shell volume or not. (Scaling will result in a display of neighbours per unit volume—which is akin to a pair-distribution function.)

You can also change the bin size (i.e., the width of individual histogram columns), edit line widths, shadows and opacity, display a graph title title, legend, labels and grid.

### Saving data and graphics

Click the toolbar's **Output** button to display a popup menu with options to:-

- Copy the graph to the clipboard.
- Export the graph to a graphics file.
- Save the graph data (histogram columns) as a text file, for use in an external charting program.
- Save the table of data (Rank, Bond, From, To…) as a text file.

Note that you can also drag-and-drop the graph into another program.

# Saving Your Document

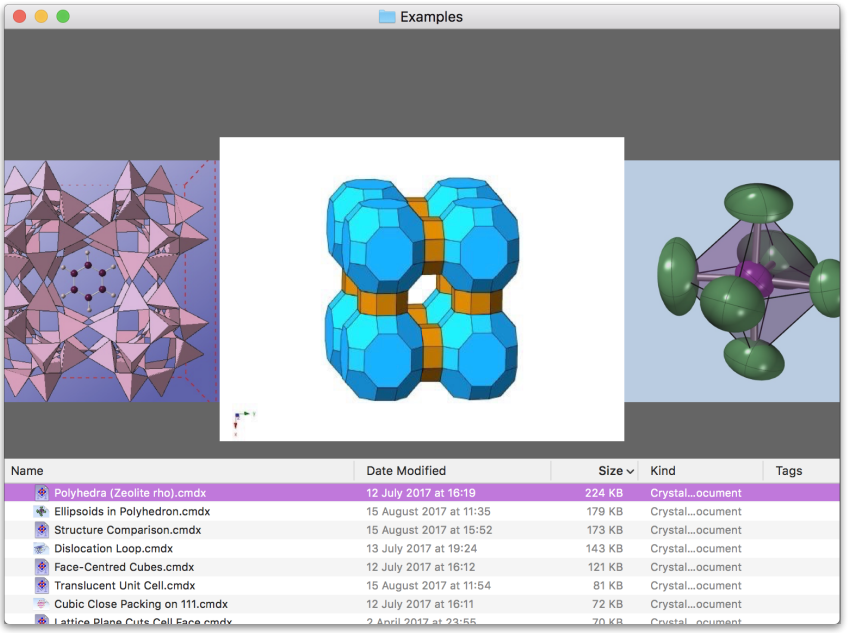
When using the **File** menu's **Save** or **Save As** commands, structures are saved using the CrystalMaker X document format (CMDX).

## CrystalMaker X Document Format

If you wish to save every detail of the current crystal plot and wish to be able to display the crystal very quickly, then you should save the crystal as a CrystalMaker X document, with extension ".cmdx".

CrystalMaker documents can contain multiple structures. Each structure retains all the atomic coordinates and bond specifications, to speed up the re-display; the downside is that some file sizes can become quite large, but this is increasingly less of a problem on modern systems.

CrystalMaker documents contain embedded previews. These images are used in the Library Browser and may also be displayed in your operating system.




CrystalMaker binary files, with their embedded previews, as displayed on Mac OS X in its "Cover Flow" mode.

## Exporting a Text File

You can export your structural information to a range of different structures files formats, some of which can be understood by other programs (e.g., the ubiquitous CIF format). Please note that none of these formats has the same richness as a CrystalMaker document: they lack embedded previews, metadata, and the full structural "snapshot" that CrystalMaker saves in its own documents.

### CrystalMaker Text Files

One of the export formats you can use, the CrystalMaker text format (CMTX), is designed to be human-readable, and is very easy to work with. This is ideal if you need to automate structure generation, using your own scripts or computer programs.

CrystalMaker text files contain the asymmetric unit (for crystals) or orthogonal coordinates (for molecules), plus a series of plot commands. The files are very compact, but can take some time to load, as CrystalMaker has to regenerate the entire structure before an image can be displayed on-screen.

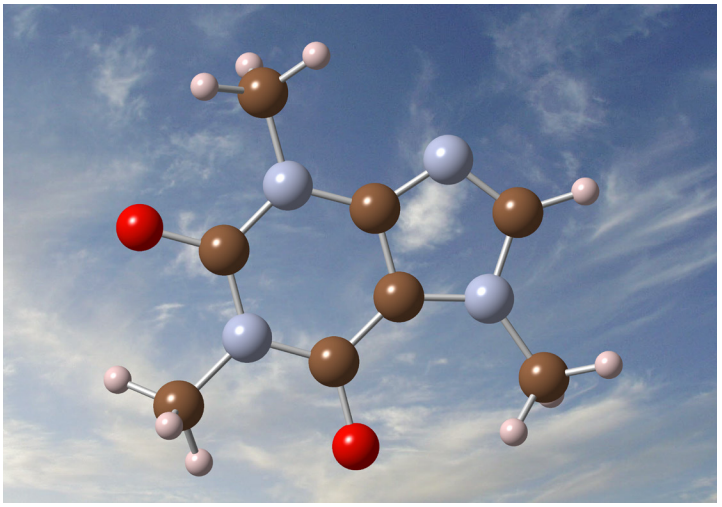
**CMTX File Format:** See *Appendix B: CrystalMaker Text Format* to learn more about this format.

Chapter 6

# Building Molecules

This chapter describes how to create new molecules (or atom clusters). It also introduces some atomic manipulation tools for designing new structures and creating defects. You can use some of these tools to edit crystals too—or you can convert a crystal into a "molecule" for extensive and interactive manipulation.

We define a "molecule" as an isolated ensemble of atoms, with no long-range periodicity (c.f. our definition of a "crystal" in Chapter 4).



## Techniques for Building a New Molecule

You can create a new molecule in one of four ways:

- By pointing-and-clicking in an empty window with the **Add Atom** tool.
- Using the Molecule Editor to enter a list of atomic positions.
- By converting an existing, *crystal* structure to an isolated "molecule".
- By creating a text file containing atomic coordinates, which can be opened by CrystalMaker (see *Chapter 14: Data Import/Export*).

## Point-and-Click Molecule Building

CrystalMaker lets you build molecules from scratch, simply by clicking with the mouse to define atomic positions and their bonding. You can opt to have hydrogen atoms added to your molecule automatically, and then minimize the molecule's energy to optimize its geometry. The basic workflow is as follows:-

1. Define your molecule's backbone.
2. Add hydrogen atoms automatically.
3. Relax the molecule.

### Define the Molecular Backbone

You can use the **Add Atom** tool to add new atoms at any clicked point. You can also generate bonds between successive clicked positions.

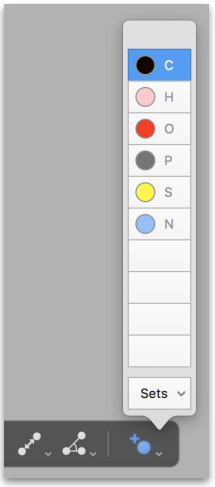
#### To build a bonded molecule:

**1** Start with an empty window (**File > New Window**) or, to add a new molecule to an *existing* window, choose: **File > Add to Window > New Empty Molecule**.

**2** Choose the **Add Atom** tool ( ) from the Tool Strip.

**3** Click the popup menu indicator just to the right of the **Add Atom** tool, to display the Atoms palette.

The Add Atom palette.



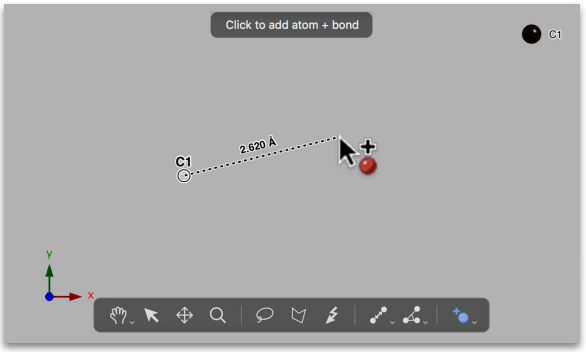

**4** Specify what sort of atom to add by selecting its element symbol from the Atoms palette.

(If the symbol you require isn't visible, click and hold an empty button to choose a symbol from a popup menu—or choose a different element set from the **Sets** popup at the bottom of the palette.)

5 Click anywhere in the empty window to add your first atom. Note that it is shown highlighted, indicating that this is an "anchor" for a possible new bond. You can change this anchor by clicking on any existing atom with the **Add Atom** tool.

6 Repeat steps 3 and 4, as necessary. If you wish to add bonds at the same time as atoms, simply hold down the **shift** key as you click and a bond will be generated to connect the new atom with the previous (highlighted) atom:-

Adding bonding by holding the shift key down with the Add Atom tool active.




If you make a mistake and add the wrong atom type, you can easily change its element type. Firstly, ensure that the atom is highlighted, then choose the correct element symbol from the Atom Picker palette, and finally click on the atom for a second time; you will then be prompted to confirm the change.

You can also add bonds to any pair of atoms: simply highlight the first atom, then **shift**-click on the second atom to bond it.

**Adding Equivalent Bonds:** Another way to quickly add bonds is to shift-click on a pair of atoms with the **Add/Delete Bond** tool. This will generate all similar bonds in one step.

## Add Hydrogens

CrystalMaker can automatically add hydrogen atoms to any molecule, via the **Transform > Add Hydrogens** command (or the **Add H** toolbar button). The program assumes that the structure needs to be *fully saturated* and performs a relaxation on the new hydrogens to yield an optimum geometry (the positions of pre-existing atoms are not relaxed, thereby making this command suitable for adding hydrogen atoms to molecular structures refined using X-ray data).

The hydrogen positions should refine quickly—but if you wish to stop the relaxation, you can do this by clicking the **Stop Relaxing** button in the toolbar, or by choosing the same command from the **Transform** menu.

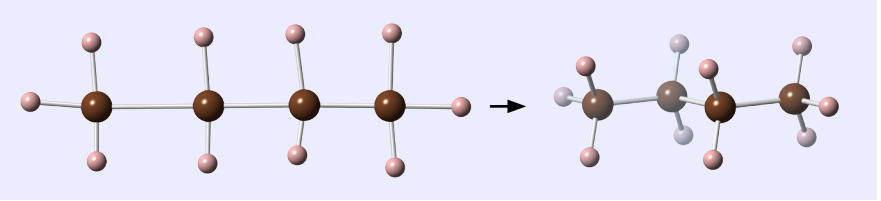
**Double or Triple Bonds:** if you require double or triple bonds (e.g., taking a C—O unit and adding hydrogens to make $H_2C{=}O$ instead of $H_3C{-}OH$), you will need to delete (not hide) some of the newly-added hydrogen atoms. To delete atoms, simply select them and press the **delete** key.

### Add Hydrogens to Selection

If you have one or more selected atoms in your molecule, the **Add Hydrogens** command changes to **Add Hydrogens to Selection**, allowing you to be specific about which sites should have hydrogens attached.

## Relax Molecule

Energy modelling is built into CrystalMaker, via the **Transform > Relax Molecule** command, making it easy for you to design your own structures and obtain realistic geometries.



Relaxing a hand-drawn propane molecule (left) to yield a 3D molecule (right).

Please note that this command is only available for *molecules*, and not for crystals. You will also need to ensure that all atoms in the molecule are bonded, as bonding information is vital for the modelling calculation.

It is also possible to relax only part of a structure, (e.g., a side-chain of a molecule, or atoms on a surface), instead of the entire molecule. One simply needs to select the atoms to be relaxed, and click the **Relax** button in the window toolbar (or choose: **Transform > Relax Selection**).

CrystalMaker uses a smart algorithm to minimize the energy of any molecule—even a crude, two-dimensional "hand-drawn" model that is way outside equilibrium. No special input is required—you don't need to specify what type of potentials to use. You can even rotate and scale the molecule during the course of the relaxation!

**Energy Minimization:** Users upgrading from CrystalMaker 9 may be interested to know that CrystalMaker X uses a very-different algorithm. Absolute energies are now employed—and displayed, interactively, during the course of the relaxation. You can also measure the energy of an arbitrary molecule via the **Calculate > Energy** command.

### How the Algorithm Works

CrystalMaker takes a rather unique approach to energy modelling. A "Force-Field" calculation (see box)—employing a hybrid *Monte Carlo* and *Least Squares* technique—uses high-quality potential parameters calibrated by "DFT" calculations.

## Energy Modelling Basics

There are essentially two ways of minimizing the energy of a molecule: a fundamental, "DFT" calculation; or a so-called "Force Field" model.

### DFT Calculation

In the DFT ("Density Functional Theory") approach, one attempts to solve the Schrödinger equation for the complete system. This sounds like an ideal way, but unfortunately, beyond hydrogen, things become a little more complicated…

For real world systems, DFT calculations become bogged down—which rules out real-time calculation—and can require a supercomputer for systems with more than a hundred-or-so atoms.

To have any hope of success, DFT calculations require a starting state very close to its final, relaxed state: so one effectively needs the answer before one begins. Note that this also rules out relaxing hand-drawn models.

Another problem is that dispersions (e.g., weak Van-der-Waals bonds in Graphite) cannot be adequately handled (a so-called Grimmé Dispersion Correction is required) which means that, for larger systems, DFT relies on parameterised terms.

### Force Field Model

By contrast, the "Force Field" approach is much faster, and can cope with more complex systems, including those with dispersion forces, and (critically for Earth Scientists, Materials Scientists and Inorganic Chemists) silicate structures: the most-important rock-forming minerals including all zeolites, natural or synthetic.

Parameterised potentials are used to model the various interactions between atoms (e.g., pair potentials, bond-bending and torsional terms). As a result, complex structures can be relaxed on a desktop system, in real time. However, the quality of the results does depend on the quality of the potentials used!

The use of the *Monte Carlo* (simulated annealing) technique means that highly non-equilibrium structures (i.e., crude, hand-drawn 2D molecules) can be relaxed. As the resulting energy is minimized there is a crossover to a second, *Least Squares* technique: this provides a finer-scale relaxation close to the molecule's equilibrium state.

CrystalMaker's algorithm is designed to be accessible and low risk. The modelling takes existing bonding and coordination environments into account, and will infer carbon hybridisation (e.g., $sp^2$ and $sp^3$)—so there is no need to specify single, double or triple bonds. CrystalMaker handles torsions and will search for rings, so that the appropriate set of potentials can be used.

As part of the modelling process, CrystalMaker uses a standardized set of interatomic potentials. These comprise the best-available *Molecular Mechanics 3* (MM3) and *Universal Force Field* (UFF) potentials for short-range interactions, plus long-range *Williams* and UFF potentials (see references below).

Multi-threading ensures that the program remains as responsive as possible during the refinement process. The structure is updated at each stage of the calculation, and can continue to be rotated at all times. Use the **Transform > Stop Relaxing Molecule** command to cancel the refinement at any time.

### Energy Graph

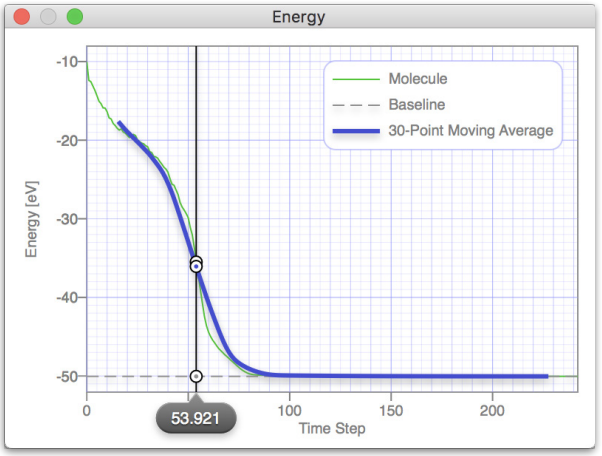
CrystalMaker displays an energy graph during the course of the relaxation; this may show a series of peaks, as the Monte Carlo algorithm explores (and rejects) different arrangements. An averaged energy curve is superimposed, as a guide to the eye. If you repeat an energy minimization in the same window, you can compare multiple curves in the same energy graph.

You can customize the Energy Graph by right-clicking in the window to display a contextual menu with commands to:

- Copy or Print the graph.
- Toggle the Legend or Grid.
- Toggle the Baseline (this shows the minimum energy).
- Toggle Zero Lines (if relevant) e.g., to emphasize a line passing through $y = 0$.
- Toggle the moving average and/or a moving minimum.
- Change the graph style (e.g., lines, markers, lines + markers).
- Clear the graph.

By default, the graph will vanish once the relaxation has been completed. However, you can bring the energy graph back at any time by choosing: **View > Show Relaxation Energy Graph**.

The energy graph, showing a cursor.




The energy graph can be resized and copied: you can click-and-drag its contents to another program, or right-click and choose various options from a contextual

menu. Clicking anywhere within the energy graph displays a cursor which can be used to measure energies (click-and-drag to move the cursor).

### Calculating Energies

You can measure the energy of a molecule at any time using the **Calculate > Energy** command. This can be useful for comparing the energies of different systems.

#### Energy Modelling References

Williams, D. E. (2001) Improved intermolecular force field for molecules containing H, C, N, and O atoms, with application to nucleoside and peptide crystals. Journal of Computational Chemistry 22:1154.

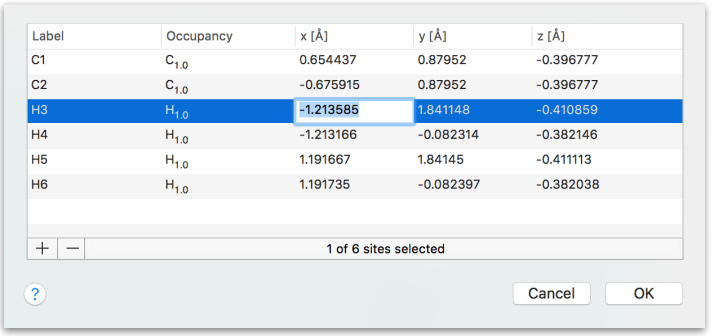
Allinger, N.L., Yuh, Y. H. , Lii, J. H. (1989) Molecular mechanics. The MM3 force field for hydrocarbons. Journal of the American Chemical Society 111:8551.

Lii, J.A. and Allinger, N. L. (1991) The MM3 force field for amides, polypeptides and proteins. Journal of Computational Chemistry 12:186.

Rappé, A. K., Casewit, C. J. , Colwell, K. S. , Goddard, W. A., Skiff W. M. (1992) UFF, a full periodic table force field for molecular mechanics and molecular dynamics simulations. Journal of the American Chemical Society 114:10024.

## The Molecule Editor

Choose **File > Add to Window > New Molecule** to add a new molecule to an existing window, or **Edit > Structure** to edit an existing one. The Edit Molecule window appears. A scrolling list of atoms displays atom labels, coordinates and occupancies. You can make the window taller to show more atoms.



| Label | Occupancy | x [Å] | y [Å] | z [Å] |
|---|---|---|---|---|
| C1 | $C_{1.0}$ | 0.654437 | 0.87952 | -0.396777 |
| C2 | $C_{1.0}$ | -0.675915 | 0.87952 | -0.396777 |
| H3 | $H_{1.0}$ | -1.213585 | 1.841148 | -0.410859 |
| H4 | $H_{1.0}$ | -1.213166 | -0.082314 | -0.382146 |
| H5 | $H_{1.0}$ | 1.191667 | 1.84145 | -0.411113 |
| H6 | $H_{1.0}$ | 1.191735 | -0.082397 | -0.382038 |

1 of 6 sites selected

Cancel OK

The Molecule Editor, showing an x-coordinate being edited.

### To add a new atom to the list:

1. Either:
   - Double-click on an empty row, *or*
   - Click the **+** button.

   A new row appears with its first field highlighted.
2. Type an atom label into the label field.
3. Press the **tab** key to move to the **Occupancy** field and enter the chemical occupancy for this atom:
   - If this atomic site is ordered with respect to a particular element, type the element symbol, e.g., "C".
   - If this site is disordered, enter up to three elements and their fractional occupancies (as a chemical formula), e.g., "`Si 0.7 Al 0.2 Ge 0.1`". The total occupancy must not exceed 1.
4. Press the **tab** key to move to the next field and enter the atom's *x* coordinate in Å units. Repeat for the *y* and *z* coordinates. Unlike for crystals, molecular coordinates are defined in absolute terms, with an orthogonal (Cartesian) basis.
5. Press the **return** key or click outside the row to finish editing.

### To edit an existing atom:

1. Double-click the cell you wish to edit.
2. Enter a new value, then press the **return** key to finish, or **tab** to the next field in the row.

### To delete an atom:

1. Select the row by clicking on it (click-and-drag to select multiple atoms).
2. Press the **–** button.

# Generating Bonds & Polyhedra

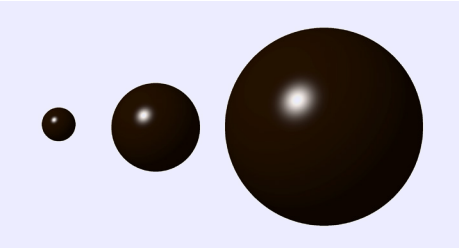
To display bonds between atoms (and hence polyhedra), bonding must be defined. This can be achieved in various ways:

- By specifying your bonding requirements in the Bonds Inspector ( in the Inspector's tab bar), as described in *Chapter 5: Building Crystals*.
- Automatically, via the **Transform** > **Auto-Generate Bonds** command.
- By defining individual bonds by shift-clicking with the **Add Atom** tool (as described earlier in this chapter).
- By defining individual bonds with the **Add/Delete Bond** tool.

## Automatic Bond Generation

The **Transform** > **Auto-Generate Bonds** command is often the most convenient way of generating bonds for a large molecule. CrystalMaker will search for atoms that lie within 15% of the sum of their radii and generate bonds accordingly. The resulting *bond specifications* may be found in the Bonds Inspector.

Auto bond generation will fail if your radii are too small—which may be the case for organo-metallic structures, if using CrystalMaker's default (ionic radius) settings. You can easily reset the radii for your structure, as described below.



Same atom, different sizes: relative sizes of a carbon atom plotted using ionic (left), covalent (centre) and Van-der-Waals radii (right).

### Applying a Different Element Table to the Current Structure

If you wish to apply a new set of element radii to the current structure you can use the Atoms Inspector:

1. Display the Atoms Inspector by clicking its icon in the Inspector tab bar (or choose: **View** > **Inspector** > **Atoms**).
2. Right-click anywhere in the Inspector to display a contextual menu.
3. Choose a new element table from the **Radii** submenu.

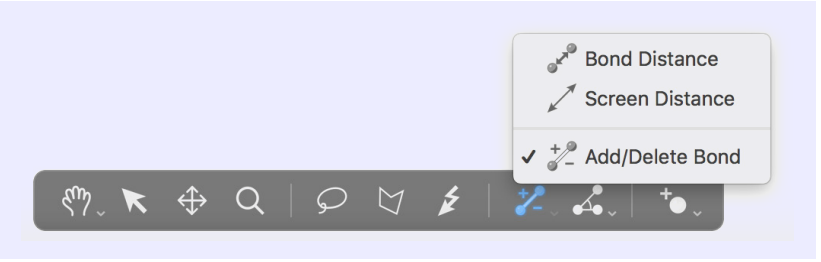
### Choosing a Default Element Table

The best approach is to define your most-appropriate set of atomic radii to be your default element table. You can do this using the **Elements** pane of the Preferences

panel (**CrystalMaker > Preferences**, Mac; **Edit > Preferences**, Windows). Once set, your default radii will be used for all new structures. You can also reset an existing structure's radii to the default values by using the **Radii > Use Default Radii** option on the Atoms Inspector's contextual menu.

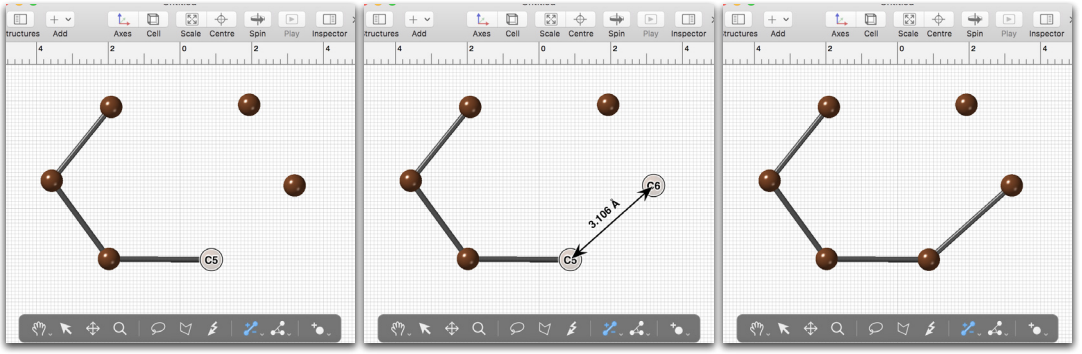
## Manual Bond Generation

You can create or destroy *individual* bonds by clicking on pairs of atoms with the **Add/Delete Bond** tool ( ). This tool is available via a popup menu in the Bonds group of the Tool Strip (click the popup menu icon—the inverted caret character—just to the right of the active Bond tool):




Choosing the Add/Delete Bond tool from the Tool Strip.

If no bond exists between the two clicked atoms then a new bond will be generated between them (using the default bond style shown in the **Bonds** pane of the Preferences panel). If, however, the two atoms are already bonded to each other, the bond will be destroyed.




Adding a bond with the Add/Delete Bond Tool. Left: The first atom is highlighted by clicking on it. Middle: the mouse is positioned over the second atom. Right: clicking on the second atom creates a bond to the first atom.

Clicking on individual bonds is fine for small molecules, but soon becomes tedious for larger ones. Fortunately, there's a shortcut: if you hold down the **shift** key when you first click with the **Add/Delete Bond** tool, CrystalMaker will search for, and generate all similar bonds in your molecule (or crystal).

# Editing Atoms Interactively

CrystalMaker has powerful tools for atom-level manipulation of crystal and molecular structures. You can *select*, *detach*, *move*, *rotate*, *duplicate*, *merge* and/or *delete* individual atoms or groups of atoms. You can also directly edit selected atoms.

**Use a Ball-and-Stick model.** For this kind of atom-level manipulation, you'll probably find it easiest to use a ball-and-stick model with perspective turned off and no depth fading. You may also find it useful to display grid lines in the graphics window (**View > Show Grid**).

## Selecting Atoms

If you wish to work with only part of the structure, you should *select* those atoms. Selected atoms are marked with yellow or red haloes, and can be saved to file, just like unselected atoms.

### To select individual atoms:

1. Choose the **Arrow** tool ( ) from the Tool Strip.
2. Click the atom you wish to select. The atom will be highlighted.
3. To select additional atoms, hold down the **shift** key whilst clicking atoms.

### To select atoms in a rectangular region:

1. With the **Arrow** tool active, click and drag to define a rectangular region.
2. On releasing the mouse, the selected atoms are shown highlighted.

### To select atoms in an angular region:

1. Choose the **Polygon** tool ( ) from the Tool Strip.
2. Click to define your first point, then release the mouse button.
3. Continue clicking at points around the atoms.
4. Click on your initial point to close the region and select atoms within.

### To select atoms in a curved region:

1. Choose the **Lasso** tool ( ) from the Tool Strip.
2. Click and drag to define an irregular, angular region around your atoms.
3. On releasing the mouse, all atoms within this region will be selected.

### To select all atoms in a molecular unit:

1. Select an atom with the **Arrow** tool.

2 Right-click anywhere in the Graphics Pane and choose: **Extend Selection > Molecule**. (Alternatively, choose: **Edit > Select > Molecule** from the menu bar)

### To select nearest neighbours:

1 Select an atom with the **Arrow** tool.

2 Right-click in the Graphics Pane and choose: **Extend Selection > Nearest Neighbours**. Repeat to select second, third, fourth… nearest neighbours (the keyboard shortcut is handy here!).

### To select all atoms in the same ring:

1 Select an atom with the **Arrow** tool.

2 Right-click in the Graphics Pane and choose: **Extend Selection > Ring**. Note that details about the ring—including a list of all atoms—are printed in the window's Output Log.

### To invert the atom selection:

- Choose: **Edit > Select > Unselected Atoms**.

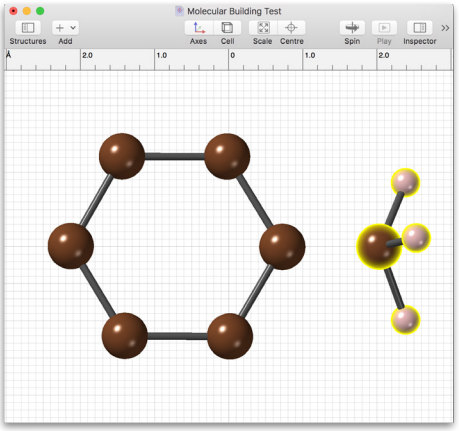
### To clear a selection:

Do one of the following:

- With the Arrow tool active, click on a blank region of the Graphics Pane.
- Choose: **Edit > Deselect All**.

## Moving Selected Atoms

With the Arrow tool you can click-and-drag selected atoms across the screen:

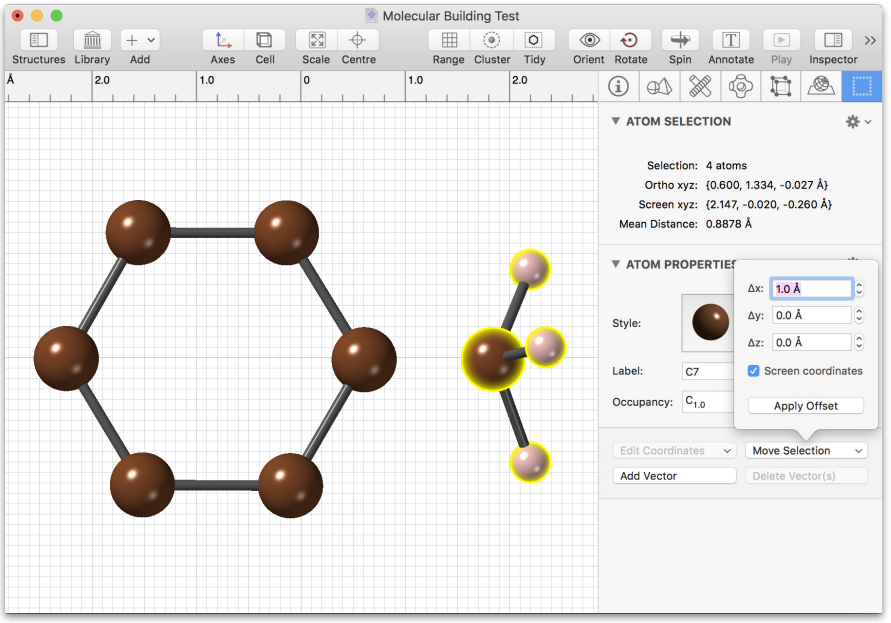



Moving a group of selected atoms (highlighted in yellow, at right) across the screen with the Arrow tool.

You can also move selected atoms using the arrow keys. Atoms are moved in one-pixel increments, or larger increments if the **shift** key is held down.

## Moving Selected Atoms

A more precise way of moving selected atoms, whilst keeping the rest of the structure intact, is to use the **Move Selection** option in the Selection Inspector.




Using the Selection Inspector to move the group of four selected atoms. A 1 Å translation along the screen *x*-axis has been specified.

### To move one or more selected atoms:

1. Select the atom(s) to be moved. The Selection Inspector appears.
2. Click the **Move Selection** button in the Atom Properties group. A popover appears displaying editing fields.
3. Enter appropriate offsets for the screen *x*, *y*, or *z* axes, and press the **Apply Offset** button to proceed. (Note that you, alternatively, specify offsets relative to the molecule's original coordinate set—these are orthogonal axes that rotate with the molecule, as opposed to the screen coordinates.)

## Editing Atomic Coordinates

You can also use the Selection Inspector to edit the coordinates of a single, selected atom. The **Edit Coordinates** button lets you either edit the screen coordinates of the atom, or its original coordinates.

**Molecular Coordinates**

As with a crystal, an atom in a molecule has two sets of coordinates: a set of (orthogonal) *molecular coordinates*, which relate to the original basis set loaded with the molecule and which remain invariant as the molecule is rotated; and a set of *screen coordinates* which change as the structure is rotated.

Mostly we'll deal with screen coordinates, as it's easiest to relate changes to the orientation of the molecule—but if you wish to refer to the original coordinates, then use can refer to the Selection Inspector, where both sets of coordinates are displayed under "**Atom Selection**".

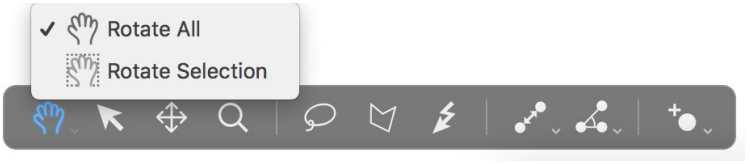
## Rotating Selected Atoms

You can use CrystalMaker's **Rotate Selection** tool to rotate only part of your structure, e.g., you have selected a $CH_3$ group, and wish to re-orientate it relative to the rest of a structure.

### To rotate selected atoms:

1. Ensure that you have selected all atoms you wish to rotate.
2. Locate the **Rotate** tool ( ) on the Tool Strip and click its popup menu to display a popup menu:

The Rotation popup menu




3. Choose the **Rotate Selection** command.
4. Click and drag with the **Rotate Selection** tool ( ) to rotate just the selected atoms. Alternatively, you can use the **Rotate** popover (on the toolbar) to rotate the selected atoms through a specified angle.

## Detaching Selected Atoms

Occasionally you may wish to separate a molecular group from a complex bonded structure. If the group is tightly bound to the rest of the structure, it may be difficult to delete the relevant bonds. In these cases, you can use the **Transform Selection > Detach** command (Graphics Pane contextual menu), which deletes any bonds between selected atoms and unselected atoms.

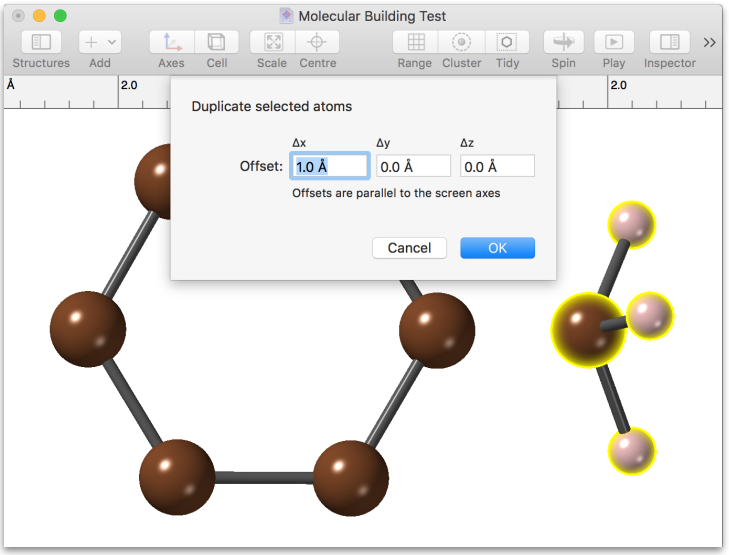
## Duplicating Selected Atoms

There are two ways of duplicating a selected atom, or group of selected atoms: either directly, via a menu command; or interactively, via a drag operation.

### To duplicate a selection directly:

1 Right-click in the Graphics Pane and choose: **Transform Selection > Duplicate** (or choose: **Transform > Selection > Duplicate**). The Duplicate Selection window appears:

Duplicating a group of selected atoms.




2 Enter offsets, in Å units, for the screen *xyz* axes, and click the **OK** button.

### To duplicate a selection interactively:

1 Choose the **Arrow** tool from the Tool Strip.

2 Hold down the **option** key on your keyboard.

3 With the **option** key still down, click and (with the mouse *still down*) drag the selection. The selected atoms and their bonds are duplicated, and the duplicate atoms move as you drag.

## Deleting Selected Atoms

You have the option of *permanently* deleting a selected atom, or group of selected atoms by choosing the **Delete** command from the Graphics Pane contextual menu (or pressing the **delete** key on your keyboard). You will be presented with an alert, giving you the option of changing your mind.

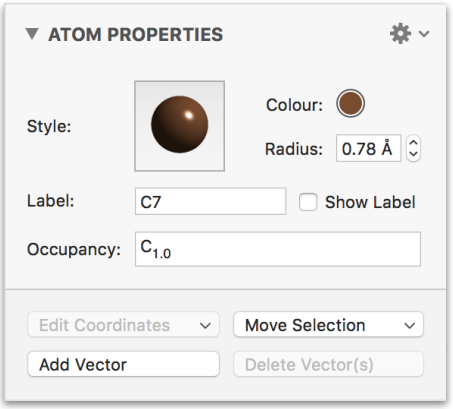
An alternative to permanently deleting atoms is simply to *hide* them (the **Hide** command on the Graphics Pane contextual menu). Hidden atoms can be made

visible using the **Show All Atoms in Range** command). You can also use the "**Vis**" checkboxes in the Atoms Inspector to show or hide specific atoms.

## Changing Atom Properties

You can edit a wide range of atomic properties using the Selection Inspector (which appears whenever atoms are selected). Properties to be edited include:-

- Chemical occupancy
- Colour
- Radius
- Style
- Labelling (text and label visibility)




The Atom Properties group in the Selection Inspector.

The Atom Properties group also includes an **Actions** menu (the cog icon, to the right of the **Atom Properties** text. Commands on this menu let you:

- Apply the current atom's properties to all related atoms in the structure.
- Reset the current atom's properties to the default settings.

## Crystal to Molecule Conversion

If you normally work with crystallographic data, but require the flexibility of CrystalMaker's Molecule mode (e.g., for placing part of a structure inside another model) you can convert your crystal to a molecule.

### To convert a crystal structure to a "molecule":

1. Ensure that you've selected the appropriate plot range, and that all the atoms you wish to work with in the new molecule are currently visible.
2. Choose **Transform > Crystal to Molecule**. A new, *molecular structure* is added to the current document (i.e., your original *crystal structure* is retained—and can be inspected by opening the document's Structures List).

   The new molecule includes all the currently-displayed atoms from your crystal, but all out-of-range and/or hidden atoms have been removed.

   Once you've converted your crystal to a molecule you can manipulate it in the same ways in which you might manipulate an ordinary molecule.

**Molecule to Crystal:** CrystalMaker also lets you work in reverse, providing an interface in which you can tile a molecule into a new crystal, whilst interactively changing symmetry, cell parameters, molecular position and orientation.

## Creating Nanotubes

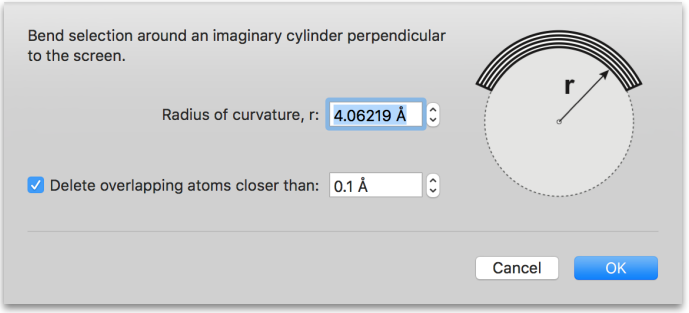
CrystalMaker lets you bend a group of *selected* atoms about an imaginary cylinder axis. You can specify a radius of curvature and repeat the command in different orientations to creating a bend, cylinder, helix, torus or dome.

The most-typical application will be to create nanotubes. CrystalMaker includes an example Graphite sheet (saved as a "crystal"), which you can extend into a large sheet, transform to a molecule, then bend to create an arbitrary nanotube; you can find the example in the Library Browser, grouped under: **Examples/Miscellaneous**.

### To create a nanotube:

1. Display a single sheet of Graphite. (If necessary, use the toolbar's **Range** command to make the sheet bigger, parallel to x and y.)
2. Convert the resulting sheet from "Crystal" to "Molecule" mode, as described in the previous section (**Transform > Crystal to Molecule**).
3. Once you have your sheet "molecule", you should rotate it into position (the sheet must be viewed "side on", and should be horizontal).
4. Select all the atoms (**Edit > Select All**).
5. Choose: **Transform > Selection > Bend**. The Bend window appears, displaying

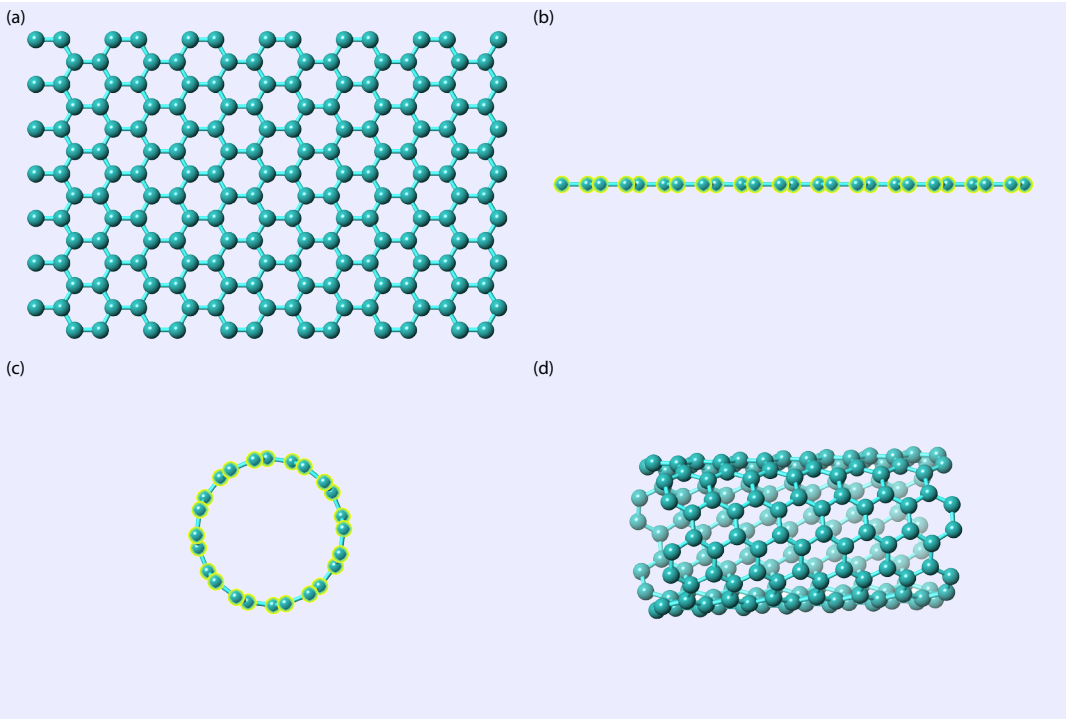
a default radius of curvature. This value should—assuming your orientation is correct—give you a nanotube.




The Bend window, showing options for making a nanotube.

## Removing Overlapping Atoms

Atom overlaps happen when convering a sheet into a cylinder: atoms on opposites sides of the sheet may come into contact (which you want, as this ensures that you have a correctly-folded sheet). You will probably want CrystalMaker to delete any "duplicate" atoms: those which fold onto an existing, and equivalent, atom.




Using the Bend command to create a carbon nanotube. (a) A Graphite sheet, oriented parallel to the screen edges. (b) The same sheet, rotated through 90° about the screen *X*-axis, with all atoms selected. (c) After using the Bend command and the default radius. (d) Rotating the model slightly reveals a carbon nanotube.

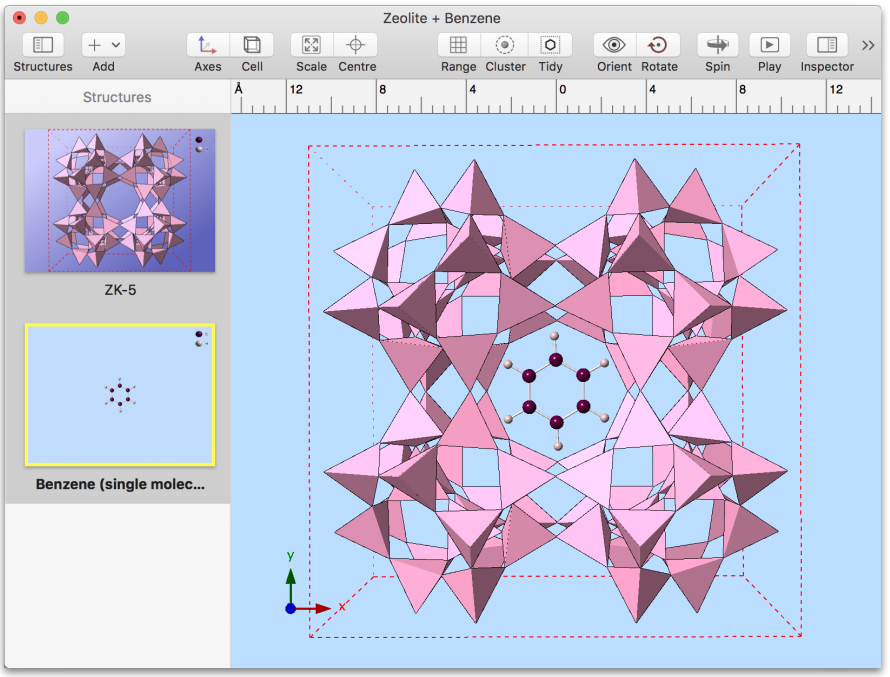
## Merging Structures

So far we have described how to create and edit a structure within CrystalMaker. Suppose that you have built your structure and would like to combine it with another, pre-existing structure. If both structures are loaded into the same document, they can be combined into a single structure.

### To Merge Two or More Structures:

1. Load all structures into the same document window (e.g., by using the toolbar's **Add** button, or by dragging-and-dropping their file icons into the window).
2. Ensure that the Structures List is visible, then select all structures to be merged by **shift**- or **command**-clicking on their thumbnails.
3. Ensure that the *host structure* is the primary selection (this should show a yellow highlight around its thumbnail).
4. Right-click in the Structures List to display a contextual menu and choose: **Merge Selection** (or choose: **Edit > Merge Structures**).

   All selected (i.e., visible) structures will now be combined into the primary-selected structure. Note that the final result will either be a *crystal* or a *molecule*, depending on whether the primary-selected structure was a crystal or a molecule.




Two structures loaded into the same document window. The pair can be merged into a single molecule.

Chapter 7

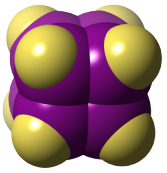
# Models

This chapter describes the ways in which you can represent a given structure using different model types, and how these can be customized and embellished using the Model menu and the Inspector.

## Model Types

The **Model** menu lists CrystalMaker's five main model types, which can be applied to any structure: simply choose a new model type, and your structure will be replotted (however, some of the models work best when you have defined bonds!)

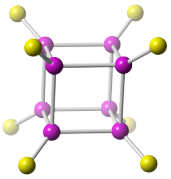
Each of the model types can be extensively customized When you save a structure, your settings for individual model types (e.g, atom colours, relative sizes, styles) will be saved—so you can freely switch between different representations for the same structure, and not lose any changes you have made.



### Space-Filling

Space-filling plots give an impression of how atoms pack together in a structure. Atoms are plotted as spheres, with radii corresponding to the actual atomic radii. If you have defined bonds, sphere overlap corrections will be applied where necessary.

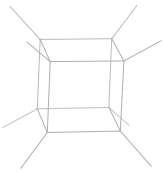
**Applying Van-der-Waals Radii.** CrystalMaker uses atomic radii from your current element table. If you would prefer to use the (larger) Van-der-Waals radii, simply right-click in the Atoms Inspector and choose the Van-der-Waals preset from the Radii submenu..



### Ball and Stick

Ball-and-stick plots depict atoms as solid spheres connected by lines or cylinders, representing chemical bonds. Each atom is plotted at a percentage of its space-filling radius subject to a minimum radius. Bond cylinders use a constant radius—to simulate the fixed width of a physical ball-and-stick model. The bond radius is a percentage of the radius of the *smallest sphere* in the current structure. Note that CrystalMaker X provides a choice of regular-width bonds or thin bonds.

**Atom and Bond Radii.** You can edit the radii of atoms using the Atoms Inspector. To adjust the relative widths of ball-and-stick spheres or bond cylinders, please see the Bond & Sphere Options group in the Model Inspector (described later in this chapter).



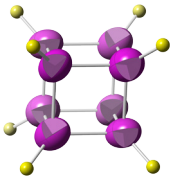
## Wire frame

For large and complex structures, wire-frame structures can be useful—and provide fast rotation. Unbonded atoms are plotted as individual pixels. Bonds are indicated by line segments between pairs of atoms. The line styles mimic the styles of the bond cylinders used for stick or ball-and-stick styles.

## Stick

This model type comprises rendered bond cylinders which begin and end at atom centres, with unbonded atoms plotted as spheres. This is useful for depicting bonded frameworks and molecular geometries—but is slower to plot than wireframe models for complex structures.

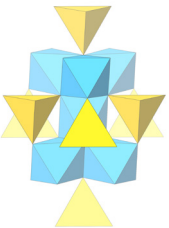
You can specify different widths for the bond cylinders used in Stick plots, compared to the bond cylinders used in Ball-and-Stick plots. For example, you can show fat cylinders to emphasize structural channels.



## Ellipsoids

This is only available if your *crystal* contains atomic displacement parameters for one or more sites. These may indicate thermal motions, positional disorder and/or uncertainty in refining positions (3D "error bars").

This model is similar to a ball-and-stick model, but with ellipsoids instead of spheres. The exact size and shape of the ellipsoids depends on their probability factor (a scale factor, set in the **Sphere & Bond Radii** group of the Model Inspector) and their individual isotropic or anisotropic displacement parameters.



## Polyhedral

Complex structures can be simplified by representing coordination groups as geometric units—polyhedra—and omitting individual atoms and bonds (e.g., an $SiO_4$ group represented as a tetrahedron with a silicon atom at the centre and oxygen atoms at the vertices). CrystalMaker can plot any kind of convex polyhedron, as well as linear and planar environments.

You have the option of mixing "polyhedral" elements with ball-and-stick, wire-frame or stick elements: all in the same model. Thus, the "Polyhedral" model type is something of a misnomer; this is really a "polymorphic" model!

**Polyhedra are Auto Generated!** CrystalMaker will automatically generate polyhedra as part of the bond-generation process. All you need to do is to edit the styles for different sites.

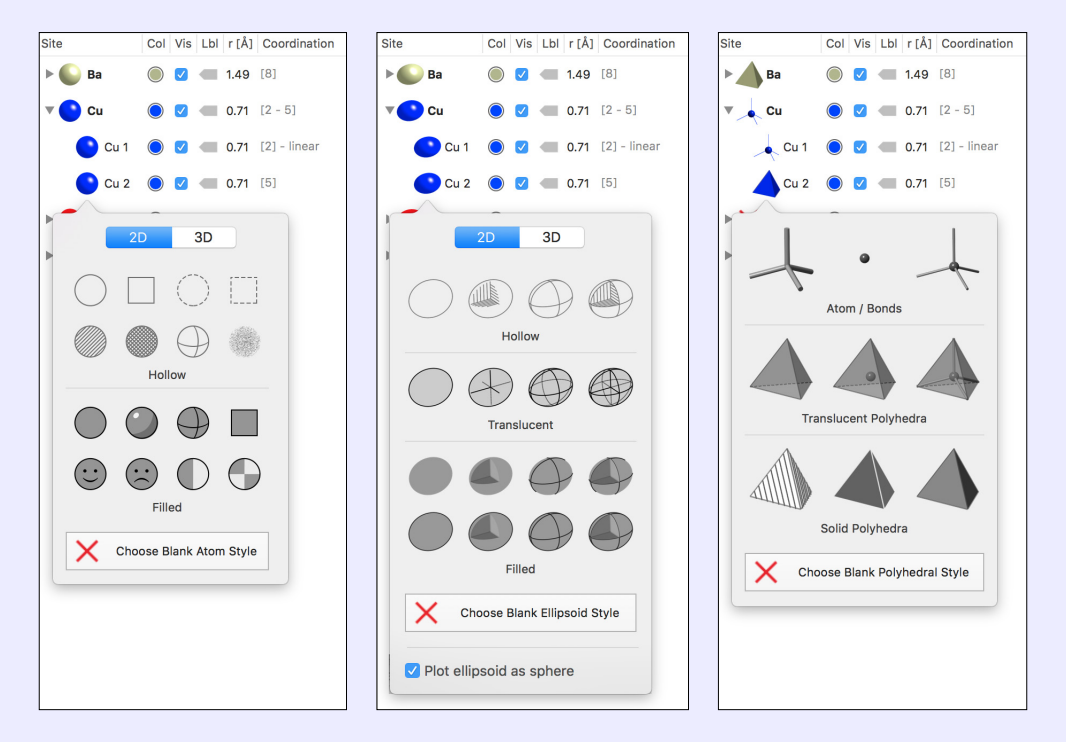
# Editing Atom Styles

The Atoms Inspector provides a wide range of sphere-, ellipsoid- and polyhedral styles. You can fine-tune the display, adjusting transparency, ellipsoid probability level, ball-and-stick radii and so on, using the Model Inspector.

## Changing Styles in the Atoms Inspector

You can use the Atoms Inspector (**View > Inspector > Atoms**) to choose different styles for spheres, ellipsoids or polyhedra—depending on the current model type. The styles include 3D photo-rendered or simpler 2D "line art" designs.

By default, the Inspector groups atoms (or in the case of crystals, sites) by element type (note the "disclosure triangle" to the left of each element row, which allows you to hide or reveal the corresponding atoms/sites). Having atoms grouped in this way lets you adjust styles settings by *element* or by atom/sites—depending on whether you click an element row or an atom row.




The Atoms Inspector displayed for Ball-and-Stick (left), Ellipsoids (middle) and Polyhedral (right) model types. For each model type, the style of the Cu2 site is being edited. Notice that the popover changes depending on model type.

CrystalMaker X also lets you *select* multiple rows in the Atoms Inspector. You can then change a property (e.g., atom style) in one row, and have your changes applied to all atoms/sites in the other selected rows.

### To set a style for a specific atom or site:

1. Locate the atom or site row in the list (you may need to open the relevant element row, to show all atoms/sites with this element symbol).
2. Click on the preview icon (shown to the left of the site label) for your site, then choose a new style from the popover that appears.

### To use the same style for a specific element:

1. Locate the relevant element row.
2. Click on the preview icon, then choose a new style from the popup menu that appears. Where possible, atoms or sites with this element symbol will be updated (some sites may not have sufficiently-high coordination numbers to display all polyhedral styles).

### To use the same style for all sites in the structure:

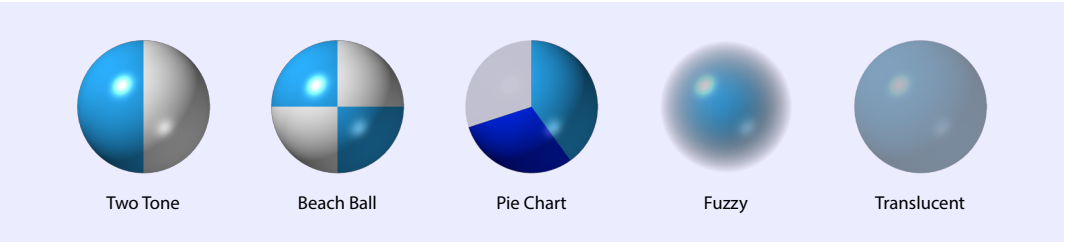
1. Select all element rows in the list (e.g., click on the first element row to select it, then choose: **Edit > Select All** to select the remaining rows; alternatively, click-and-drag the mouse across all element rows).
2. Choose a new style from any element row; this will be applied to all selected rows.

## Indicating Site Disorder

If you have a disordered site—perhaps with mixed occupancy, such as $Al_{0.5}Si_{0.5}$, or with partial occupancy, such as $Li_{0.5}$—CrystalMaker provides various sphere styles you can use to emphasize the disorder.

The "two tone" and "beachball" atom styles are good for indicating mixed occupancy, or flagging "difficult" sites. "Fuzzy" and translucent styles are also available; the degree of translucency can be adjusted using the General group in the Model Inspector.

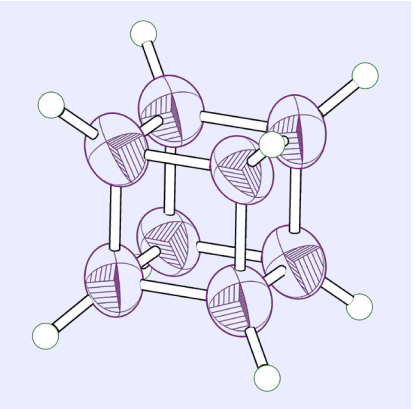
The new "Pie-Chart" sphere style provides a visual summary of the site occupancy, showing different *sectors* which are colour-coded according to the occupancy. For the case of partial occupancy, a translucent sector is used; for fill occupancy, colours are chosen from the current *Element Table* (Preferences panel).




Sphere styles for showing site disorder. The Pie-Chart atom here corresponds to an occupancy of $Al_{0.4}Si_{0.3}$.

## Ellipsoids as Small Spheres

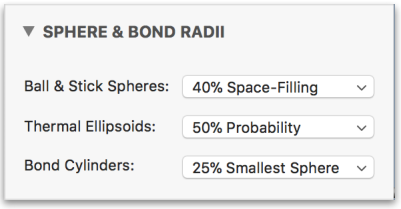
Small atoms such as hydrogen are difficult to refine, and may have large ellipsoids which obscure more important parts of a structure. You may therefore wish to disable ellipsoid display for these atoms. You can do this by choosing the **Plot ellipsoid as sphere** option in the Ellipsoid Style popover. The atom will continue to use the same ellipsoid style (which you can edit in the same popover), but will be drawn as a sphere. You can choose a specific radius for "ellipsoid-as-sphere" atoms using the Sphere & Bond Radii group (see below).



The cubane structure plotted with small spheres for the H atoms (green) and thermal ellipsoids for the C atoms (purple).

## Sphere and Ellipsoid Radii

CrystalMaker's Model Inspector includes controls for setting *relative* radii for ball-and-stick spheres, ellipsoids—and also bond cylinders. These options are all grouped under **Sphere & Bond Radii**:-




The Sphere & Bond Radii group.

The relative sizes of ball-and-stick spheres, ellipsoids and bond cylinders are summarized in the button titles. Clicking a button displays a popover with editing controls.

For ball-and-stick and polyhedral plots, atom spheres generally need to be smaller than their true, space-filling radii (otherwise any bonds would be hidden!). You can customize how much smaller the spheres should be, as a percentage of the space-filling radius (note that the space-filling radii are edited in the Atoms Inspector).

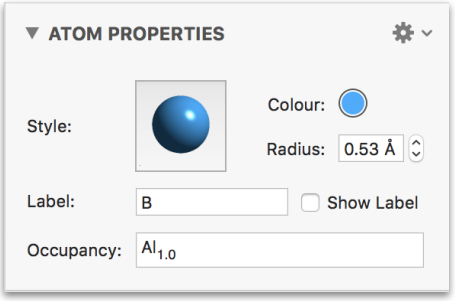
You can also specify a *minimum* radius, in Ångstrøm units: this lets you ensure that smaller spheres (such as hydrogen)—and any bonds (see below) remain visible.

Ellipsoids are sized according to the probability level that you enter. If you choose to display an ellipsoid as an atom sphere, you can specify the radius—which will be the same for all "ellipsoid-as-sphere" atoms.

**Saving Defaults:** You can make the current settings your default settings by right-clicking in the Bond & Sphere Options pane and choosing: Save as Defaults. Alternatively, use the Atoms or Bonds panes in the Preferences panel to inspect your settings.

## Local Atom Styles

The Selection Inspector lets you edit the appearance and properties of individually-selected atoms or bonds. You can apply custom colours and styles which are independent of the global settings (shown in the Atoms or Bonds Inspectors). These can be useful in highlighting areas of interest.




The Selection Inspector provides controls for changing properties of selected atoms.

The Selection Inspector lets you change the atom style (sphere, ellipsoid or polyhedron, depending on the current model type), its colour, space-filling radius, labelling and site occupancy.

**Resetting Range May Reset Atoms:** Custom colours and styles applied to a specific atom in a crystal structure may be reset when the crystal is recalculated (e.g., after editing atomic coordinates) or if the plot range is significantly altered. This may happen if the program needs to replace the existing atoms array with a new array. For best results, try to define styles at the site level, using the Atoms Inspector, wherever possible.

### To reset custom settings:

- Click the Actions button (cog icon) in the **Atom Properties** group to display a drop-down menu, then choose: **Reset Atom Properties**.

# Polyhedral Models

If your structure has sufficient bonding, switching to a **Polyhedral** model will *automatically* display coordination polyhedra. Note that, unlike other programs, you do *not* need to take any special action: CrystalMaker has already calculated coordination polyhedra as part of the bond-generation process. Your coordination polyhedra might comprise two-dimension shapes such as triangles, or three-dimensional rendered polyhedra, such as tetrahedra or octahedra—or much larger units such as icositetrahedra.

## Default Polyhedral Styles

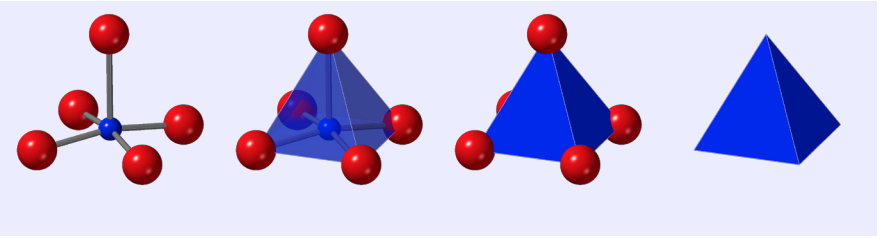
By default, rendered polyhedra are shown for atoms or sites (generally cations) that have coordination numbers (i.e., numbers of primary bonds) of 3 or higher. Atoms with lower coordination numbers may appear hidden—i.e., they have "blank" styles (e.g., if they are at the vertices of existing coordination polyhedra) or depicted as spheres (e.g., if they have no bonds).

You can specify default polyhedral styles for both cations and anions (O, F, Cl…) using the **Model/Polyhedra** tab in the **Preferences** panel. By default, cations are shown as rendered polyhedra (bonding permitted) and anions are blank.

**Cation and Anion Defaults:** CrystalMaker 10.4 introduced the ability to specify separate default styles for cations and anions. Earlier versions of the program only had a single style option, which caused problems with dense structures such as orthosilicates, resulting in inter-penetrating oxygen- *and* metal-centred polyhedra.

## Overriding Default Styles

You can edit styles using the Atoms Inspector: simply click a style preview for a site- or element row, and choose a new style from the popover that appears. (The style preview changes depending on the model type, so to edit polyhedral styles you will need to be working with a polyhedral model.)



Representations of a $CuO_5$ cluster in a polyhedral model. Blank styles were applied to the (red) oxygen atoms in the right-hand image.

### Ball-and-Stick Styles

The Polyhedral model type isn't just for coordination polyhedra: you can regard this as being a "poly-morphic" model and combine different representations, e.g.,

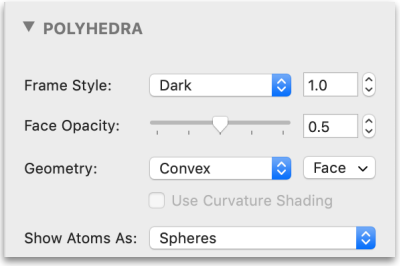
ball-and-stick, stick, spheres and rendered polyhedra—all in the same plot. Note that any spheres shown in a polyhedral plot will be plotted using the same style as for a Ball-and-Stick plot. To change this style, simply switch back to a Ball-and-Stick plot and click the atom's preview icon to edit its sphere style.

### Blank Styles

Blank atom, ellipsoid or polyhedral styles can be handy ways of simplifying complex structures. For example, in a polyhedral plot, it's generally useful to have highly-coordinated ions displayed as rendered polyhedra, but with their vertex atoms assigned a blank style (i.e., not drawn).

## Polyhedral Options

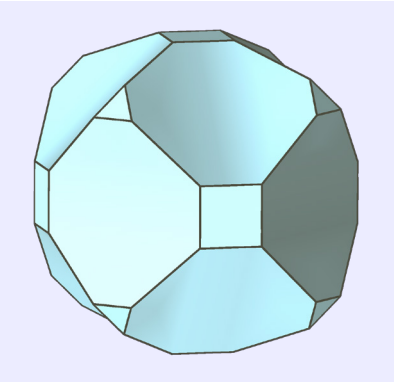
Once you have chosen a polyhedral style for a site, you can tweak its display using the **Polyhedra** group in the Model Inspector. Commonly-used options include the frame style and width and whether ability to display any vertex atoms as spheres or ellipsoids.




The Polyhedra group in the Model Inspector.

### Concave Faces

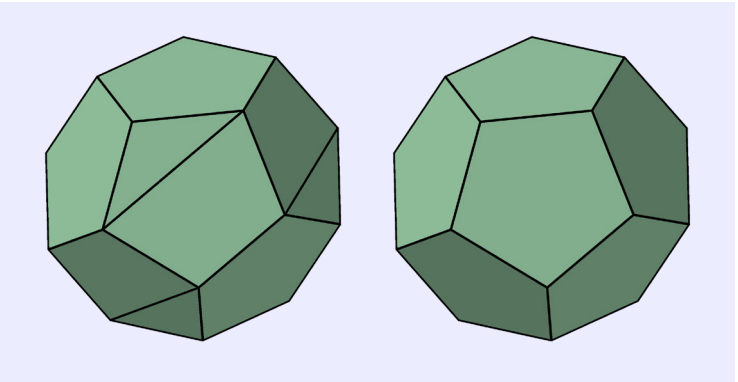
Very-large polyhedra can be displayed conventionally, using convex models, or as a concave version. For the latter case, CrystalMaker can, optionally, render the convex faces using smooth shading with emphasizes their inward curvature.



A large cage from a molecular-organic framework (MOF) displayed as a concave polyhedron.

### Face Generation

CrystalMaker X lets you control how faces are generated, adjusting the maximum out-of-plane tolerance value to permit larger faces with more vertices. Most of the time you won't need to adjust the default value, but if you are working with low-density structures with very large cages (such as clathrates or molecular-organic-frameworks), you might wish to have greater control.



Increasing the out-of-plane tolerance allows one to represent imperfect polyhedra (left) more clearly (right).

As an example, consider the large, 20-vertex cage in Dodecasil 3C (pictured above). The cage can be idealized as consisting of 12 pentagonal faces, but because some of the (silicon) vertex atoms are not exactly co-planar, one might see the pentagonal faces subdivided into smaller faces (top left). By increasing the out-of-plane tolerance, a more idealized view is seen (top right). Note that continuing to increase the tolerance becomes counter-productive as vertices from other faces are added and the polyhedron ends up breaking down into a series of small triangles.

### Opacity

You can control the opacity of any *translucent* polyhedral styles. CrystalMaker provides three such styles, showing an empty polyhedron, one with a central atom, or one with a central atom and bonds to the vertex atoms.

### Edge Highlights

Polyhedra generally look better if their edges (the polyhedral frame) are highlighted. CrystalMaker lets you choose what type of highlight to use:

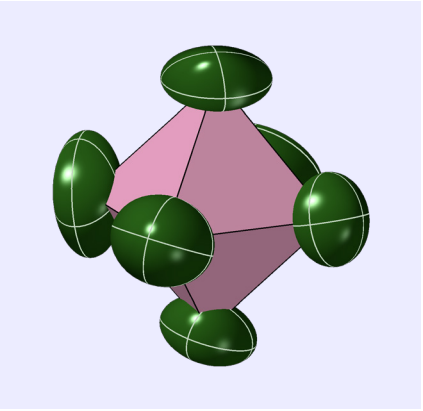
- Light
- Dark
- Subtle (a blend of light and dark that depends on the face colour)
- No highlight.

You can adjust the width of the frame. Very-thick frames use rendered cylinders, rather than flat line segments; this gives a powerful, 3D effect.

**Use Dummy Bonds for Thicker Edges:** If you can't quite get the edges you require (perhaps your faces are too distorted to plot with enough vertices) you could try adding bonds between the vertex atoms (for the case of Dodecasil, pictured above, we would require Si–Si bonds). In a polyhedral plot, you would specify that the central, cage atom, plots as a solid polyhedron, and that the vertex atoms plot as sticks.

### Ellipsoids in Polyhedra

If you have opted to display some atoms as spheres (i.e., you chose the "atom sphere" polyhedral style for the corresponding sites), you have a further option to show "**Ellipsoids (where possible)**". This option will replace any atom spheres with their corresponding ellipsoids (assuming that your structure contains atomic displacement parameters for those sites).



A $PF_6$ polyhedral group, with atoms represented by thermal ellipsoids.

## Bond Styles

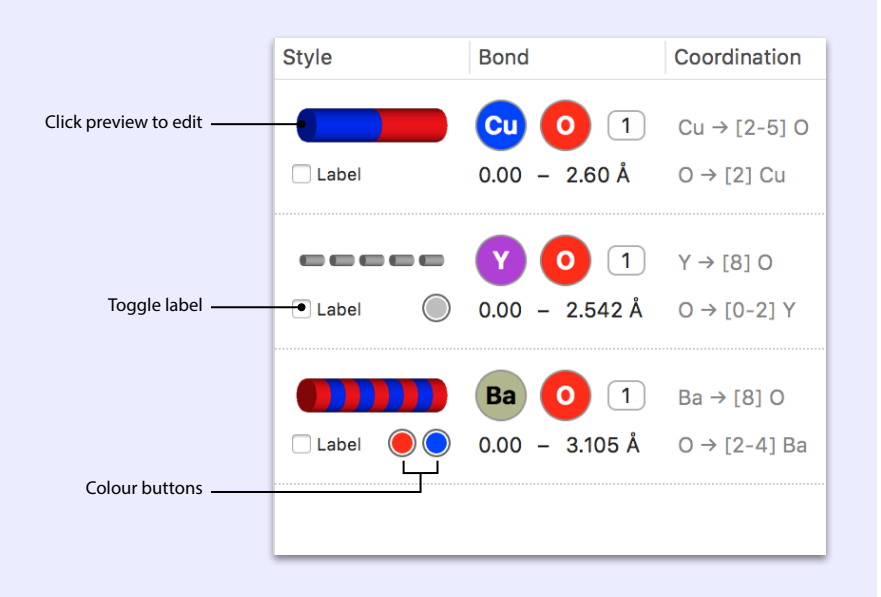
Bonds are drawn as cylinders or lines between atoms. You can choose different styles and colours using the Bonds Inspector or, for bond selections, using the Selection Inspector.

### Changing Styles in the Bonds Inspector

The Bonds Inspector lists all of the "global" bond specifications defined for the current structure. These are effectively requests for certain bonds to be generated throughout the structure, in terms of element-pair combinations and distance ranges. The Inspector also lets you edit style information for each specification:

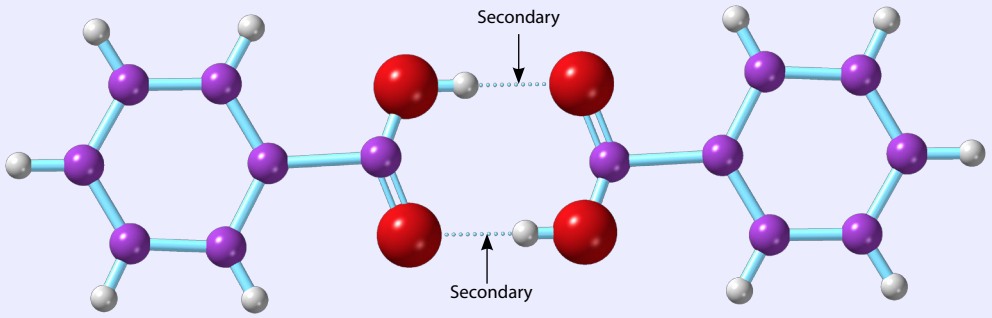
- Bond style and colouring
- Label visibility
- Primary or secondary status

The Bonds Inspector with some of its editing controls.




Some bonds use two colours, others are monochromatic. The "two-tone" bond style (shown in the top row of the previous figure) has no colour buttons because this style is automatically coloured according to its atom pair (blue=Cu, red=O).

### Primary or Secondary Bonds




CrystalMaker X offers you a choice of two bond classes: primary or secondary bonds. Most of the time you'll be using primary bonds: these represent strong interactions in the structure and are used to auto-generate coordination polyhedra.

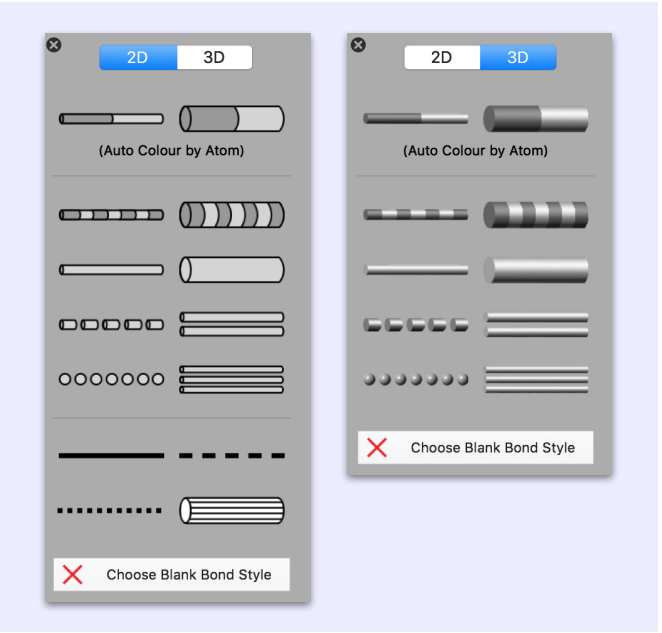
Occasionally you may wish to show some secondary bonds; use these to:-

- Show weak (inter-molecular) interactions—as for dotted lines in the benzoic acid dimer, shown above.
- Show non-bonded distances (e.g., ring or channel diameter).

Secondary bonds are *ignored* for the purposes of generating polyhedra.

### To change a bond style:

1 Click on a bond preview and choose a new style from the popover that appears.




The Bond Style popover showing a selection of 2D "line art" styles (left) and 3D rendered styles (right).

2 Choose a bond colour(s) by clicking on the round colour button(s) and selecting a new colour from the colour palette that appears (option-click to display the colour wheel directly).

3 Use the Label checkbox to turn bond labels (distance display) on or off.

### To edit multiple bond styles simultaneously:

1 Select the rows to be edited (shift- or command-click to extend your selection).

2 Edit the bond style, labelling and/or colouring for one selected row; the other selected rows will also be updated.

## Changing the Bond Width

CrystalMaker offers you three options for bond widths:-

- Lines (stylized, "2D" bond styles)
- Thin cylinders
- Regular cylinders

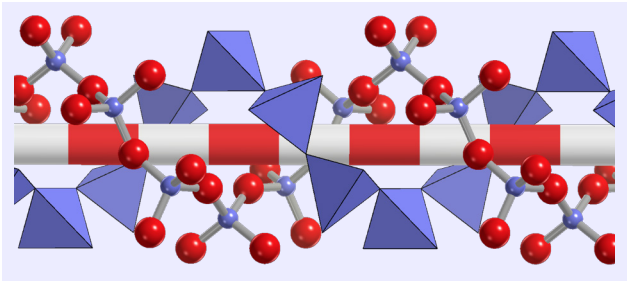
We recommend using the regular cylinders (shown in the right-hand column of the Bond Style popover) for most primary bonds. The thin cylinders are designed to illustrate weaker interactions or secondary bonds—but the choice is yours.

CrystalMaker tries to replicate the appearance of a traditional "ball-and-spoke" model in which metal wires—of constant width—connect wooden or plastic spheres. Hence, you cannot adjust the widths of *individual* bonds; however, you can adjust the widths of *all* bonds, relative to the smallest atom in your structure.

### To adjust the width of bond cylinders:

1. Show the Model Inspector (**View > Inspector > Model**).
2. Open the **Sphere & Bond Radii** group.
3. Click the Bond Cylinders button to edit Ball & Stick, Stick and Thin Bond radii. Note that ball-and-stick cylinders cannot be wider than the smallest atom in your structure–but that this limitation does not apply to Stick cylinders (so you can show "fat" cylinders—perhaps to emphasize structural channels, as illustrated below).

Using a fat "stick" cylinder (red-and-white pole) to emphasize a channel in the quartz structure.



**Saving Defaults:** Use the Bonds pane of the Preferences panel to specify a default bond style, colouring and radius settings.

## Unit Cell

New crystals are displayed with the outline of a single unit cell. Initially the unit cell shown is the centremost cell in the current plot range (and does not necessarily correspond to the unit cell closest to the origin).

### To show/hide the unit cell display:

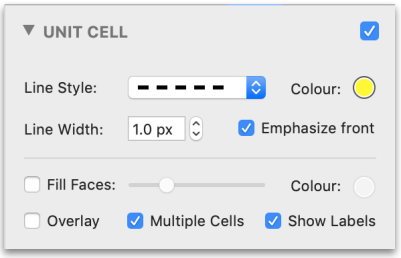
Do one of the following:

- Choose the **Model > Show Unit Cell**, or **Model > Hide Unit Cell** commands.
- Click the **Cell** button in the toolbar.
- Click the **Unit Cell** checkbox in the Model Inspector (see below).

## Unit Cell Options

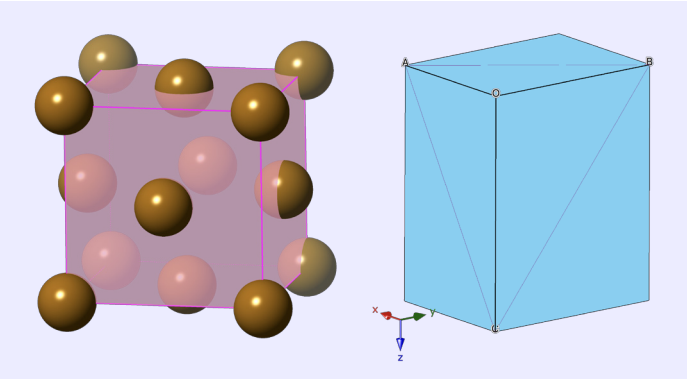
You can use the **Unit Cell** group in the Model Inspector (**View > Inspector > Model**) to change the way that the unit is displayed.

The Unit Cell group in the Model Inspector




A new feature in CrystalMaker X is the ability to shade the unit cell *faces*. You can define a colour and transparency—and even make the cell faces opaque.

Models with translucent unit cells. Left: emphasizing the number of atoms in the unit cell; Right: showing the trace of a (111) plane cutting the unit cell—a useful aid for learning about Miller Indices.




Translucent unit cells are useful for teaching, showing traces of planes (teaching Miller Indices) or helping to illustrate the number of atoms in one unit cell.

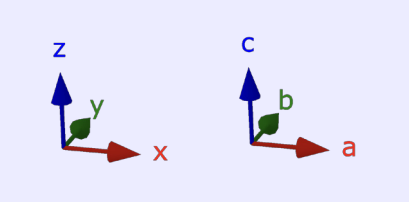
You can choose between solid, dashed or dotted lines for the frame, and specify the line width. You can also make the frontmost edges thicker, which helps to emphasize depth and avoids false perspective.

For densely-packed structures, where the unit cell frame might become hidden, you can opt to turn off the **Overlap correction** so the cell frame is then superimposed over the structure. You can also opt to display a single, central unit cell, or multiple unit cells, with or without labelled corners.

# Axial Vectors

As a guide to the crystal orientation, you can display a set of axes, parallel to your structure's crystallographic axes.

Axial vectors can use xyz or abc labels.




### To display axial vectors:

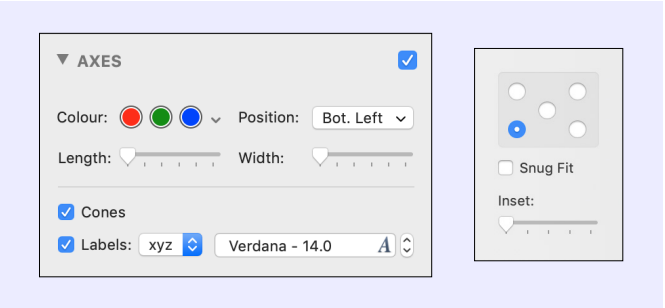
Do one of the following:

- Choose: **Model > Show Axes**.
- Click the **Axes** button in the toolbar.
- Click the **Axes** checkbox in the Model Inspector.

## Customizing the Axes Display

Use the **Axes** group in the Model Inspector to change the colours of individual axes, adjust their lengths and widths, toggle the display of vector cones and specify your preferred labelling: either "*xyz*" or "*abc*" (or none at all). The axis label font and its size can also be set here.

The Axes group in the Model Inspector (left) with its Position popover (right).




### Moving the Axes

You can use the **Position** button to specify where you would like the labels to be displayed. A popover is shown with radio buttons, letting you specify positions in the four corners, or at the centre of your model. A "**Snug Fit**" option ensures that the axial vectors rotate about their centre of gravity, rather than their origin. This means they take up less space—and might be useful when preparing a figure for publication.

For greater control, you can increase the "**Inset**" amount, which moves the axes closer to the centre of the screen.

**Screen Aspect Ratio:** When printing, or exporting graphics, remember that CrystalMaker preserves the aspect ratio of your Graphics pane. We recommend resizing your document window to ensure that the Graphics Pane is the appropriate shape; that way, when you export graphics, you won't have masses of "white space" between the axial vectors and your structure.

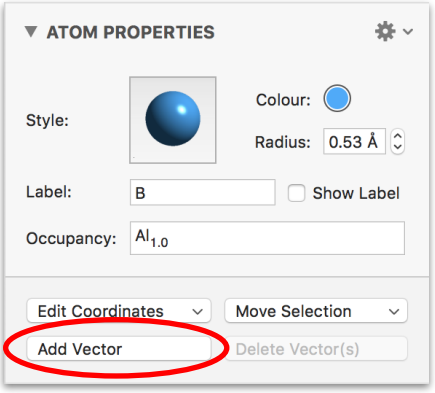
## Atom Vectors

CrystalMaker allows you to attach one or more arrowed "vectors" to an atom. You could use these to indicate the direction of atom offsets, a ferroelectric polarisation, or perhaps a magnetic moment. Individual vectors can be edited to change their orientation, length and colour, and it is possible to select and edit multiple vectors.

**Import Vectors:** If you have large numbers of vectors to add or visualize, we recommend entering these in a CrystalMaker text file, using the AVEC card to specify each vector's host atom, orientation, length, colour and style. See *Appendix B: CrystalMaker Text Format* for details.

### To add a vector to an atom:

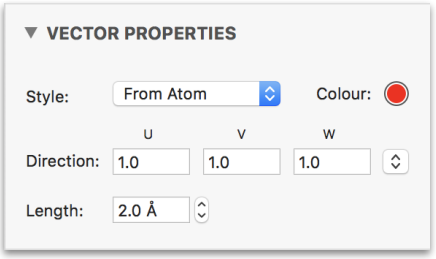
1. Select the atom or group of atoms.
2. Ensure the Selection Inspector is visible (if not, choose: **View > Inspector > Selection**).
3. Click the **Add Vector** button in the **Atom Properties** group:




The Atom Properties group showing the Add Vector button.

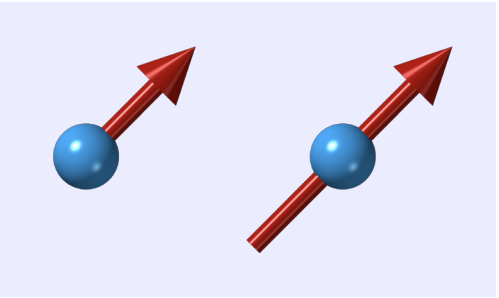
A vector will be added to any selected atoms. Any new vectors will be selected, so their properties can be edited in the **Vector Properties** group which appears:

The Vector Properties group.




4 Using the **Vector Properties** group, specify a vector style (either "From Atom" or "Through Atom"), a colour, the orientation (i.e., U**a** + V**b** + W**c**, where **abc** are the unit cell vectors) and a length (the distance from the *centre* of the host atom to the *tip* of the vector; the "tail" of a "through-atom" vector style is not included in this length). Remember to press the **enter** key to update your structure's display.

Two vector styles: "from atom" (left) and "through atom" (right). Note that both styles have the same nominal length.



### To edit an existing atom vector:

1 Select the vectors you wish to edit: click anywhere on a vector to select it; shift-click to select multiple vectors.

2 Ensure the Selection Inspector is visible, then use the **Vector Properties** group to make your changes.

### To edit a vector interactively:

1 Select the vector(s) with the Arrow tool.

2 Click and drag the vector cone to a new orientation.

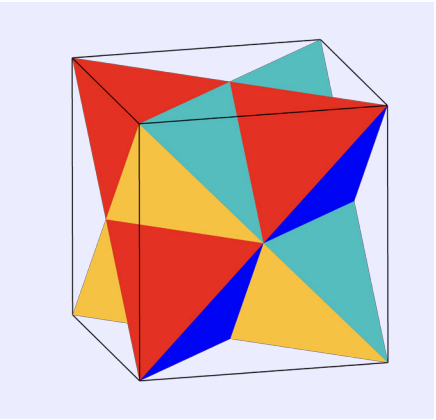
### To delete vectors:

Do one of the following:

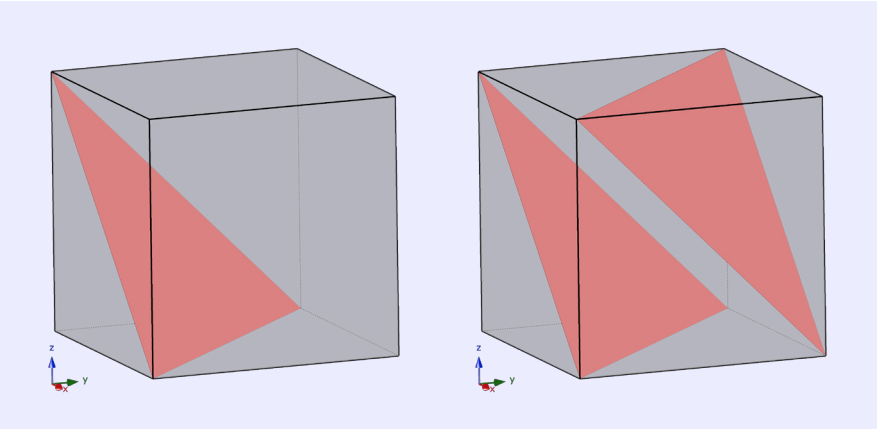
- Select the vectors to be deleted, then press the **Delete** key
- Select the host atom(s) the press the **Delete Vector(s)** button in the **Atom Properties** group of the Selection Inspector.

## Lattice Planes

CrystalMaker allows you to display multiple lattice planes slicing through a structure. You can move any plane along the direction of its plane normal, change its colour and opacity, and toggle between showing a single plane, or a set of parallel planes. A plane can also be used to slice away part of a structure, e.g., to reveal a surface, as detailed later in this chapter.



A set of {111} planes, colour-coded by orientation, centred in a cubic unit cell.



Single (left) and parallel (right) planes in a (translucent) unit cell.

### Displaying Lattice Planes

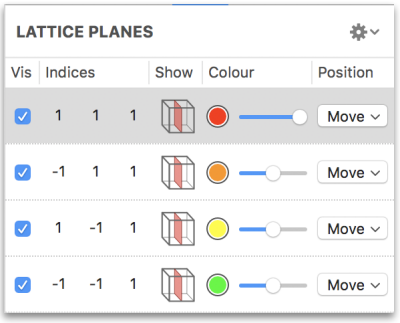
You can display a single lattice plane by specifying its Miller indices (hkl), or by fitting a plane through a group of selected atoms.

Most of the time, you'll probably want to specify the precise orientations of the planes you wish to add. You can do this by using the **Lattice Planes** group in the Volume Inspector. This lets you add multiple planes, with or without different orientations (different Miller Indices) to a list. You can use the list row controls to change the visibility of a particular plane, toggle between viewing a single plane or

a set of parallel planes, to change the plane's colour, and to edit the plane's opacity. The list box also includes an Actions popup menu button (cog icon) with preset orientations, plus controls to:-

- Add a new plane.
- Duplicate one or more selected rows.
- Add an inverse (e.g., add $\overline{111}$ to an existing 111 plane).
- Add symmetry-related planes.
- Slice the crystal with the selected plane.
- Create a slab from two visible planes.

The Lattice Planes group in the Volume Inspector.




### To add a lattice plane:

1. Locate the **Lattice Planes** group in the Volume Inspector.
2. Choose one of the following methods to add a dummy plane to the list:
   - Double-click on a blank row.
   - Click the Lattice Planes **Actions** button (cog icon) to display a pull-down menu, then choose: **Add New Plane** to add a new plane to the list.
   - Right-click in the list and choose **Add New Plane** from the contextual menu that appears.
3. Edit the Miller Indices, then presss the Return key to replot.

### To display a set of parallel planes:

◆ Click the button in the **Show** column so its icon changes to from a single plane to a set of planes.

### To show symmetry-related planes:

◆ Click the list's Actions button (cog icon) and choose: **Add Symmetry Related**.

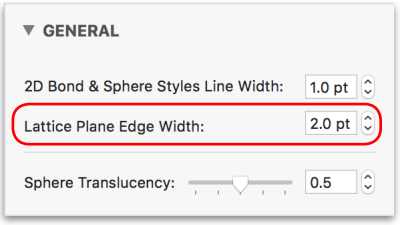
## Changing Lattice Plane Display Properties

Each lattice plane comprises a solid or translucent planar region, bounded by a solid edge. You can change the colour and opacity of the planar region using the Colour button and slider control in the corresponding list row. You can also use the Actions menu to automatically assign colours (so that each plane has a unique colour). The thickness of the lattice plane edges is a global setting, which can be adjusted using the Model Inspector:

### To change the thickness of the plane's edge:

1. Navigate to the Model Inspector.
2. Locate the **General** group.
3. Adjust the **Lattice Plane Edge Width** controls.

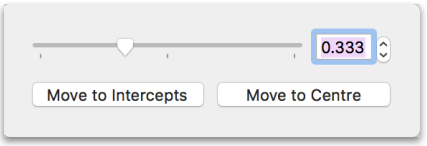
Adjusting the thickness of lattice plane edges.




## Moving a Lattice Plane

Each list row has a Move button which, when clicked, displays a popover. This provides a slider control, to move the plane along its normal. For finer control, use the little arrows control on the right-hand side of the slider (numeric values range from 0 to 1).

The Move Lattice Plane popover.




**Smoothly Does It:** Mac users can use their multi-touch trackpad to smoothly adjust the slider value, without any clicking required. Simply position the mouse pointer over the slider control then slide two fingers across the trackpad in the intended direction of slider movement.

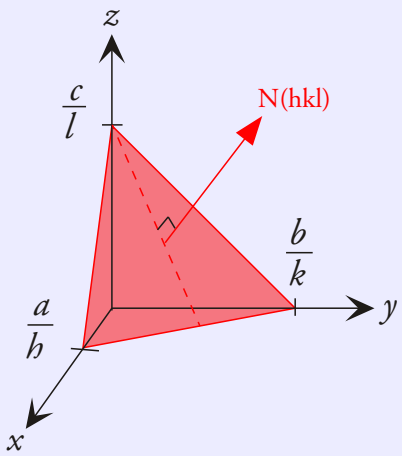
A pair of buttons lets you reset the plane's position to either its "intercepts", or to the centre of the unit cell. The "intercepts" are the locations along the $x$, $y$ and $z$ axes where the first plane *from the origin* would lie, e.g., for the set of parallel planes ($hkl$), if one plane were at the origin, the next plane would cut the $x$-axis at $a/h$, the $y$-axis at $b/k$ and the $z$-axis at $c/l$.

**View Horizontally:** The Lattice Planes **Actions** menu includes a handy **View Horizontally** command which will rotate your structure so it is seen sideways on: this is particularly useful when you need to move a lattice plane in order to slice through part of a crystal.

## Lattice Planes Aren't Fixed in Space!

There seems to be a common misconception (especially amongst Materials Scientists) that the Miller Indices of a lattice plane somehow uniquely fix it at a particular point in space—so that the plane (200) would be half-way up the unit cell's **a** axis. This is wrong!

Miller Indices define the *orientation* of a plane's normal and, if one is referring to a *set* of lattice planes, their *relative spacing*. However, they provide absolutely no information about the *position* of the planes along their normal.




Miller Indices (hkl) define the orientation of a lattice plane and its normal, N(hkl), relative to the unit cell dimensions a, b and c.

Miller Indices were derived long before scientists understood about the atomic structures of crystals. They were used for specifying the relative orientations of external crystal *faces* in hand specimens. The ratios of the three indices *h, k* and *l* gave the orientation of a single face, relative to a bulk crystal.

The origin of the "fixed-in-space" misconception probably stems from an over-simplistic approach when teaching crystallography. It is usual to start with a block model of a unit cell, and then explain Miller Indices in terms of the first intercepts from the origin made by a particular plane. However, that does not mean that the plane has to be fixed in space. After all, most crystals have billions of unit cells—so which unit cell would the plane be fixed to?

Furthermore, there is nothing sacrosanct about the crystal's origin: it can be anywhere within the lattice. Indeed, crystallographers often move the origin for convenience; this does not mean that planes have to change their indices: (100) doesn't suddenly become (200) or some other value!

**Summary:**

1. For a single lattice plane, the Miller Indices define only the orientation of its plane normal—not its absolute position.

2. When dealing with a set of parallel planes, the Miller Indices also define the separation (d-spacing) of the planes. Thus, a set of (200) planes would have one-half the d-spacing of a set of (100) planes.

Please see *Appendix D: Basic Crystallography* for more information about Miller Indices.

## Surface Overlay

CrystalMaker lets you visualize the overall shape of your structure via a translucent "surface" overlay. You can vary the size (radius) of the overlay to describe one of three different types of surface:-

- Space-Filling Surface
- Van-der-Waals Surface
- Solvent-Excluded Surface

Before discussing the differences between these surfaces in more detail, we should point out that the surface overlay applies to *all visible atoms* in the structure. If you require more flexibility—perhaps you want to show some atoms inside a surface, and not others—then you can create a surface as a "Volumetric Dataset" (see *Surface Maps* in *Chapter 12: Measurement*).

### Space-Filling Surface

A surface is calculated using the existing space-filling atomic radii. This is useful if you wish to combine, say, an open, polyhedral representation of your model, with an indication of the true size of your atoms—with the latter implied by a translucent space-filling surface.

*Please note that if you are currently viewing your structure as a "space-filling" model then, because of the limitations of OpenGL, some or all of the surface overlay may be hidden.*

### Van-der-Waals Surface

For molecular crystals, it is often useful to visualize an extended region of influence (the interaction volume) around a molecule. This is achieved by having a surface extend out to the Van der Waals radius of each atom. CrystalMaker uses its own table of Van der Waals radii, which you can browse in the Elements pane of the Preferences panel.

### Solvent-Excluded Surface

Similar to a Van der Waals surface, a "Solvent-Excluded Surface" lets you determine the possible contacts between a "probe sphere" of a defined radius and the surface of your structure.

The surface is generated by rolling the "probe sphere" over the Van der Waals surface. This smooths out any cusps where atoms overlap. CrystalMaker applies a default probe sphere radius of 1.4 Å, which is the approximate Van der Waals radius of a water molecule; thus, your default Solvent-Excluded Surface provides a visualization of your structure from the perspective of a water molecule (an excellent solvent) or a hydroxyl ion.

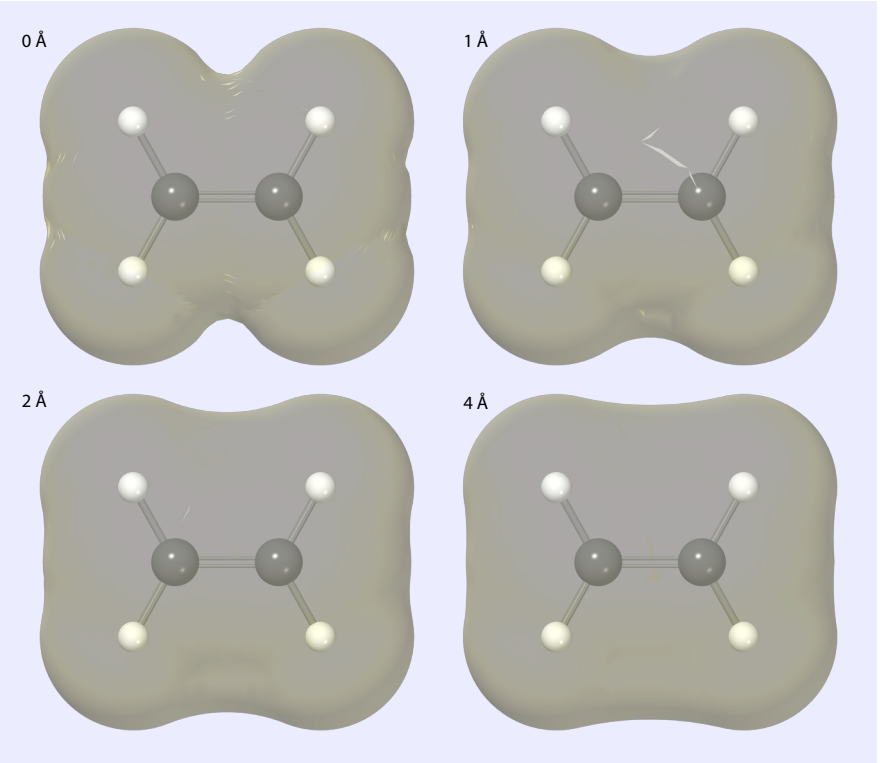
### To display a surface overlay:

Do one of the following:

- Choose **Model > Show Surface**.
- Click the **Surface** checkbox in the Model Inspector.

## Editing Surface properties

Use the **Surface** group in the Model Inspector to choose a surface type, its colour and its opacity. If you have opted to display a *Solvent-Excluded Surface*, you can use the slider control to adjust the "rolling" probe sphere radius.



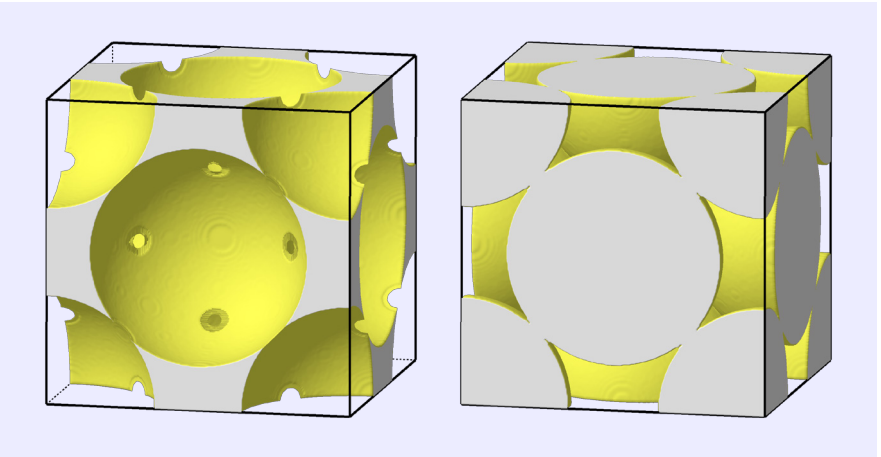

Solvent-excluded surfaces for ethene, showing the effect of increasing probe radius.

**Legacy Surfaces:** Earlier versions of CrystalMaker displayed essentially a translucent space-filling model as a surface overlay, with the option of increasing the surface radius. This would be an intermediate between a Space-Filling and a Van-der-Waals surface.

# Volumetric Data

CrystalMaker lets you visualize volumetric data imported from text files, or generated within the program in electron density, porosity or surface map calculations.

Negative (void) and positive (filled) space in one unit cell of copper.

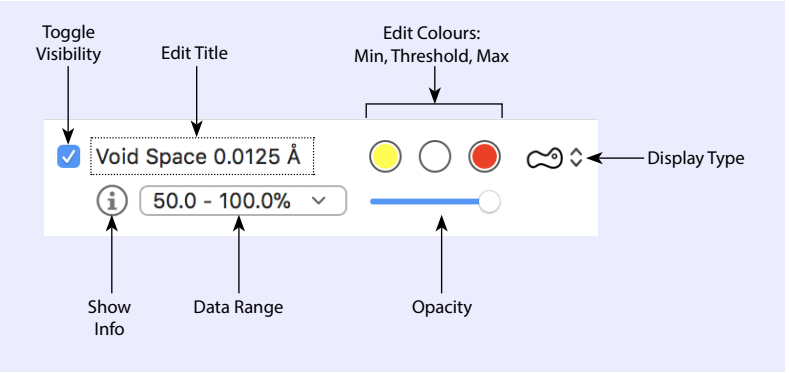


You can manage multiple volumetric datasets in the same window, using the **Volumetric Data** group in the Volume Inspector.

## Volumetric Display

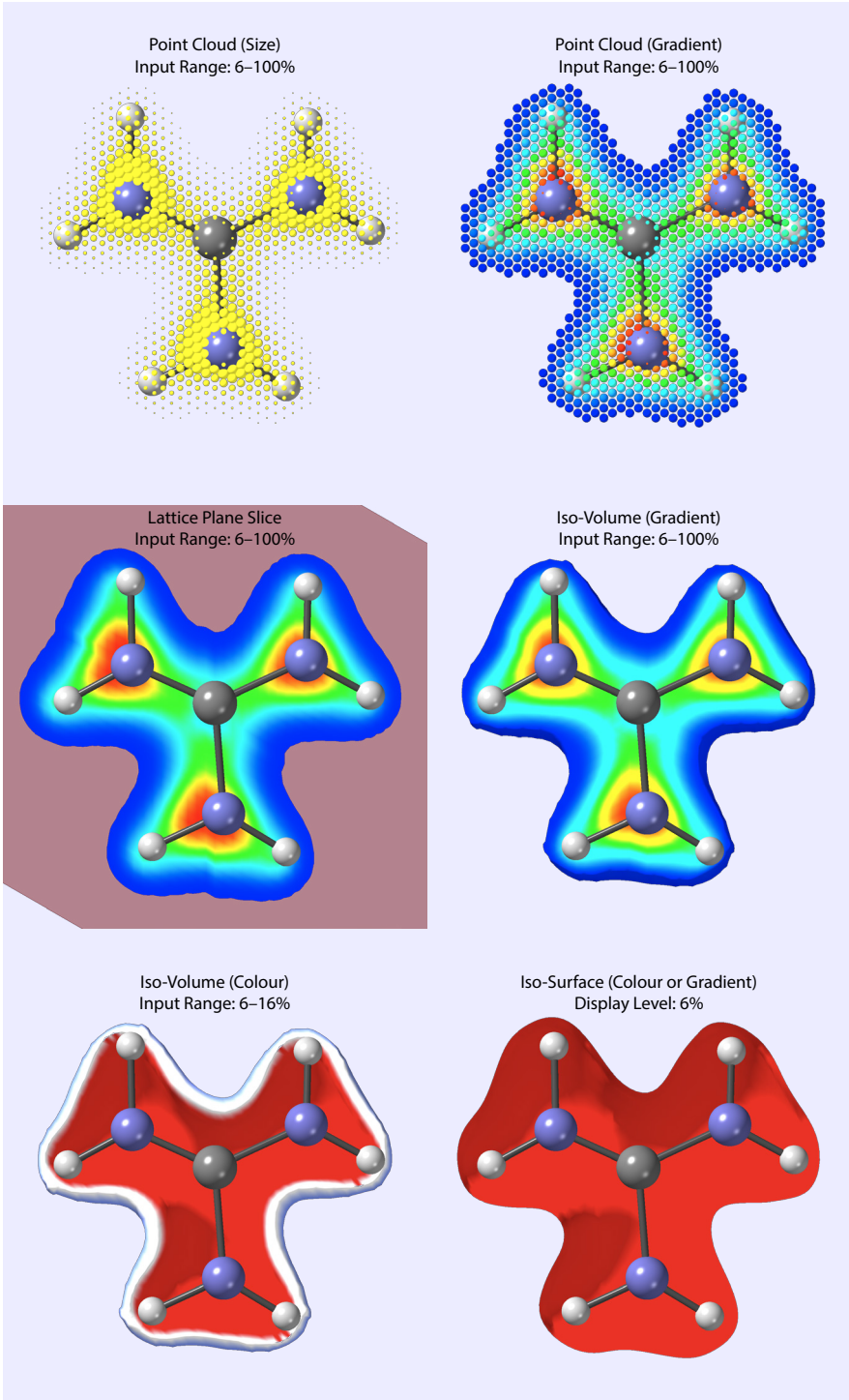
Each volumetric dataset is represented by a row in the Volumetric Data list. Controls embedded within the row let you toggle the dataset's visibility (**Vis** checkbox), change its colouring, opacity, display type, point size and input thresholds (i.e., opt to display a subset of the overall data).

One row from the Volumetric Data list, showing the controls available.



Volumetric display styles for a small organic molecule. The minimum input threshold for all plots is 6% and the maximum threshold was reduced to 16% for the bottom row.

Note that in the "Lattice Plane Projection", the red colour of the unfilled lattice plane shines through.



### Volumetric Display Type

CrystalMaker provides a choice of three main types of volumetric display:

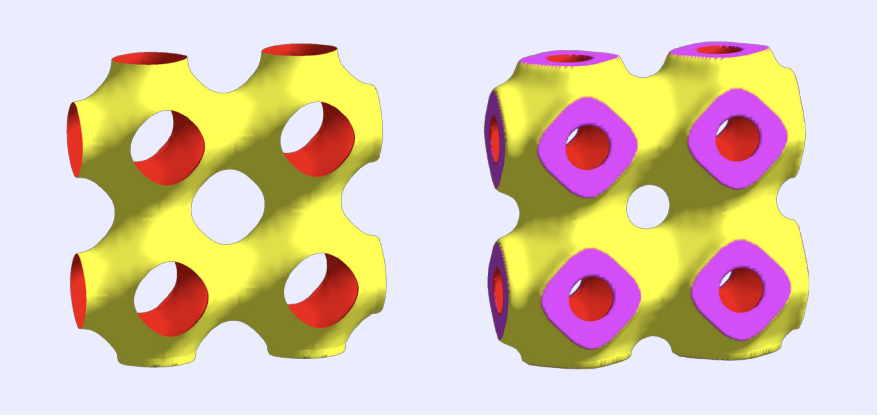
- **Point Cloud** (gradient or size). Each datapoint is plotted as a sphere, so this is a good option for directly visualizing your data. The value of each data point is communicated either by its colour (gradient option), or its size. You can scale sizes using the **Point Size** slider.
- **Lattice Plane Section**. Data are rendered onto any visible lattice planes using a gradient. Each lattice plane effectively shows a slice through the 3D dataset. You can move lattice planes through the structure, and add as many planes, in as many orientations as you require, using the **Lattice Planes** group of the Volume Inspector.
- **Iso-Surface** or Iso-Volume (gradient or single colour). All data between the minimum and maximum input thresholds are shown. If you specify the complete data range, you will end up with a solid block of data.

### Dataset Colouring

Depending on the display type, you can choose one or three colours—or specify a gradient display.

If you have selected a gradient option, the gradient is shown in the **Colouring** column of the list. You can click this and choose an alternative gradient from a popup menu. Options include rainbow, blue-white-red, greyscale, "fire", plus a selection of contour gradients: providing repeating bands at 10% intervals.

For "isosurface" displays, three colours can be chosen, corresponding to the minimum surface value, the maximum surface value, and the truncation area: where the surface is cut by the plot range or any selection boundary.



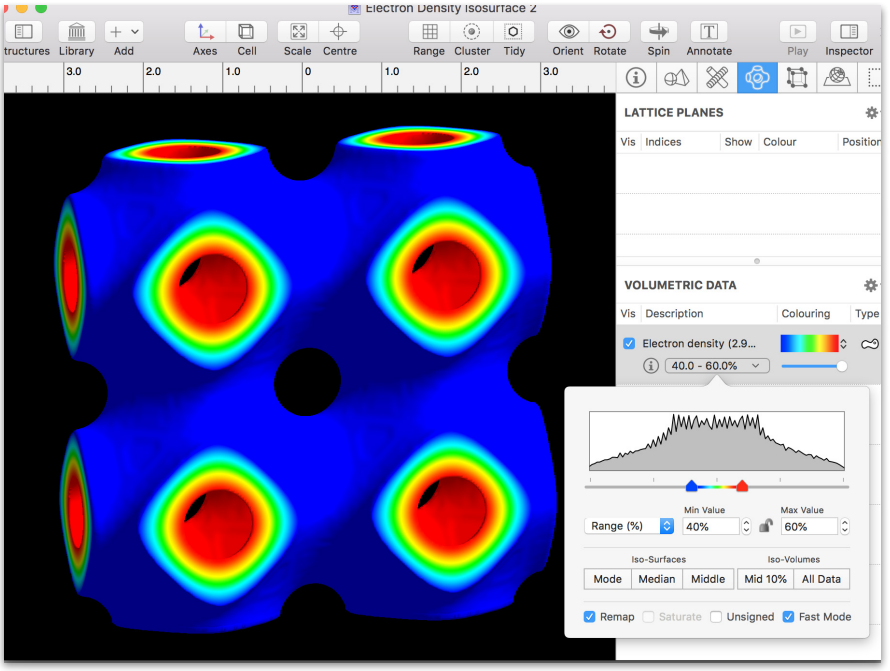
Visualizing electron density in a simple lattice. Left: 50% iso-surface showing "minimum" (yellow) and "maximum" (red) colouring. Right: 40-60% iso-volume showing a purple "truncation" colour, where the data are cut by the plot range.

## Data Range

CrystalMaker lets you control the range of data values to be plotted. For example, you might wish to hide any data points below a minimum threshold, so you can focus on the high values; or you might wish to hide any "saturated" values, using the maximum input slider.

If you are displaying an "isosurface", all values between the minimum and maximum values will be displayed—in other words, the thickness of your "surface" is the difference between maximum and minimum input thresholds (strictly speaking, unless the minimum and maximum values are the same, this is an "iso-volume", not an "iso-surface").

The current display range is shown in the list row, next to the Info button. Clicking the **Range** button displays a popover with a histogram (numbers of data points with a particular value), range slider (adjust minimum and maximum threshold values), text fields and preset buttons.




Editing the input threshold for an iso-volume display. Note the gradient display in the Range Slider, beneath the data histogram.

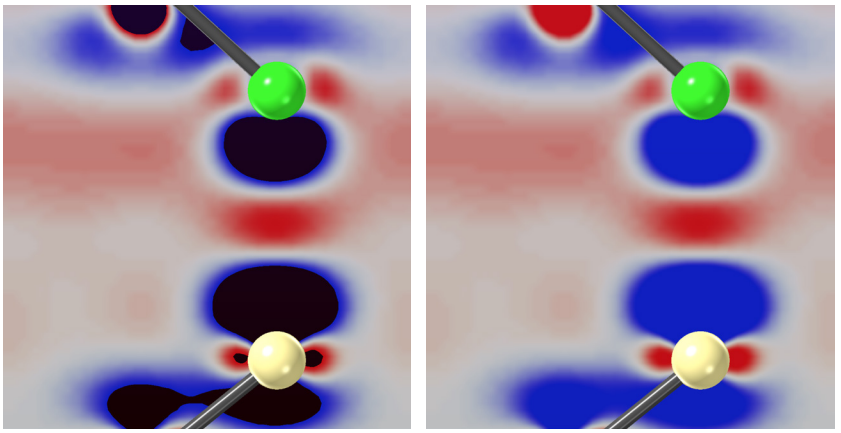
At the bottom of the Range popover are some checkboxes, letting you customize the gradient display, the speed at which updates are performed, whether to show out-of-range "saturation", and the option to show unsigned data.

### Remap Gradient

If you are working with a gradient display, you have the option of squeezing ("remapping") the gradient so it fits snuggly into a sub-range, rather than the full intensity range. This can help highlight areas of interest.

### Saturation

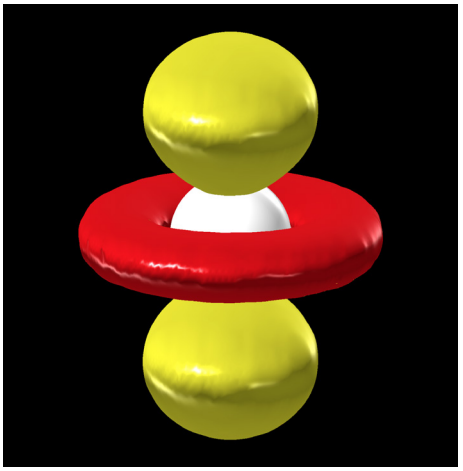
When visualizing lattice plane sections, the default option is to hide any data points which are outside the min/max thresholds, thereby revealing open areas on the lattice plane (which may be masked if you have specified a lattice plane colour and opacity). An alternative is to fill these areas with the minimum or maximum gradient colours, to emphasize which part of the intensity scale (minimum or maximum) these points correspond to.



Default Lattice Plane section (left), showing "holes" in the display where out-of-range data are excluded. The Saturation option (right) fills these holes. *Dataset courtesy of Giovanni Cantele.*

### Unsigned Values

The **Unsigned** checkbox which lets you display negative and positive values within the specified unsigned (absolute) value range. This is useful if you have data on either side of zero and wish to exclude values close to zero, regardless of their sign. If you are displaying an iso-surface with the colour option, different colours will be used for the positive and negatives parts of your visible data range.



An electron orbital visualized as an "unsigned" isosurface, using the Colour option. "Positive" and "negative" regions of the dataset use contrasting colours. The central atom is shown in white. *Dataset courtesy of Zack Gainsforth.*

### Fast Mode

Another option is for faster redrawing of volumetric datasets whilst you adjust the range using the slider. This option is designed for iso-surfaces or iso-volumes where interpolation is used to improve the rendering of sparse datasets. With the "Fast Mode" in effect, interpolation is temporarily disabled as you adjust the range slider; once your system is idle, your structure will be redrawn at maximum quality. (If your data are already detailed, no interpolation will be necessary and so this option will have no effect.)

## Dataset Info

The Info Button ⓘ embedded in each list row lets you display a summary of the dataset in a popover, including the number of voxels, physical dimensions of a voxel, dataset minima, maxima, mean, median and modal values.

## Adding Volumetric Data to an Existing Structure

CrystalMaker can import volumetric data in a range of formats (3ED, CASTEP, Gaussian CUBE, DEN, GRD, GULP, VASP). Most of these formats include unit cell (periodicity) and structural data, and so can be opened as documents in their own right. However, you can also add the volumetric data from such files to an existing structure; in this case, any structural data (atoms, cell parameters, etc.) in the text file will be discarded, and its volumetric data will be mapped onto the current crystal lattice.

### To add volumetric data to an existing structure:

Do one of the following:

- Drag-and-drop a text file into the list.
- Click the **Actions** popup button (cog icon) to display a popup menu, then choose an option from its **Import Data File** submenu.

### To remove a volumetric dataset:

1. Select the dataset to be removed by selecting its row in the list.
2. Click the **Delete** button on your keyboard to delete the dataset.

## Combining Volumetric Datasets

The Volumetric Data group's Actions menu includes a Combine submenu. This lets you take two *selected* datasets and either Add or Subtract their values (when subtracting, the second dataset is subtracted from the first). CrystalMaker will up-sample (i.e., linearly-interpolate) any dataset with a lower number of voxels in any dimension. This ensures that mismatched datasets can still be combined, and that maximum precision is used.

Chapter 8

# Labelling & Annotation

In this chapter we explore the various ways in which you can add text to your document, including Atom and Bond labels, as well as titles and text boxes, with or without arrows.

## Labels Versus Annotations

CrystalMaker lets you add two kinds of text objects to your document and it is important to be clear as to their differences.

- Structure-specific *labels* help identify individual atoms, bonds and unit cell edges. These labels are attached to their corresponding model objects and so they move with your structure as it is rotated or scaled.
- General *annotations* include lines, arrows and textboxes. These exist in an overlay layer—and remain fixed as any structures in your window are rotated or scaled below.

In addition to model labels and annotation objects, you also have the option of displaying a Legend (a key to the colours and styles of atoms or bonds). As with annotation objects, the Legend "floats" above the dynamical content of the window.

## Bond Labels

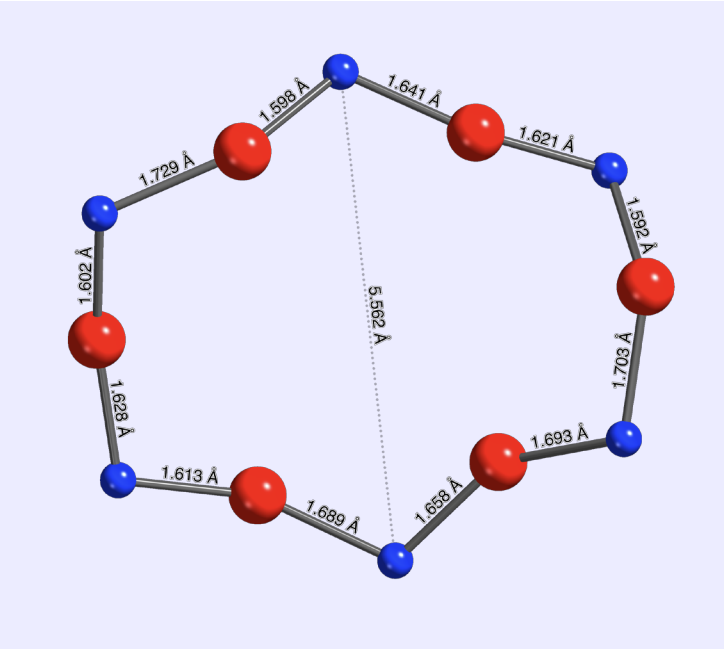
A new feature in CrystalMaker X is the ability to label individual bonds in your structure. Currently, all bond labels are of the same type: they give the length of their bond in crystallographic (Ångstrøm) units. You can also define rotatable distance measurements; these are effectively "secondary" bonds with line or thin bond cylinder styles.

### Displaying Bond Labels

Bond labels can be applied *globally*, via the Label checkboxes in the Bonds Inspector. All corresponding bonds will then be displayed with labels shown.

Alternatively, you can choose to label bonds *locally*, by selecting the bonds of interest and then enabling the Label checkbox in the Bond Properties group of the Selection Inspector.

Bond distance measurements can be created using the Bond Distance tool. We will explore this in more detail in *Chapter 12: Measurement*.




Labelled bonds in a zeolite ring, with a (rotatable) distance measurement across the centre of the ring.

As we will see with Atom Labels in the next section, bond labels are always drawn in the current highlight colour. Their size and font is set using the Labels group in the Model Inspector.

# Atom Labels

You can display atom labels which move with the structure as it is rotated or scaled. These are displayed in the current highlight colour (black or white) and can contain different kinds of information, including atom or site labels, element symbol, atom number, the height or coordinate information.

## Displaying Labels

You can apply labels to individually-selected atoms or opt to automatically all labels of a certain site or element type. Alternatively, you can label every single atom on screen.

### To label all atoms:

Do one of the following:

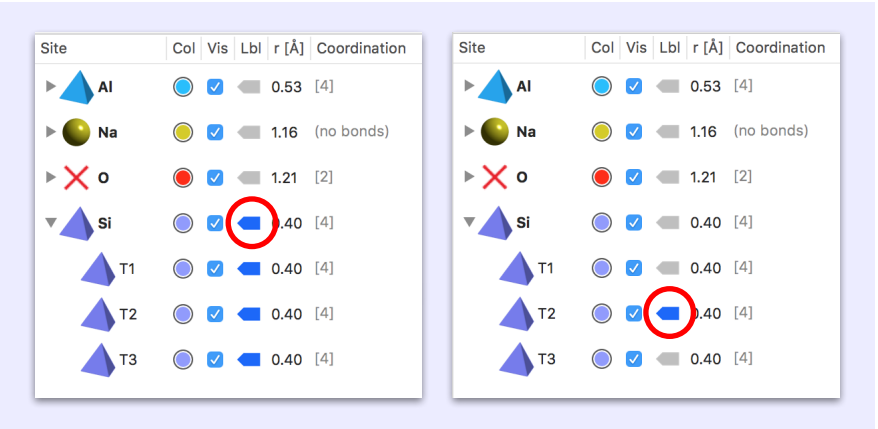
- Click the **Labels** button in the toolbar. (By default, this button may not be visible, but you can add it to your toolbar layout by customizing the toolbar.)
- Choose: **Model > Show Atom Labels** button.

### To label all atoms with a particular element symbol:

1. Display the Atoms Inspector and ensure it shows atoms grouped by element.
2. Locate the *element row* (this will have a disclosure triangle in front of it) and click the label icon so it shows a blue highlight.

### To label all atoms correponding to a particular site:

- Locate the site row in the Atoms Inspector and click the label icon.

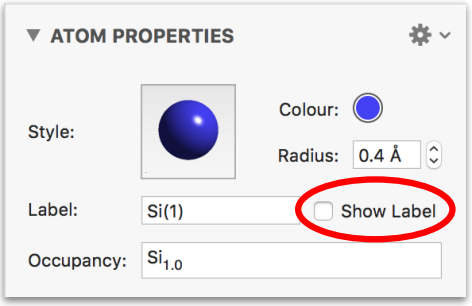



Toggling atom labels using the Atoms Inspector. Left: labelling all Si atoms; Right: labelling all atoms on the T2 site.

### To label specific atoms on screen:

1. Select the atoms to be labelled (e.g., by shift-clicking on them). If the Inspector is visible, the Selection Inspector pane should appear.
2. Click the **Show Label** checkbox in the **Atom Properties** group of the Selection Inspector.

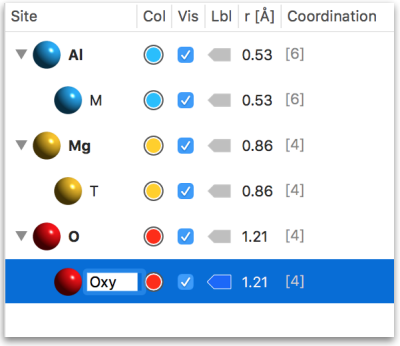
Part of the Selection Inspector, showing the control to toggle atom labels for the current selection.



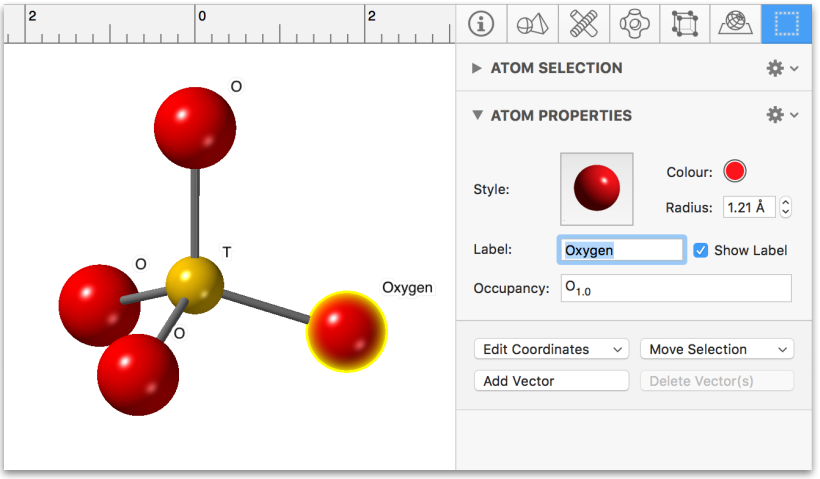

## Editing Atom Labels

You can edit atom labels in the Crystal or Molecule editor windows. Alternatively, you can use double-click an atom or site row's label in the Atoms Inspector to edit this. If this is a crystal structure, all atoms for that site will have their atom label displays updated.

Editing a site label using the Atoms Inspector.



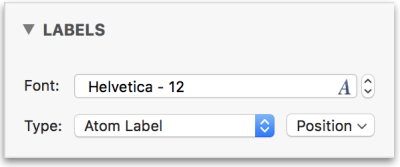

A third way is to select the atoms whose labels you wish to edit, then use the **Atom Properties** group in the Selection inspector to edit the label. Note that, if you are working with a crystal structure, this will give the selected atoms *different* labels to other (unselected) atoms on the same site (as illustrated below).




Labelling a selected atom in the spinel structure. Note that this atom is displaying a unique *atom label*, whereas the other atoms are displaying their *site labels*.

## Changing Label Styles

Global label settings (type, position, font, etc.) can be set using the **Labels** Group in the Model Inspector:




The Labels group in the Model Inspector

## Label Content

By default, atoms display a text string, the "atom label", which is usually set when you build or import a structure (but which can be edited at any time). However, you can use the **Labels** group to display other information, including heights, element symbol or coordinates.

Please note that all labelled sites share the same label content type—so you can't mix chemical elements, atom numbers and z-coordinates on the same plot.

### Atom or site label

*Example:* "Ca(2)"

For a molecule, every atom has its own label, which you can inspect in the Atoms Inspector. For a crystal, atoms usually display the label for their corresponding *site*. However, you can override this, and give atoms a *unique* atom label, using the Selection Inspector: simply select the atom whose label you wish to change and enter a new label in the **Atom Properties** group.

### Chemical Element Symbol

*Example:* "Ca"

This corresponds to the *principal* element symbol for the site. For example, if a site were disordered, with average composition, say $Al_{0.5}Si_{0.4}Ti_{0.1}$, then the site would be labelled "Al".

### Atom number

*Example:* "`597`"

Atom numbers are used internally, within the program, but can be useful if you need to track atoms.

### Height

*Example:* "`-13.234 Å`"

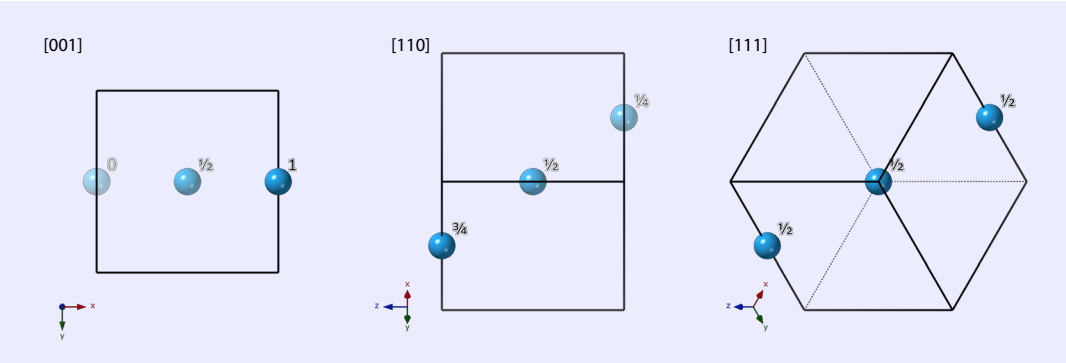
This is the *z*-coordinate of the atom, measured in Ångstrøm units, relative to the *screen axes*. In other words, it is the vertical distance of the atom from the plane of the screen. As you rotate your structure, the heights will change.

### Relative Height (crystals only)

*Example:* "½"

This is the height of atoms relative to the *unit cell repeat distance* normal to the screen. The heights will be expressed relative to the closest lattice vector to the screen normal. For clarity, CrystalMaker finds the closest lattice vector in one of the sets <100>, <110> or <111>, and then uses this to compute the fractional height. This avoids massive changes in the fractional height as the unit cell is tilted slightly, e.g., if the view direction changes from [001] to [1 1 10000000] !

*For example, if the crystal is viewed approximately down the [001] direction, then heights will be fractions of the c parameter, whereas if the crystal is viewed approximately down [110] then heights will be fractions of the vector a + b.*




Atoms labelled by relative height, shown in different orientations.

### Individual X, Y or Z Coordinates

*Example:* "½" *(crystal) or* "7.32 Å" *(molecule)*

You can opt to display an *x*, *y* or *z* coordinate. These will be *fractional* coordinates for crystals or structural (orthogonal) coordinates for molecules. Because these are coordinates are defined relative to the structure (not the screen), they do not change as you rotate your model.

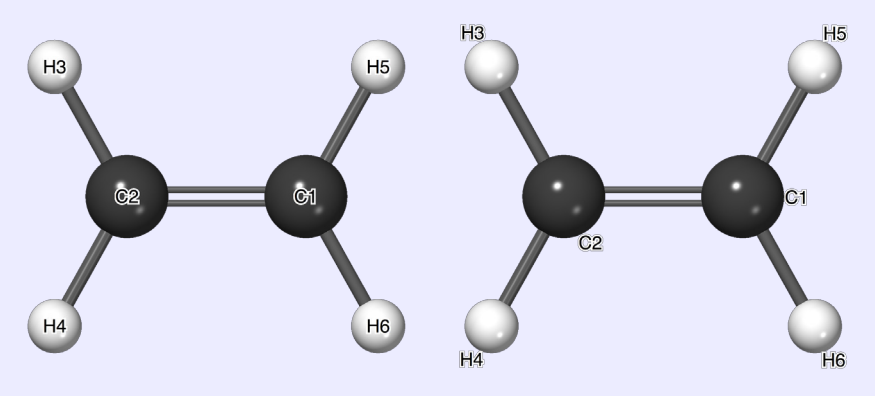
### Coordinates

*Example:* "0 ½ ¾" *(crystal) or* "7.12 3.32 –0.75 Å" *(molecule)*

This option displays the set of *xyz* fractional (crystal) or structural (molecule) cordinates.

## Label Position

You can specify the position of labels, relative to the host atom, or you can opt to let CrystalMaker automatically position the labels, so as to avoid overlap with neighbouring bonds.

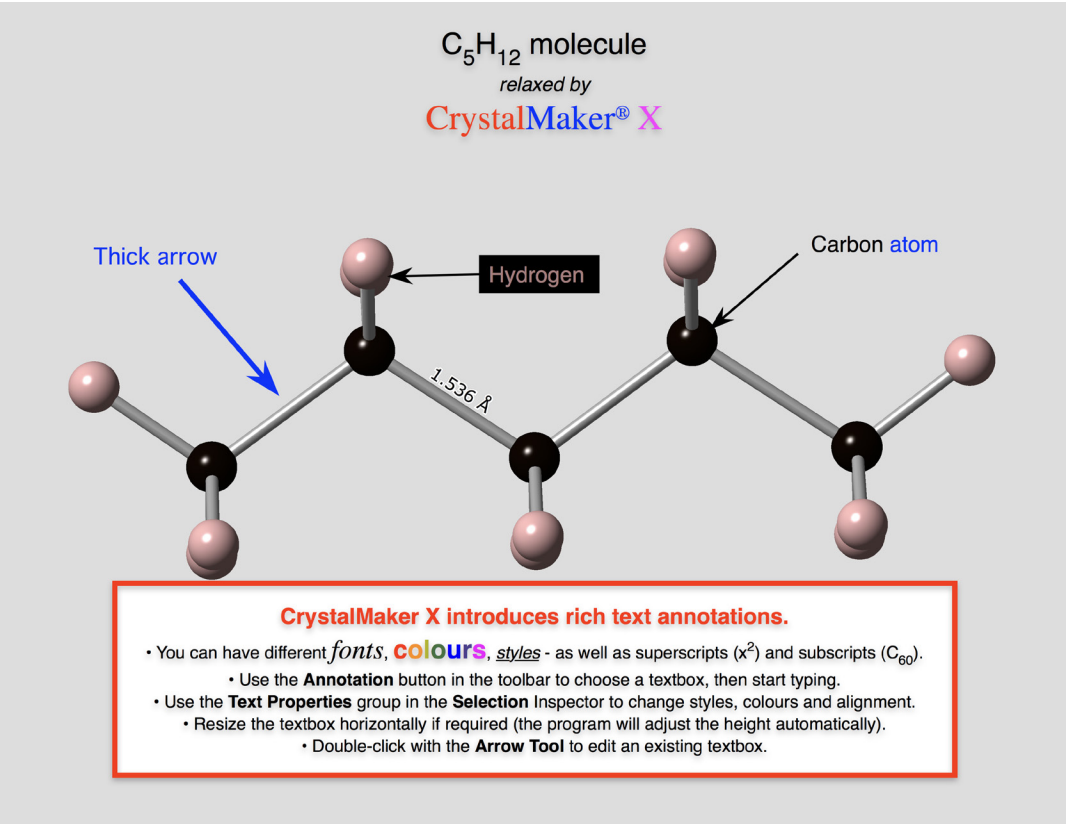



Different label positioning in ethene. Left: centred; Right: auto-positioned to avoid overlaps between labels and bonds.

**Annotation Option:** CrystalMaker provides powerful annotation capabilities, letting you overlay rich-text boxes, lines and arrows above your structure: ideal for final publication output.

## Annotation

CrystalMaker lets you overlay rich-text annotations, lines and arrows above your structure. Please note that, unlike atom and bond labels, annotation objects exist in a separate layer, *above* your structure—and do not rotate when the structure is rotated (hence it is best to add annotation once you have finalized the orientation and appearance of your structure).

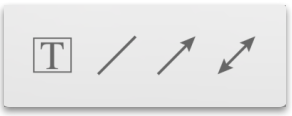



Annotation includes textboxes with rich-text plus lines and arrows.

### Creating Annotation Objects

CrystalMaker provides an **Annotate** button in the toolbar; clicking this reveals a popover, letting you choose: text, line, arrow or double-arrow:

The Annotation Popover.



Newly created annotation objects use default settings and are positioned in the centre of the screen; they are selected, so you can easily move or edit them.

### To add a plot title:

- Choose: **Model > Add Title**.

The title is, by default, positioned in the top left-hand corner of the Graphics pane—but this can be customized using the **Workspace** pane of the Preferences window.

### To create a text annotation from an atom label:

1. Select the atom(s) whose atom labels should be converted into text annotations.
2. Choose: **Model > Convert Labels to Textboxes**.

Converting atom labels to text boxes can be useful as a final stage in the production of a figure for publication. It provides the flexibility to reposition labels, adjust their content and change their fonts or styles.

### To duplicate an existing annotation object:

1. Choose the Arrow tool from the Tool Strip.
2. Select the annotation objects you wish to duplicate (shift-click for multiple selection).
3. **Option**/**Alt**-click and drag one of the selected objects.

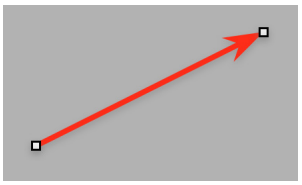
### To delete an annotation object:

1. Select the annotation objects you wish to delete (e.g., by **shift**-clicking on them with the Arrow tool).
2. Press the **Delete** (backspace) key on your keyboard.

**Select All:** To select all annotation objects (useful if you wish to edit or delete them *en masse*, choose: **Edit > Select > All Annotations**.

## Moving Annotation Objects

Any selected annotation object shows a pair of control handles: these indicate that the *entire* object is selected; you can then drag the object to a new position, or edit its position using the Selection Inspector.



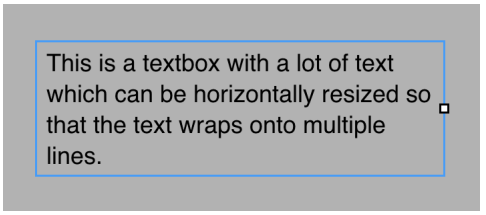
A selected arrow object: note the two control handles at either end.

The positions of annotation objects are defined in a *relative* sense to the rest of the graphics window, so that they maintain their correct relative positions when

you copy or print graphics at high resolution, or when the window is resized (as long as you maintain the window's aspect ratio). Because CrystalMaker X saves a document's size and position on the screen, you can be sure that your annotations will be correctly displayed the next time you open your document.

## Resizing an Annotation Object

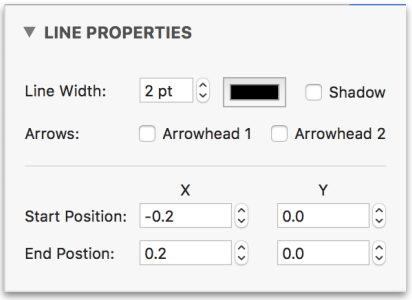
To resize an annotation object you simply click-and-drag one of its two control handles (the unclicked handle vanishes when you do this).




A textbox being resized horizontally using its right-hand control handle. (The inactive left-hand control hand is hidden.)

## Editing Annotation Objects

To edit an annotation object you need to first select it (e.g., using the Arrow tool). You can then use Selection Inspector to change properties such as line width, colour, shadow, position and height (relative to other annotation objects).



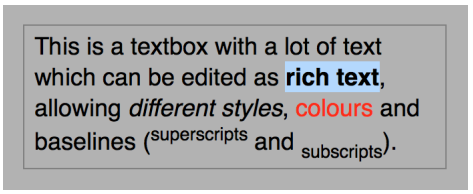

The Line Properties group in the Selection Inspector.

Note that line-, arrow- and double-arrow objects are interchangeable: you can use the **Line Properties** group to toggle arrow heads on or off.

## Editing Rich Text

Selecting a text box lets you change its overall settings. However, if you wish to change text styles *within* the box, you need to *select* part of the text first. To do this, simply double-click on the text so that it appears highlighted:

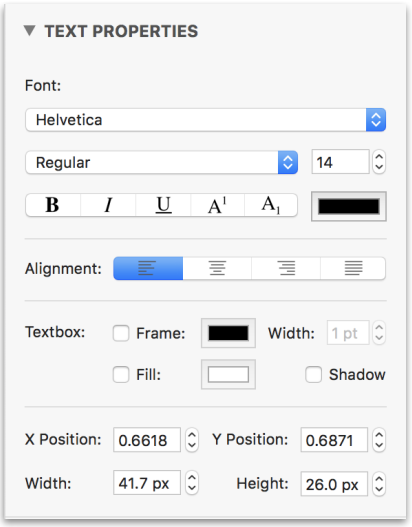
Editing rich text in a text box: the words "rich text" have been selected and a bold style applied.




You can then edit the text in one of three ways:

- Using the **Edit > Format** submenu. The Font submenu lets you change fonts, styles and sizes; the Text submenu lets you change alignment.
- Using the standard system font panel (Mac users: **command-T**) to edit font size, style and colour.
- Using the **Text Properties** group in the Selection Inspector to change font, size, style, text alignment, baseline (superscript, subscript or normal), etc. (as illustrated below).

The Text Properties group in the Selection Inspector.




**Cross Platform Issues:** Mac and Windows computers generally use different fonts and even the same fonts have different metrics. This means that text displayed correctly on, say, the Mac version, may not display correctly on the Windows version: the font may be substituted and may appear at an incorrect size.

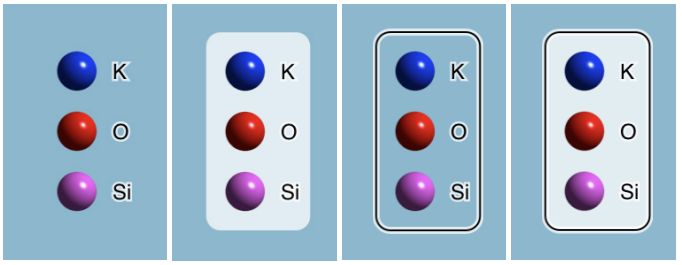
**Windows Subscripts:** Another issue concerns using superscripts and subscripts on Windows computers. Whilst the Mac version lets you do this with any fonts, on Windows, this is only possible if you use the newer *OpenType* fonts.

## Legend

A new option in CrystalMaker X is the ability to display a legend in the Graphics Pane. The legend provides a key to the colours and styles in your structure. Only the visible atoms are included and, for very-large numbers of atoms, only different element types are shown.

You can drag the legend to one of eight different locations on the screen: the four corners and the centres of the four edges. You can also customize the legend display by right-clicking on it and choosing options from its contextual menu:

- Position on screen: top left, top centre, top right…
- Frame
- Translucent background




Examples of the Legend display with and without a frame and a translucent background.

**Double-Click Tip:** If you double-click the Legend, the Atoms Inspector is made visible, allowing you to customize atom/site visibilities, styles, labelling and more.

Chapter 9

# Rendering

This chapter covers the process of "rendering" your three-dimensional structural model on screen. All of this happens automatically, but CrystalMaker lets you override the default behaviour, using a range of controls in the Rendering Inspector. You can change the way that atoms are bonds are depicted, emphasizing the three-dimensional aspect of a model, and enable a thrilling 3D red/blue viewing mode, for dramatic "out-of-the-screen" graphics.

## Principles of Rendering

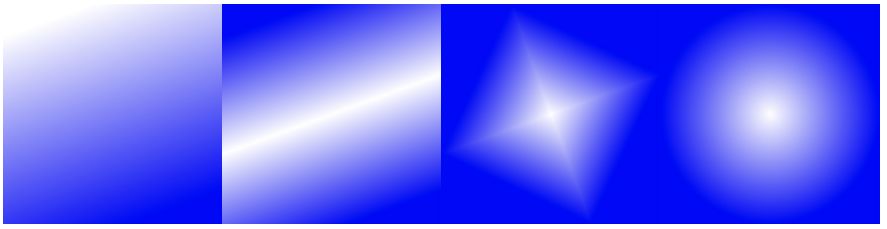
Rendering is the process of turning your abstract crystal or molecular model into a vivid image on your screen. This involves a series of different stages:-

- Assign a background: a colour, gradient or image, above which the structure will be displayed.
- Define the reflectivities for the different model objects: atoms, bonds, polyhedra, surfaces, lattice planes.
- Apply lighting to illuminate the scene.
- Simulate the effect of atmospheric fog or haze ("depth fading").
- Apply a perspective correction.

CrystalMaker can also show this "rendered" scene from a pair of angles, thereby giving a true three-dimensional image. This can be viewed as a "stereo pair" in full colour, or as a red-blue anaglyph.

# Background

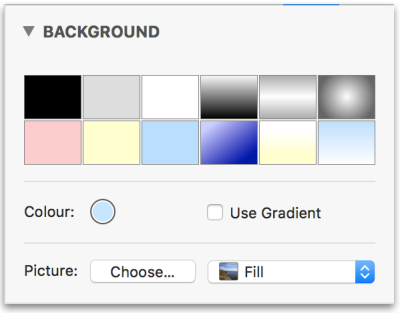
CrystalMaker lets you display plain or gradient-filled backgrounds with the option of a background picture.



Background gradients available in CrystalMaker. From left-to-right: Linear, Reflected, Diamond, Radial.

## Editing Background Settings

You can adjust background settings using the **Background** group of the Rendering Inspector :




Part of the Rendering Inspector, showing the Background group.

The Background Inspector also includes a range of one-click presets, which are previewed in the colourful boxes at the top of this group. These include examples of different gradients, as well as plain colours.

### To display the Background group:

Do one of the following:

- Right-click in the Graphics Pane to display a contextual menu and choose: **Change Background**.
- Display the Rendering Inspector (**View > Inspector > Rendering**) and open the **Background** group.

### To change the background colour(s):

1 Choose a fill pattern option:

- Choose **Plain background** to specify a background with a single colour.
- Choose **Gradient fill** to display one of a number of gradient options. You have

the option of changing the scale or angle for some of these options.

2 Choose the background colour(s) from the corresponding **Colour** button(s).

## Adding a Background Picture

You have the option of display a background picture. This can be displayed in various ways, according to the **Fill** popup menu in the Background Group:-

- **Tile**. The picture is displayed at its natural size in the top left-hand corner of the Graphics Pane. It is then repeated horizontally and vertically to fill all the available space. This option is best suited to small textures.
- **Centre**. The picture is displayed at its natural size in the centre of the Graphics Pane. Depending on the size of your picture, your background colour/gradient may be shown around the edges of the picture—or the picture may be clipped. This might be useful if you have, say, a two-dimensional contour map over which you wish to overlay a crystal structural model.
- **Scale**. The picture is rescaled so that it spans either the full width or full height of the Graphics Pane (depending on the relative aspect ratios of the picture and the Graphics Pane).
- **Fill**. The picture is scaled horizontally and vertically to fill the entire Graphics Pane. If the picture's aspect ratio differs from that of the Graphics Pane, the picture will be distorted.

### To add a background picture:

Do one of the following:

- Click the **Choose…** button in the **Background** group and choose a graphics file from the file dialog that appears.
- Drag-and-drop your picture directly into the Graphics Pane.

### To remove an existing background picture:

- Click the Source **Clear** button in the Background Picture group.

**Saving the Picture:** The background picture is saved in your document, together with all structural and other display information. This contrasts with earlier versions of the program, where only a link ("alias") to the original picture files was stored. Saving a copy of the picture with your document gives you more flexibility—but please bear in mind that the file size will increase.

## Reflectance and Shading

CrystalMaker lets you adjust the *reflectance* of solid objects, making them look as if they are made of different materials such as plastic, metal or wax.

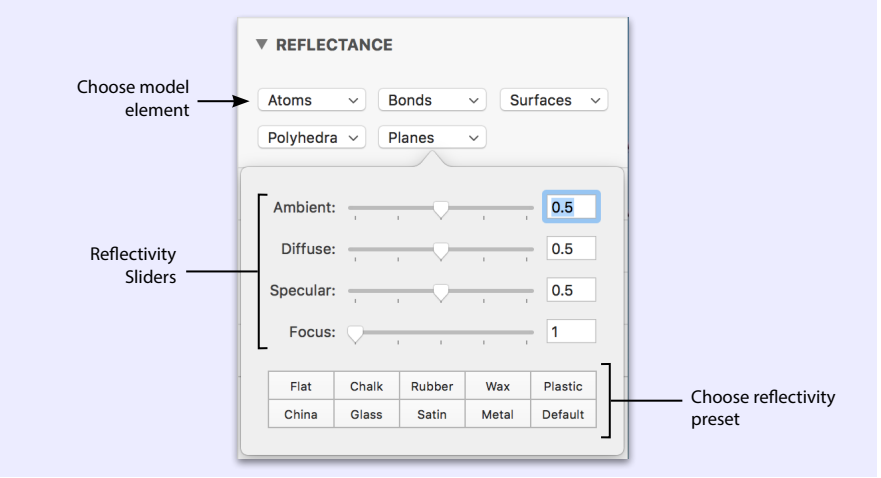
### Reflectance Explained

The intensity of light reflected from a solid body depends not only on the light source, but also on the intrinsic reflectivity of the material.

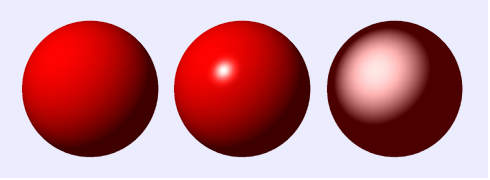
- Ambient illumination causes the solid body to glow evenly in all directions, as if the body itself were the source of the illumination.
- Diffuse reflection varies with direction; strong diffuse reflection gives objects a "chalky" lustre.
- Specular reflection is characteristic of shiny or waxy surfaces, where a surface "gloss" causes intense reflection from a point light source.

### Adjusting Reflectance Properties

Use the **Reflectance** group of the Rendering Inspector to adjust settings for atom spheres, bonds, polyhedra, surfaces or lattice planes. Choose which model element to edit by clicking its button, then use the popover to adjust reflectance in real time (or apply a preset).




Part of the Rendering Inspector, showing the Reflectance group.

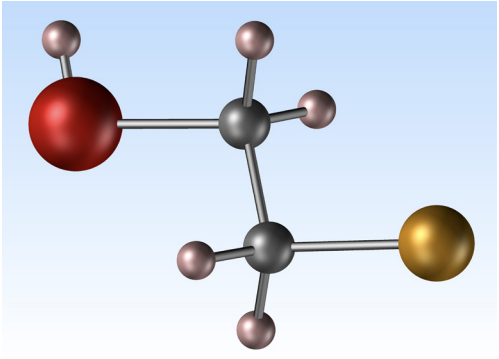


Reflectivity presets in action. From left to right: "Chalk", "China", "Metal".

## Lighting

You can also adjust the type of *illumination* required: its intensity and direction. CrystalMaker X provides up to five light sources: one ambient (omnidirectional) light plus up to four spotlights, each with customizable intensity and direction.

By default, CrystalMaker X uses two spotlights. The second spotlight makes models look more realistic, emulating a spread of light as found in a typical office environment (desk light, window, etc.). Adding three spotlights (as illustrated below) makes the specular reflections appear to be reflections of real objects.

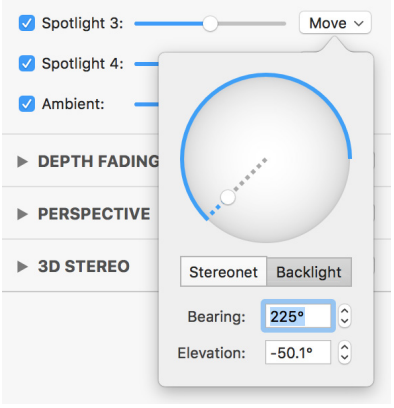


Using multiple spotlights gives this dummy molecular a realistic, metallic look.

The **Lighting** group in the Rendering Inspector provides interactive controls for enabling or disabling spotlights, changing their intensities (sliders) or changing the orientation of the light source. Click the **Move** button to display a stereogram control; click and drag the indicator inside the stereogram to move the light source, or enter an explicit bearing and elevation in the text fields.

**Multi-Touch Lighting Control:** Mac users with trackpads can use "pinch" and "expand" gestures to change the elevation of the spotlight; use the "rotate" gesture to change its bearing.

The **Backlight** option lets you change the sign of the elevation. Negative values work well with specular illumination, e.g., highlighting the edge of a sphere.

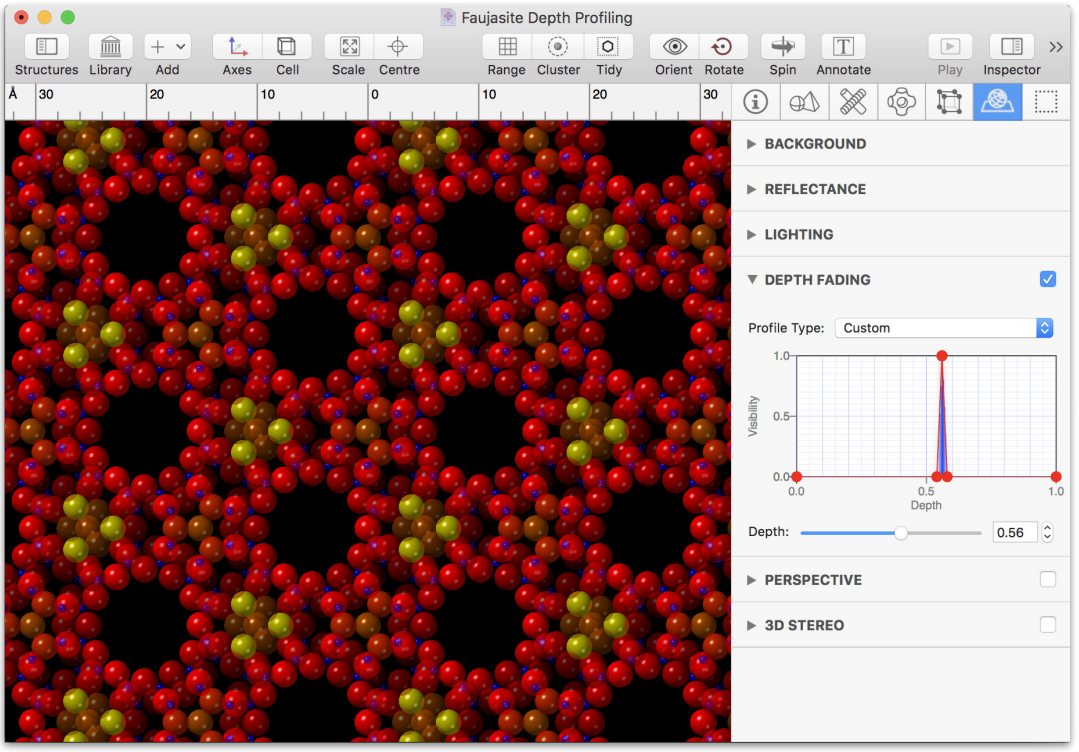



Adjusting the orientation of a spotlight using the LIghting group in the Rendering Inspector. In this case, the spotlight is behind the model ("Backlight") and hence has a negative Elevation.

## Depth Fading

Conventional "depth fading" simulates the effect of atmospheric haze or fog: so that distance atoms appear to blend into the background. This is useful for complex structures with many atoms. With large amounts of depth fading, atoms become invisible beyond a certain, critical depth.

A special feature in CrystalMaker is the ability to control the opacity of foreground atoms, so that you can focus on a slab of structure at a particular depth; we call this "Depth Profiling".




Using Depth Profiling to reveal hidden cavities inside a zeolite framework.

Applications of Depth Profiling include:-

- **Seeing inside dense materials.** Using a slider control, you can progressively "zoom" through different depths of material, profiling the structure that would otherwise be hidden by frontmost atoms.
- **Rapidly scanning a computer simulation model.** You might have a massive block of atoms and need to rapidly scan through this, in search of anomalies or other areas of interest.

- **Viewing surfaces as a function of height.** For a given plane, the arrangement of atoms varies according to the height of the surface. If you set your view direction to be perpendicular to your desired surface plane, then you can rapidly scan through the range of atomic patterns at different depths.

### To turn on depth fading:

◆ Choose: **Model > Turn Depth Fading On**.

### To control the extent of depth fading:

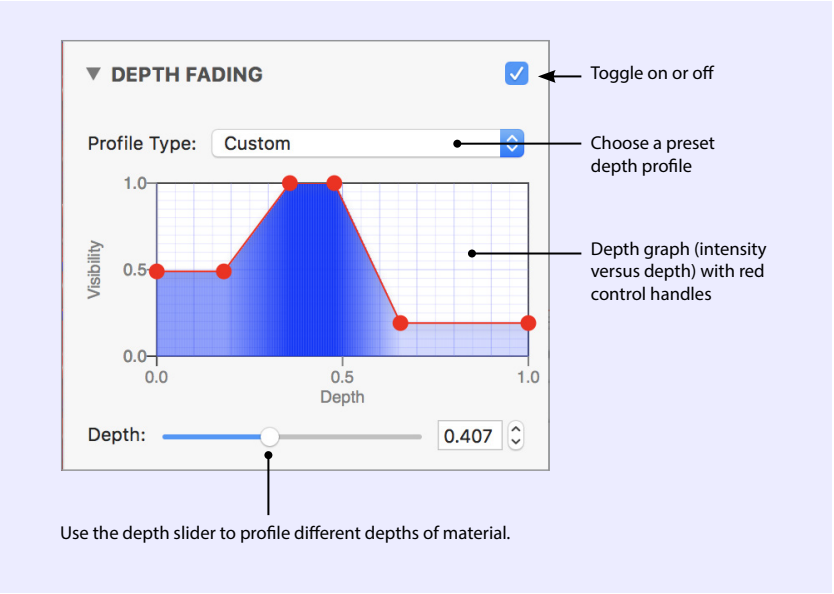
◆ Choose a preset from the **Profile Type** popup, or drag the red control handles in the graph to adjust how the opacity of an atom varies with depth.

### To "profile" different depths of material:

1 Choose an appropriate depth profile (e.g., a "Needle" profile).

2 Click and drag the slider control to visualize different depths of material.

> **Multi-Touch:** You can use "pinch" and "expand" gestures to control the extent of depth fading in your structure (e.g., the width of the central maximum in your "Needle" profile). Use a two-finger horizontal swipe to shift the maximum to the left or right. Use a two-finger vertical swipe to adjust the baseline intensity.




The Depth Fading group in the Rendering Inspector.

## Perspective

A perspective correction can be used to emphasize the three-dimensional nature of any model. Use the **Model > Turn Perspective On/Off** command to enable to disable perspective.

You can vary the amount of perspective distortion using the **Perspective** group in the Depth Inspector: editing the view distance (the distance between you and the nearest part of the structure). Small view distances enhance the sense of perspective, but can make the structure appear distorted. For best results, choose a view distance in proportion to the maximum dimension of the structure: larger structures can be viewed from afar, whilst very small structures may require closer viewing.

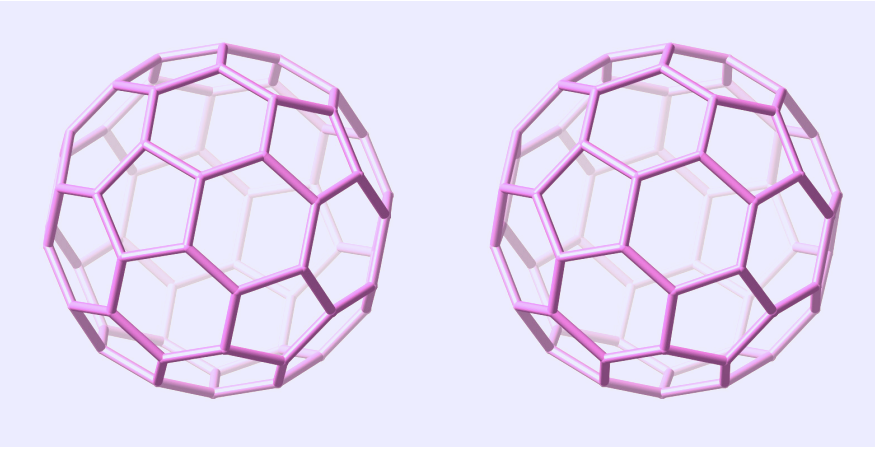
## Stereo 3D

CrystalMaker provides two built-in 3D viewing modes: Stereo-Pair plots; and Red-Blue Stereo. The latter requires a pair of red/blue glasses—simple, cheap and readily obtainable—and can give a thrilling "out-of-the-screen" effect.

### Stereo-Pair Plots

Stereo-pair plots show two side-by-side images, representing left- and right-eye views of a model. The two views are slightly rotated relative to each other (i.e., they have an angular offset) and ideally, the distance between the two images should match the distance between your eyes.

You can adjust the angular offset using the **3D Stereo** group of the Rendering Inspector. The best way to adjust the separation of the image pairs is to manually resize the graphics window—or, if you are printing, to use the Page Setup (**File > Page Setup**) to specify a final print size (twice the pair separation).

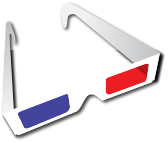


Stereo-pair image of a "buckyball" molecule. The images are recorded at slightly different angles.

### 3D Stereo Projection

It is possible to *project* stereo-pair images in such a way that true-colour 3D images can be created. The technique involves superimposing the left-eye and right-eye views from a stereo pair plot, using two computer projectors, polarizing filters, a silvered screen—and polarizing spectacles.

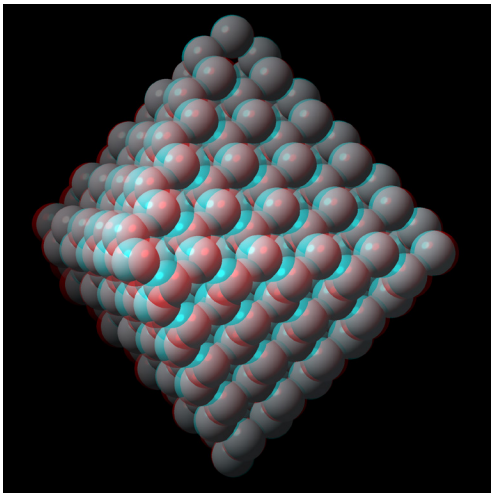
You would need to expand your Graphics window so that each half of the stereo pair lies on a different virtual screen, covered by a projector. Each projector would require a polarizing filter, with one filter rotated through 90° relative to the other. 3D images could then be viewed using polarizing spectacles (again, with one lens rotated through 90° relative to the other). For best results, you should use a silvered screen (a white screen results in light scattering, and reduces the polarization of the projected light).



## Red/Blue Stereo

Red/Blue stereo superimposes two views of a model at an angular offset, as defined in the **Separation** field of the Depth group. The views are filtered so that one uses shades of red and the other shades of cyan. When stereo glasses are used (a red lens over the left eye, and a blue, cyan or green lens over the right eye), impressive three-dimensional views may be seen.

Red/blue stereo is a great way to demonstrate 3D structures in a lecture theatre. Graphics can be projected onto a projector screen and your audience require only low-cost cardboard-framed red/blue spectacles. Educational institutions will particularly appreciate the much higher resolution and considerably lower cost of this method, as compared with proprietary 3D colour display systems.



Red/Blue stereo image of the diamond structure, showing (111) octahedral faces.

In some cases, stereo models may appear to emerge from the screen towards you. We call this phenomenon **Stereo Standout**. For the most relaxed viewing, a neutral standout value (zero) is preferred, with the model centred on the screen surface.

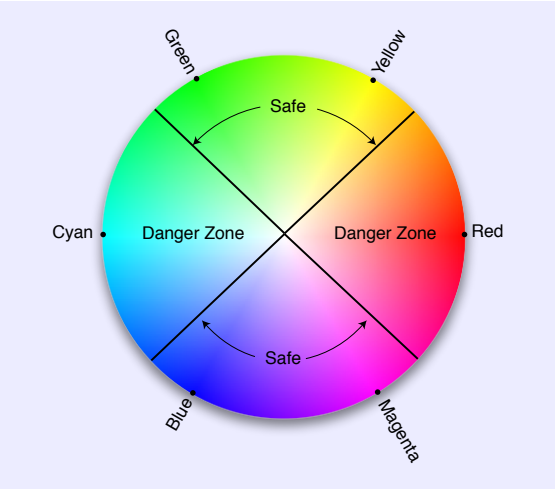
**Relaxing the Eyes:** You may find it helpful to slowly rotate the structure, as this helps to relax the eyes and enhances the 3D effect, particularly if you are using a large 'standout' value.

There are some limitations to the range of colours that can be used in Red/Blue Stereo:-

- Red is blocked by the cyan filter;
- Cyan is blocked by the red filter.

For the best results, you may wish to tweak the colours in your structure, so that they correspond to hues away from red and cyan (the "danger zones" in the colour wheel shown below), and instead use hues in the "safe" areas between yellow/green and blue/magenta.

Colour wheel showing "safe" colours for use in red/blue stereo.




As a convenience, you can use the **Colour > Optimize for Red/Blue Stereo** command, which is located on the Atom Inspector's contextual menu and also on its **Actions** menu (the cog icon, in the inspector's top right-hand corner). This command automatically shifts colour hues away from the "danger zones" of red and cyan.

# Saving Model or Rendering Preferences

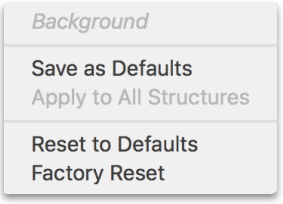
If you save your structure in a CrystalMaker document, all of its model options will be saved with the structural data, ready for the next time you open the document.

You can also opt to save your favourite settings as default settings, so they will be used for all new structures. We have already met the **Preferences** panel; this includes dedicated panes for Model objects (atoms, ellipsoids, bonds, polyhedra), Model "Extras" (e.g., unit cell, lattice planes, etc.) as well as Rendering settings too. However, you might find it easier to adjust some of these settings (particularly reflectance and depth fading) using the Inspector instead.

## Customizing Specific Options

All of the Model and Rendering Inspector groups let you save their settings as defaults, which will then be applied to new structures. You can also reset the current group's settings (e.g., the unit cell settings) to your default settings, or to the "factory settings". Simply **control**-click anywhere in a control group to display a contextual menu.

Contextual menu for the Background Group.




**Apply to All Structures:** Use the contextual menu's **Apply to All Structures** command to propagate any changes to all structures in the current document.

## Customizing All Inspector Options

If you wish to apply the settings for *every* control group, you can use an Inspector-wide contextual menu instead.

### To Display an Inspector-Wide Contextual Menu

Do one of the following:

- Right-click below the lowest control group.
- Right-click in the Inspector tab.

Chapter 10

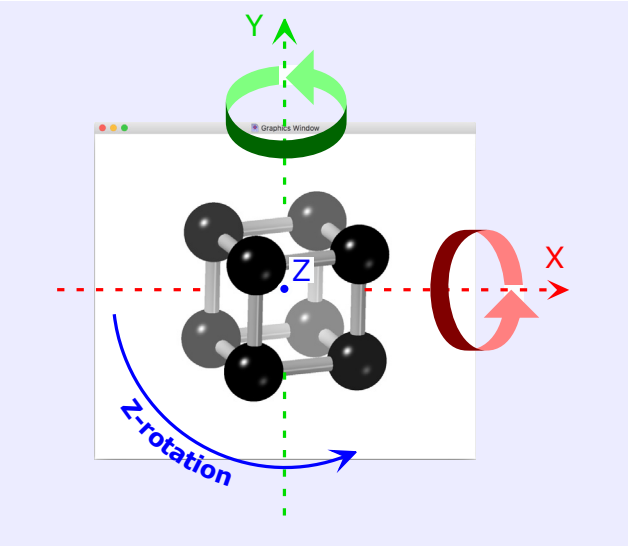
# Manipulation

This chapter describes ways in which a structural model can be manipulated on screen: changing its orientation, scale, and the range of atoms plotted (including the creation of crystal surfaces).

## Rotating the Structure

CrystalMaker uses a set of orthogonal *screen axes* as a reference for rotations. These should not be confused with the *crystallographic axes* in your model! As their name might suggest, the screen axes remain fixed, relative to the computer screen, whereas your crystallographic axes are fixed relative to your structure (and so will appear to rotate as your structural model rotates).

The scheme of the screen axes is as follows: X runs left-to-right across the screen; Y from bottom–to–top, and Z directly out of the screen. Rotations are defined as being positive if they occur in a right-handed sense relative to the screen axes:

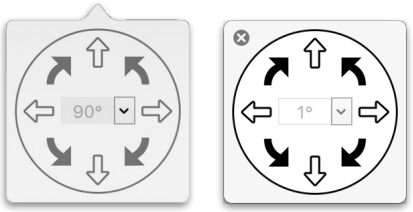



CrystalMaker screen axes: the sense of positive rotation is indicated.

## Rotation Popover

You can use the toolbar's **Rotate** button to display the Rotation popover. This lets you apply precise rotations about specific screen axes, with the sense of rotation indicated by the arrows.

The Rotation Popover, shown here in its attached (left) and detached (right) states.




**Tear Away:** As with many of the toolbar's popovers, you can click-and-drag the Rotation popover away from its toolbar button, to keep it open on the screen as a floating palette. Note that, in this, detached state, the popover has a small Close box in its top left-hand corner.

### To rotate about a screen axis:

Do one of the following:

- Click an arrow in the Rotation Popover.
- If the Rotate tool is active, you can click one of your keyboard's arrow keys to rotate left, right, up or down. (To rotate about the screen Z axis, hold down the **shift** key as you press an arrow key.)
- Press a button on your keyboard's numeric keypad, using the scheme below:-

Keyboard rotation buttons.

| | | |
|---|---|---|
| –Z | –X | +X |
| –Y | | +Y |
| +Z | +X | –Z |

| | | |
|---|---|---|
| 7 | 8 | 9 |
| 4 | 5 | 6 |
| 1 | 2 | 3 |

At each button press the structure is rotated through a rotation angle step.

**Rotating the Selection:** Use the Rotate Selection tool to apply any rotation only to selected atoms. (The Rotation Selection tool can be located using the drop-down menu next to the Rotate Tool in the Tool Strip—its icon shows a hand inside a dashed rectangle.)

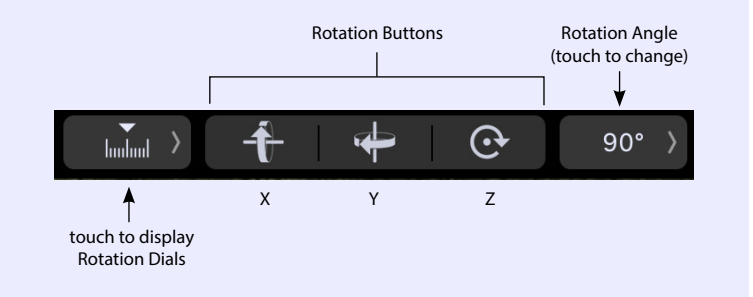
### To change the rotation angle step:

1. Click the rotation angle field in the centre of the popover.
2. Type a new rotation angle—or choose one from the drop-down menu.

## Touch Bar Rotation Popover

If you have a MacBook Pro with Touch Bar you can use the rotation controls provided in the default touch bar:

Rotation Buttons in the default Touch Bar interface.




The sense of rotation is shown by the rotation icons; to switch sense, hold down the shift key on your keyboard and the little rotation icons will update.

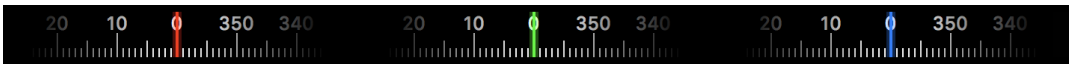
### To change the rotation angle step:

Do one of the following:

- Touch-and-hold the Rotation Angle popover button (it has a ">" symbol indicating that it is a popover control), then slide your finger over to the rotation angle you require, and release.
- Touch the Rotation Angle popover then, when its angle popover appears in the Touch Bar, touch the angle you require.

## Touch Bar Rotation Dials

CrystalMaker for Mac also provides a set of rotation dials in its Touch Bar interface, one for each axis. To display the dials, touch the Rotation Dials button (illustrated above). A set of three dials appears, from left-to-right: X-rotation (red dial), Y-rotation (green dial) and Z-rotation (blue dial):




Rotation Dials in the Touch Bar interface. The dials provide rotation about the screen axes: X (left), Y (middle) and Z (right).

You can turn the dials with your finger, letting you precisely orientate your model.

## Auto-Rotation (Spin)

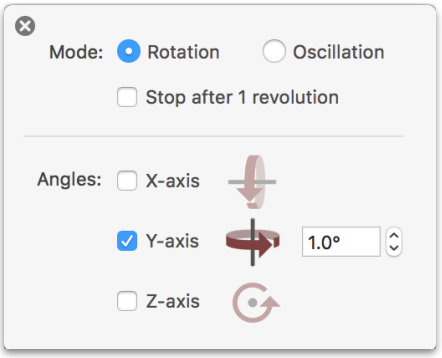
CrystalMaker lets you automatically *rotate* or *oscillate* your structure. Each involves step-wise rotation about one or more screen axes, and you can limit the rotation to one complete revolution, or allow continuous rotation.

### To start auto-rotation:

- Click the **Spin** button in the toolbar (or choose: **Transform > Spin**). The structure starts spinning about the currently-defined rotation axis and through the currently-define rotation step.

### To control auto-rotation:

1. Click-and-hold the **Spin** button in the toolbar. After a short delay, the Spin Popover appears:




The Spin Popover showing default Y-axis auto-rotation.

2. Do one of the following:
   - For same-sense rotation (spinning) choose the **Rotation** radio button.
   - For oscillation, select the **Oscillation** radio button.
3. Specify which axes should be used for rotation (using the **Angles** checkboxes), and enter the rotation steps for each axis.
4. Close the popover by clicking outside its bounds or, if the popover has been detached from the toolbar, simply click the popover's close box.

> **Performance Metrics:** You can use the **Auto Rotate** command to measure system performance: if the **Stop after 1 revolution** option is checked, timings are printed in the Output Log.

### To halt auto-rotation:

Do one of the following:

- Click the **Spin** button in the toolbar (or choose: **Transform > Stop Spinning**).
- Press the **escape** key.

Note that the structure returns to its original orientation when auto-rotation ends.

## Interactive Rotation

You can use the mouse or your trackpad to rotate a structure in real time, with the **Rotate** tool from the Tool Strip.

### To rotate about the screen X axis:

Do one of the following:

- Drag the mouse vertically in the window.
- Slide two fingers up or down the trackpad (Mac).

### To rotate about the screen Y axis:

Do one of the following:

- Drag the mouse horizontally.
- Slide two fingers from left-to-right, across the trackpad (Mac).

### To rotate about the screen Z axis:

Do one of the following:

- Hold the **shift** key, then drag the mouse in a circular direction.
- Use a "rotate" gesture on the trackpad (Mac).

A common mistake is to drag the mouse too quickly so that rotation appears erratic. For best results, drag gently so the structure follows the mouse.

### To rotate only part of the structure:

1. Select the atoms you wish to rotate (e.g., using Arrow, Lasso or Polygon tools).
2. Choose the Rotate Selection tool from the Tool Strip (hint: click the drop-down menu to the right of the Rotate tool and choose: **Rotate Selection**).
3. Click-and-drag to rotate the selection, or use the Rotation popover.

### Rotating whilst another tool is active:

You can still rotate the structure when another tool (e.g., the Arrow tool) is active. Hold down the **space** key, then click and drag with the mouse to rotate your model. When you have finished, release the **space** key and your original tool is active once more.

## Mouse Wheel Structure Rotation

If your mouse has a scroll wheel, trackball or trackpad, you can use this to rotate your structure:

### To rotate about the screen X axis:

- Turn the mouse wheel or trackball up or down.

### To rotate about the screen Y axis:

Do one of the following:

- Hold down the **option/alt** key and turn the mouse wheel
- Rotate the trackball from left to right.

### To rotate about the screen Z axis:

- Hold down the **shift** key on your keyboard and turn the mouse wheel.

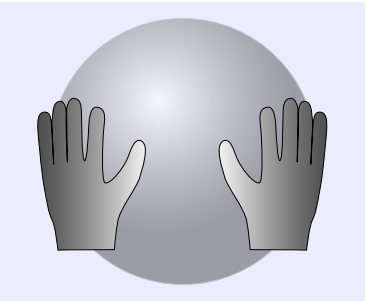
## Leap Motion Control

CrystalMaker supports the Leap Motion Controller (`www.leapmotion.com`) for gesture-controlled rotation and scaling. This is a small USB device that detects hand movements using an optical transmitter and a pair of video cameras. We have programmed CrystalMaker to respond to such movements by generating rotation angles and/or scaling commands.

The Leap Motion controller is a small USB device for Mac or Windows.

You can use one or both hands to rotate your structure. Use natural gestures such as twisting one hand, or making turning motions with both hands. For example, imagine that you are holding a squishy beach ball between your hands; think how you would rotate the ball—then use the same gestures to rotate a structure on the screen; you can also squeeze or stretch the (virtual) ball.

The easiest way to use the Leap Motion controller is to imagine that you are turning, stretching or squeezing a virtual ball between your hands.



### To rotate about a horizontal (X) axis (left-to-right):

Do one of the following:-

- Place one hand above the Leap controller with your palm facing downwards. With your fingers spread out, twist your hand to turn the structure.
- Hold your arms out towards the screen so that your hands are side-by-side above the Leap Motion controller, facing down about 45°. Move your hands in opposite directions, forwards and backwards to turn the structure.

### To rotate about a vertical (Y) axis (top-to-bottom):

Do one of the following:-

- Place one hand above the Leap controller, with your palm facing downwards and your fingers bent towards the controller, and twist in the direction you wish your structure to rotate.
- Hold your arms parallel to the screen, so that your hands are side-by-side above the Leap Motion controller, and inclined at about 45°. Raise one hand and lower the other to turn the structure.

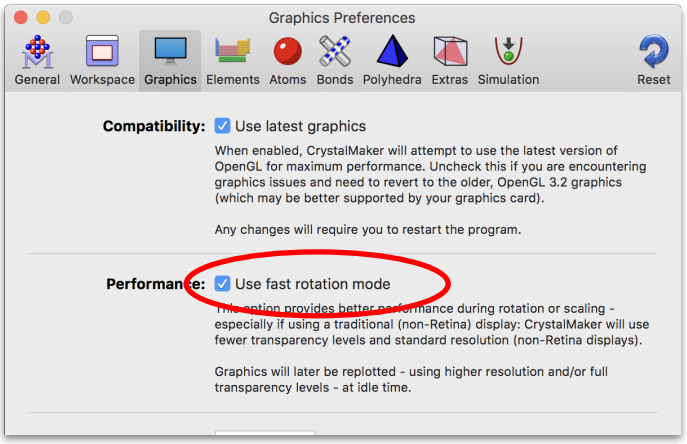
### To rotate about an axis out of the screen (Z):

Do one of the following:-

- Place one hand parallel to the screen, above the Leap Motion controller, with your fingers facing forwards slightly. Twist your hand to turn the structure.
- Position your hands above the Leap Motion controller, one on the left, and one on the right. Move them clockwise or anti-clockwise to turn the structure.

## Fast Rotation Mode

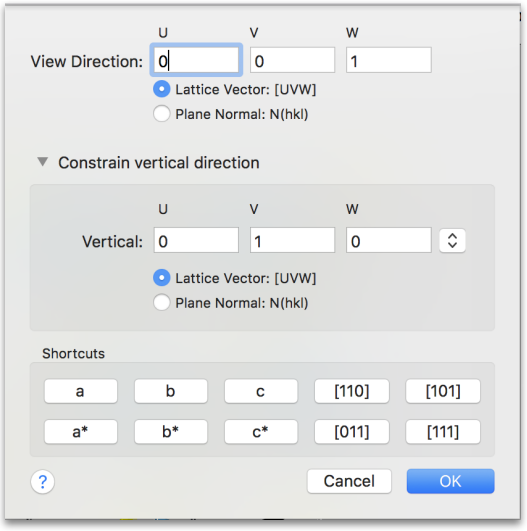
CrystalMaker can use a fast drawing mode which suppresses graphics smoothing (anti-aliasing) until idle time and also uses fewer transparency layers, thereby increasing rotation speed. This is particularly noticeable in full-screen mode. To control this setting, please see the Graphics pane of the Preferences panel:




The Fast Rotation Mode setting in the Preferences Panel.

## Defining a View Direction

You may view a crystal structure along a lattice vector, [UVW], or along the normal to a lattice plane, (hkl), using the View Direction sheet (**Transform > View Direction > Set View Direction**). Specify either a Lattice Vector or Plane Normal, then type the appropriate indices in the three fields shown. The structure will be replotted such that your view direction vector is oriented directly *into* the screen, in other words, one is viewing the structure *along the vector.*




The View Direction sheet, showing a constrained orientation setting. Here, the view direction of [001] is combined with a vertical direction of [010] to uniquely define the crystal's orientation.

### View Direction Presets

A series of buttons at the bottom of the sheet lets you quickly specify view directions, such as the a-axis, or the [111] direction.

### Constrained Orientation

Specifying a view direction along one axis does not uniquely define the crystal's orientation: it could still be rotated about the view direction. To uniquely define the orientation, you can opt to specify a second vector, perpendicular to (or nearly perpendicular to) the view direction, which should be displayed vertically on the screen—that is, parallel to the screen Y axis, which runs from the bottom to the top of the screen.

You can enter this second vector in the View Direction sheet, by clicking on the **Constrain vertical direction** disclosure button, to reveal the **Vertical** direction fields.

## Moving a Structure

CrystalMaker allows you to move all of, or part of, a structure across the screen. You may need to move the entire structure so that you can:

- Scroll to different parts of a structure viewed at high magnification.
- Move objects of interest to the centre of rotation (which is always the centre of the Graphics window).

### To move the entire structure:

Do one of the following:

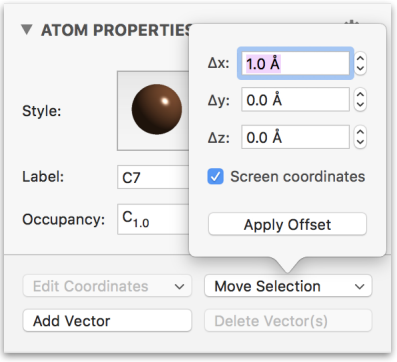
◆ With the Move tool active:

- Click and drag the structure across the screen (hold the **shift** key down to constrain your movements to horizontal or vertical). Mac users with a force-touch trackpad will feel a slight vibration as the structure crosses over the horizontal or vertical centre lines.
- Use the arrow keys on your keyboard to move the structure.

◆ Use the **Transform > Scale & Centre > Move Structures** command to specify a precise distance to move (in Å units).

### To move part of an existing structure:

1. Select the atoms you wish to move.
2. Do one of the following:
   - Click-and-drag the atoms with the Arrow tool.
   - Click the Move Selection button in the Selection Inspector and define an offset relative to screen (orthogonal) or structural coordinates.




Using the Move Selection popover to move a group of selected atoms in a structure.

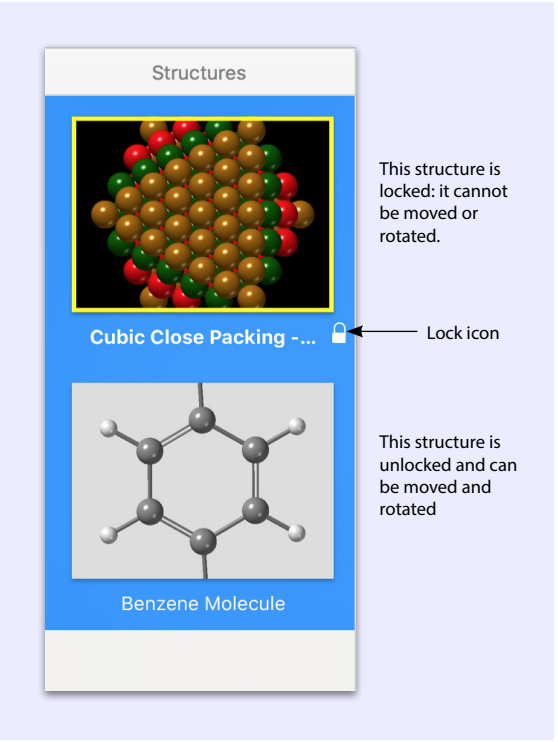
## Moving One Structure Relative to Another

One of the very-powerful features of CrystalMaker X is the ability to display multiple structures simultaneously. This allows you to compare structures, visualize topotactic relationships, place molecules onto crystal surfaces or inside cavities. In each of these scenarios you probably want to be able to reposition one structure, relative to another.

The easiest way of doing this is to *lock* one structure, so it remains fixed in space and orientation, then move (or rotate) another structure.

You can easily lock and unlock structures using the Structures List: move the mouse over a structure's title and a lock icon appears on the right; you can click this to lock or unlock the structure.

The Structures List lets you lock structures so they cannot be moved or rotated.




**Learn More:** Fore more information about using the Structures LIst to work with multiple structures, please see *Chapter 4: Document Window*.

# Scaling the Structure

When you display a new structure it is automatically scaled to fit the Graphics Pane in any orientation. As you resize your window, the structure is also resized.

## Defining a Scale

CrystalMaker lets you scale a structure using a trackpad, mouse or Leap Motion controller. You can also use the **Magnify** tool to reveal details in any clicked region.

### To scale the structure:

Do one of the following:

- Use a pinch or zoom gesture with a multi-touch trackpad (Mac) or screen (Win).
- Hold down the **command** key (Mac) or **control** key (Windows), then click-and-drag the mouse up or down the screen.
- With two hands positioned above the Leap Motion controller, move them closer together or further apart.
- Press and hold the **Zoom Out** or **Zoom In** buttons on the toolbar (if these buttons are not visible, you can customize the toolbar and add them). For faster scaling, hold down the **shift** key as you click a zoom button.
- If you have a MacBook Pro with Touch Bar, you can quickly zoom by touching-and-holding a zoom button in the Touch Bar.

### To magnify a specific area of interest:

1. Choose the **Magnify** tool from the Tool Strip.
2. Click an area of interest. The structure is replotted with doubled scale, and with your clicked point at the centre of the screen. (To zoom out, hold down the **shift** or **option/alt** keys on your keyboard as you click with the **Magnify** tool).

### To set an explicit scale:

1. Choose: **Transform** > **Scale & Centre** > **Set Scale**. The Scale dialog appears.
2. Enter a scale in pixels-per-Ångstrøm.
3. Click the **OK** button to replot your structure with the new scale.

## Automatic Scaling & Centring

Clicking the **Auto-Scale** button in the toolbar will rescale the current plot so that its maximum dimension fits snugly within the graphics window. The **Auto-Centre** button moves the *centroid* of the structure to the centre of the screen, but does not change the current scale, or scale mode. If you prefer to centre the structure's outer bounds (rather than its centroid), choose: **Transform** > **Scale & Centre** > **Centre on Bounding Box**.

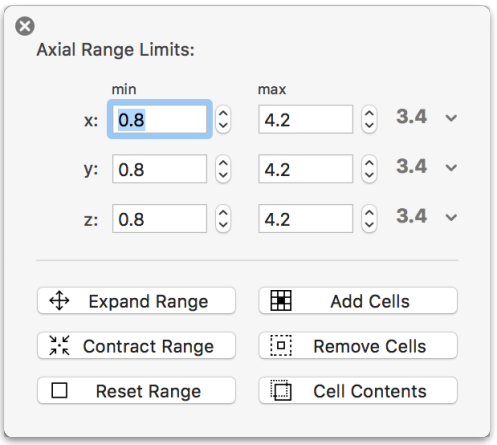
## Specifying a Plot Range

There are several ways of changing the number of atoms plotted. Atoms can be hidden according to their site or chemical element symbol (e.g., using the Site Browser); a precise plot range can be specified; you can use selection tools to prune extraneous atoms; or you can opt to "grow" atoms and bonds to repair a selected coordination environment or molecule.

### The Range Popover

The Plot Range popover lets you define a plot range for crystal structures in terms of minimum and maximum distances along the crystallographic *x*, *y* and *z* axes. Plot limits should be entered as fractions of the unit cell repeats, thus a range specified as from $x_{min}$ = 0.1 to $x_{max}$ = 1.1 would result in all atoms lying between 0.1**a** and 1.1**a** being plotted.

The Range Popover.




#### To set a plot range:

1. Click the **Range** button in the toolbar (or choose: **Transform > Atom Range > Set Range**). The Range popover appears.
2. Enter your range limits for the *xyz* axes (press the tab key to move between fields) or use the **Expand Range** or **Contract Range** buttons to change the range by 10% along each axis.

#### To show just the contents of one unit cell:

- Click the **Cell Contents** button. The range limits are reset to $0 \leq xyz \leq 0.99999$.

#### To add another unit cell along one axis:

1. Locate the axial range fields for the axis (*x*, *y* or *z*) you wish to change.
2. Click on the number displayed to the right of the "max" field (this shows the

number of cells for that axis). A popup menu appears.

3 Choose: **Add cell along x/y/z**. The plot range is updated.

4 Click **Apply** to replot your structure.

> **Beware Vanishing Polyhedra:** Changing the range may cause some polyhedra to disappear. Polyhedra can only be plotted if all of the coordinating atoms (vertices) lie in range.

## Refining the Plot Range

CrystalMaker allows you to hide selected atoms, polyhedra, or groups of atoms. To select one or more atoms, use the selection tools:

- The Arrow tool allows a rectangular selection in the structure by clicking and dragging across your chosen atoms. Alternatively, shift-click on atoms or polyhedra to add or remove them from the selection.

  *Clicking on a polyhedron selects all atoms in the polyhedron, unless the polyhedron is translucent, in which case you can select any visible atoms or, if you click on a blank part of the polyhedron, all atoms are selected.*

- The Polygon tool lets you define an angular selection region. You must close this shape by clicking on the starting point, in order to complete your selection.
- The Lasso tool allows you to define a freehand selection region. With this tool, click and drag a closed loop around the atoms you wish to select.

### To quickly hide individual atoms or polyhedra:

1 Choose the Zapper tool from the Tool Strip.

2 Click on the atom or polyhedron you wish to hide. As you release the mouse button, the atom vanishes in a puff of smoke.

### To hide a group of atoms:

1 Select the atoms you wish to hide. (Shift-click with the Arrow tool, or outline a selection region using the Arrow, Polygon or Lasso tools).

2 Right-click in the Graphics Pane and choose: **Hide Selection** (or choose: **Transform > Selection > Hide**).

### To hide all atoms with missing bonds:

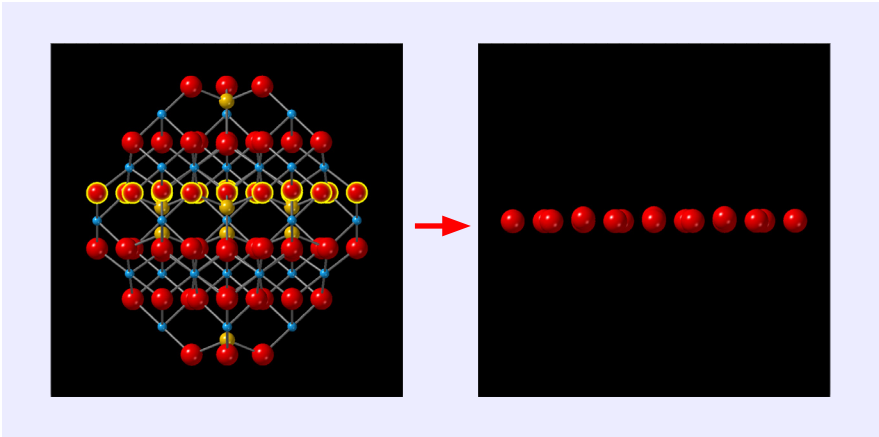
◆ Choose: **Transform > Atom Range > Hide Stranded Atoms**. All atoms which do not show their full complement of bonds (e.g., because one or more of their coordinating atoms is out of range) are hidden.

### To hide all atoms with fewer than 2 bonds:

- Choose: **Transform** > **Atom Range** > **Hide Minimally-Bonded Atoms**.

### To isolate a group of atoms:

1. Select the atoms you wish to isolate.
2. Right-click in the Graphics Pane and choose: **Isolate Selection** (or choose: **Transform** > **Selection** > **Isolate**).



Using the Isolate Selection command to reveal a single layer of oxygen atoms (red) in the Spinel structure.

### Trim Plot Range to Selection

Using the selection tools to isolate regions of interest is very powerful, but CrystalMaker still retains the hidden atoms in memory and this can make operations slower than they need to be—and increase the size of your document when you come to save it. To avoid these problems, you can reduce the plot range to match the range of visible atoms. To do this, simply choose: **Transform** > **Atom Range** > **Trim to Selection**.

### To reveal hidden atoms:

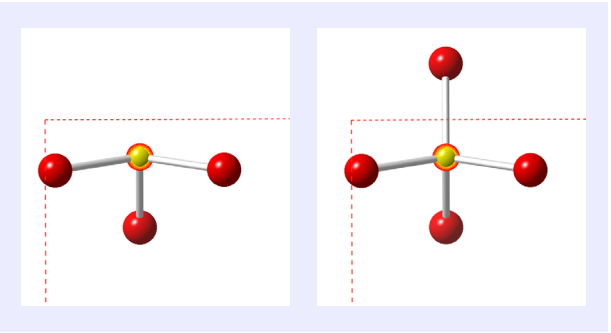
- Right-click in the Graphics Pane and choose: **Show All Atoms In Range** (or choose: **Transform** > **Atom Range** > **Show All Atoms in Range**).

## "Growing" Atoms and Bonds

Atoms with incomplete bonding can have their coordination repaired, making nearest-neighbour atoms and their bonds visible. Similarly, "broken" molecules can be repaired. In both cases, missing atoms and bonds are caused by plot range truncation. CrystalMaker can intelligently expand the plot range in the appropriate directions, to "grow" the selection, whilst keeping the rest of the structure the same.

### To repair nearest-neighbour bonding around an atom:

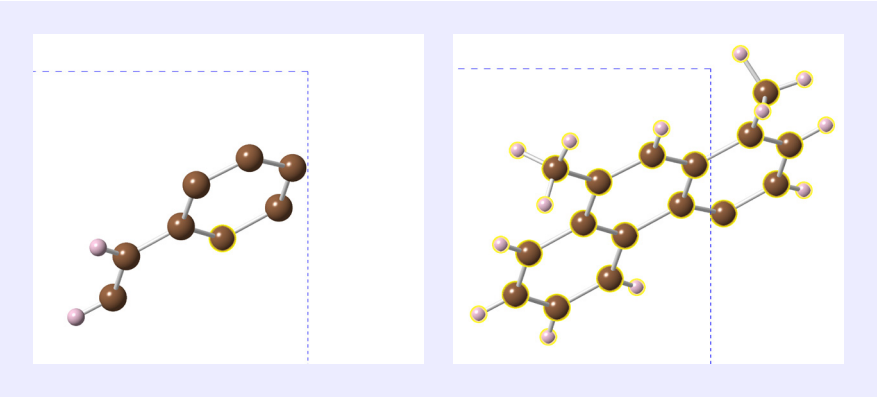
1. Select the atom (e.g., by clicking on it with the Arrow tool).
2. Right-click in the Graphics Pane and choose: **Repair > Bonding Around Selection**. Any hidden neighbours will be shown, and their bonds drawn to the selected atom.



The Repair > Bonding Around Selection command in action: repairing a partial sulphate group (left) to reveal the full coordination (right).

### To repair a "broken" molecule:

1. Select one atom in the molecule.
2. Right-click in the Graphics Pane and choose: **Repair > Selected Molecules**. Any hidden atoms will be made visible and bonded to the rest of the molecule. (Note that this command is not suitable for a fully-interconnected framework structure.)



The Repair > Selected Molecules command in action: repairing a fragment of a molecule (left) to reveal the full molecule (right).

## Working with Molecular Crystals

If you are dealing with a *molecular* crystal, you probably want to display only intact molecules. However, using the **Set Range** command typically results in molecules at the edge of the plot range being broken into fragments—and tidying up the plot using selection tools can get tedious.

**What is a Molecular Crystal?** We define a "molecular crystal" as one whose unit cell comprises one or more *discrete* molecules, i.e., molecules which are *separate*, and not connected via *primary* bonds. This definition excludes framework structures (where all atoms are interconnected throughout space) as well as chain- and sheet-structures. Polymer crystals are also excluded, since they comprise infinite chains.

CrystalMaker's **Transform > Atom Range** submenu provides automated commands for tidying up the display of molecular crystals. A related series of commands can be found by clicking the **Tidy** button in the toolbar.

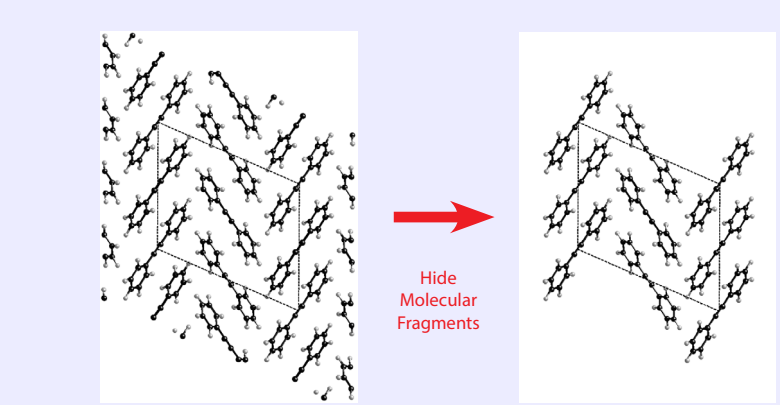
**Check Your Bonding:** Please ensure that your bonding is adequate *before* attempting to use the molecular crystal commands. In particular, you may wish to review your default element table (see the Elements pane in the Preferences panel) before you start to import text files.

### Hide Stranded Atoms

Stranded atoms are atoms which should be bonded, but which appear isolated because their neighbours are hidden or out of range.

### Hide Molecular Fragments

This command hides all molecules that have missing atoms in the current screen view (the missing atoms are generally outside the plot limits).




Using the Hide Molecular Fragments command to reveal intact molecules: before (left) and after (right)

## Repair Molecular Fragments

This command examines the currently-displayed atoms on screen, identifies any incomplete molecules ("fragments"), and then if required, generates additional atoms and bonds so that all of the original atoms are now part of fully-intact molecules.

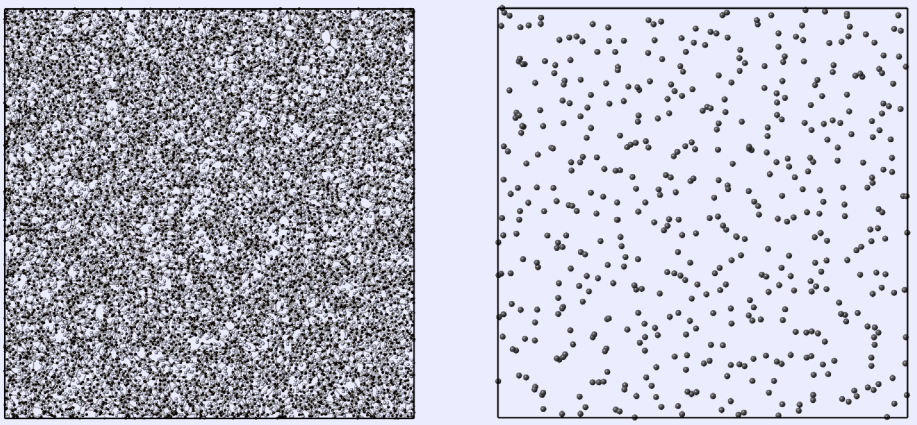
## Add Molecular Centroids

If you are working with a complex structure containing hundreds or thousands of different molecules in the unit cell, you can simplify it replacing each molecule by a single dummy atom: the *molecular centroid*.

CrystalMaker's **Transform > Add Molecular Centroids** command will first verify that the structure is indeed a molecular crystal (and not, say, an infinite framework), and will then prompt for an element symbol to be used for the centroid atoms. Your structure's atoms are then hidden, with only the centroid atoms visible.

**Dummy Sites:** We recommend that you use a distinctive element symbol for the centroid sites—something crazy like "Zz" makes it easy to locate these sites in the Atoms Inspector and further distinguishes them from the true sites in your crystal.

To revert to the original structure, simply navigate to the Atoms Inspector and use its **Vis** checkboxes to hide your centroid sites (which will all be listed under your chosen dummy element symbol), and make your original sites visible.



Simplifying a complex molecular crystal (left) by showing just its molecular centroids (right).

## Show Asymmetric Unit

This command will display the original asymmetric unit (as loaded from a raw text file). Depending on how the asymmetric unit was defined, this may—or may not—correspond to one or more intact molecules.

*Please note that if fractional coordinates in the asymmetric unit have been changed (e.g., earlier versions of CrystalMaker automatically wrapped sites into the same unit cell), the results may be unpredictable, and some molecules may appear broken.*

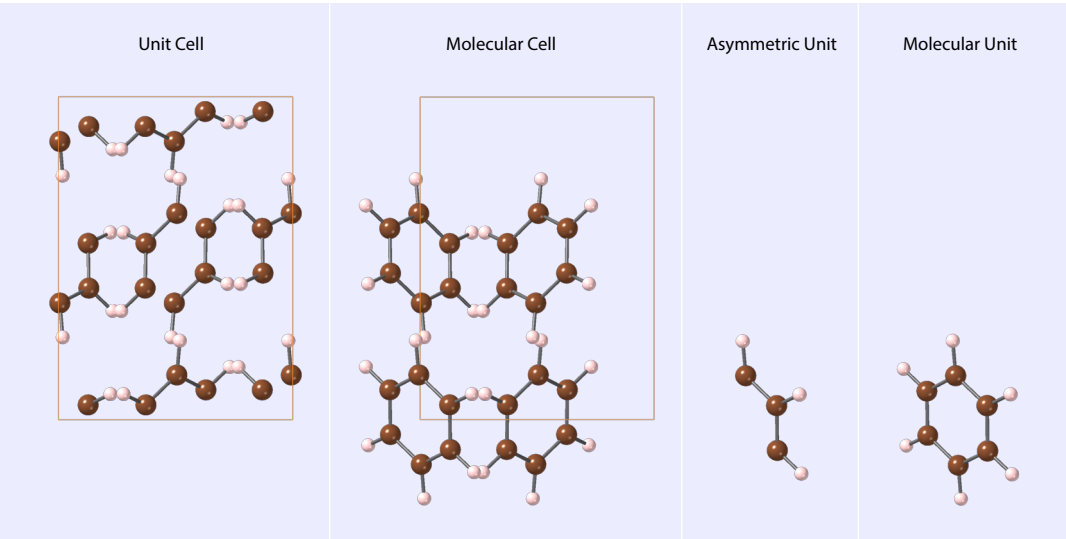
## Show Molecular Unit

A safer alternative to showing the asymmetric unit is to use **Show Molecular Unit** command. This identifies *fully-intact* molecules which contain at least one atom in the asymmetric unit. (This is equivalent to displaying the asymmetric unit and then repairing any fragmented molecules.) The end result may show more atoms than are present in the asymmetric unit—but the molecule(s) shown will be intact!

## Show Molecular Cell

This command generates the optimum view of a molecular crystal's complete cell contents. The program searches for intact molecules associated with a single unit cell, including those which lie partly outside the cell bounds. The full unit cell contents are then displayed, without any fragmented molecules.

This command does not depend on any existing range limits or unit cell settings. A single unit cell frame will be displayed, together with its optimum content.




Different views of a molecular crystal (benzene). Only the "molecular cell" and "molecular unit" show intact molecules.

## Isolating Single Molecules

You can easily select an individual molecule and isolate this from the rest of the structure.

> **Tip:** You may find it easier to use the **Show Molecular Unit** or **Show Molecular Cell** commands before you choose a single molecule to isolate.

### To isolate a single molecule:

1. Choose the Arrow tool from the Tool Strip.
2. Click on one atom in the molecule you wish to isolate.
3. Right-click in the Graphics Pane and choose: **Isolate Selected Molecules** (or choose: **Transform > Selection > Isolate Molecules**). All molecules which do not contain selected atoms will be hidden.

### To select an entire molecule:

1. Select one or more atoms in the molecule you wish to select (e.g., using the Arrow tool).
2. Right-click in the Graphics Pane and choose: **Extend Selection > Molecule** (or choose: **Edit > Select > Molecule**). All atoms in the molecule will be marked as selected.

This procedure is useful if you wish to move or rotate a molecule relative to the rest of the structure.

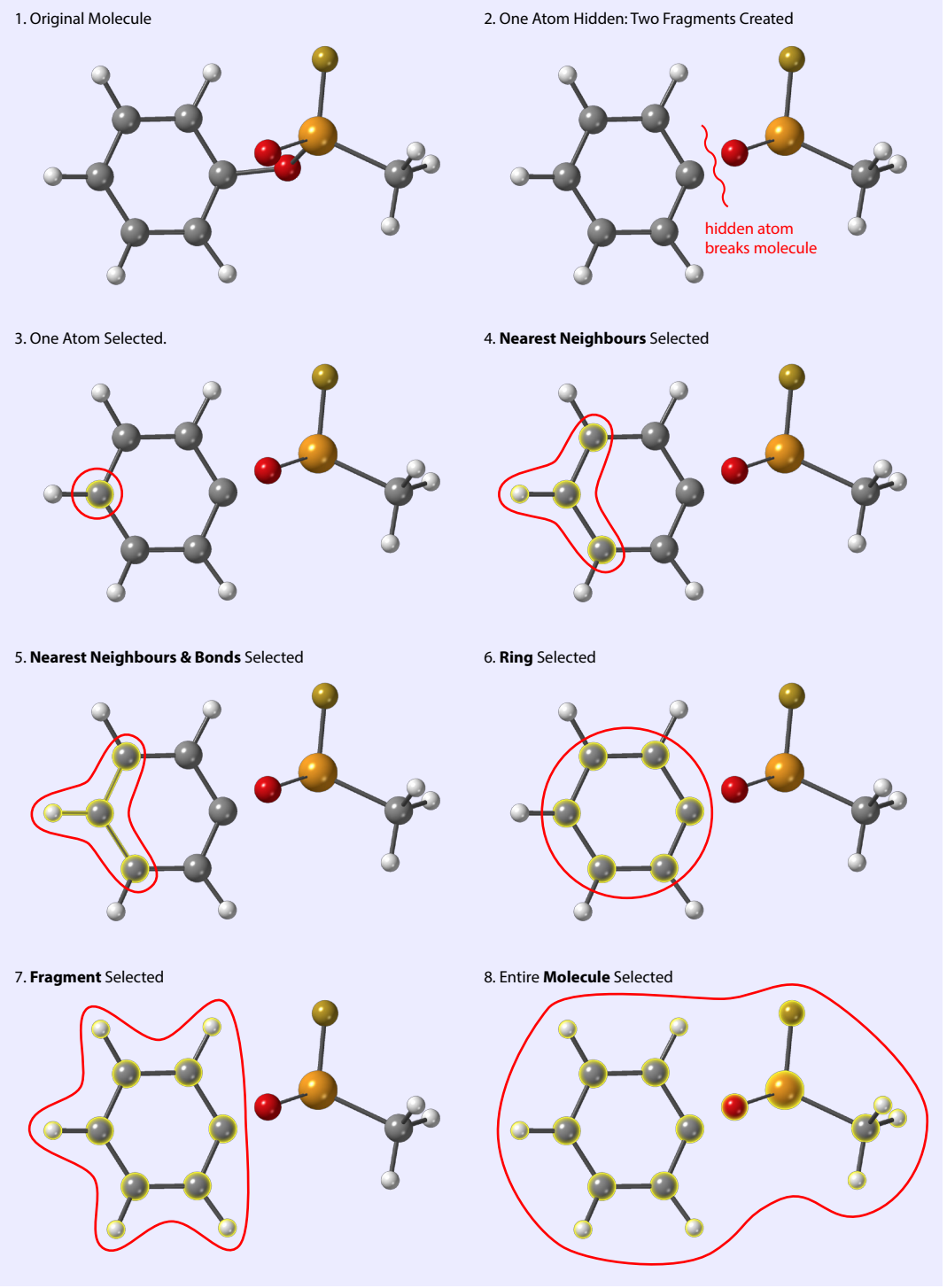
> **Molecular Crystals Only:** These commands are only appropriate for structures which contain discrete molecular units. The commands are not appropriate for structures with long-range bonding such as most inorganic structures including framework silicates.

## Ring and Fragment Selection

Other commands available from the Graphics Pane's contextual menu let you extend a selection to include:

- Nearest neighbours (with the option of including bonds)
- Ring
- Fragment
- Molecule

By "fragment" we mean a distinct part of the structure that is internally bonded, without any breaks; this is subtly different from a "molecule", which might contain hidden atoms and/or bonds. These options are illustrated on the next page.




Options for extending a selection

## Crystal Surfaces

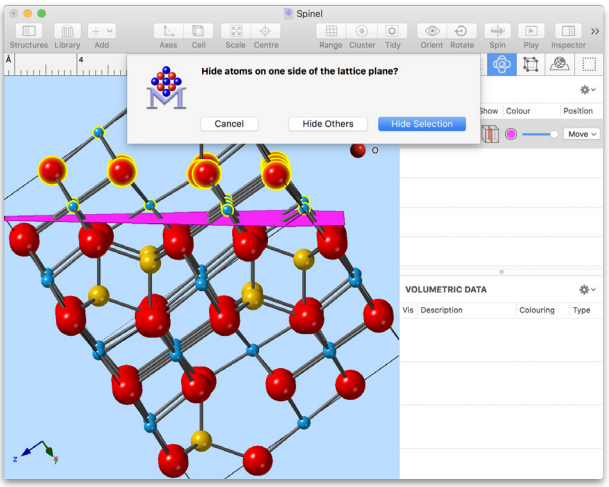
You have the option of hiding atoms on either side of a displayed lattice plane, which then lets you visualize the arrangement of atoms in a surface.

It is important to emphasize that the surface corresponds to an unrelaxed lattice (i.e., bulk material). This may differ from a real surface, where atoms tend to move slightly, in order to increase their coordination and lower the surface energy. In order to visualize such changes, one would require a sophisticated energy-minimization program, which is currently beyond the scope of CrystalMaker

### To create a surface:

1. Use the **Set Range** command to generate a sufficiently-large block of atoms.
2. Add the plane you are interested in to the **Lattice Planes** group in the Volume Inspector.
3. Click the corresponding row's **Move** button to display a popover, then use the slider control to move the lattice plane to the position in the structure where you want to create a surface.
4. Choose: **Transform > Slice Crystal**. All atoms above the lattice plane are shown highlighted, and a dialog lets you choose between hiding these atoms, hiding the other (unselected) atoms, or cancelling.

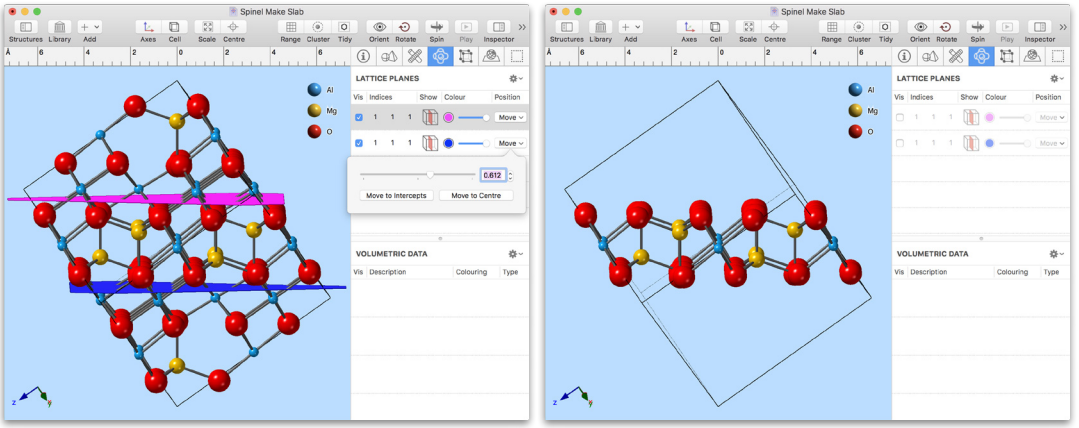
Using the Slice Structure command. The atoms above the plane have been selected,




4. Choose which side of the plane you wish to hide, and click the appropriate button in the dialog. The structure is replotted with the appropriate atoms hidden and the lattice plane hidden.

### To create an oriented slab:

1. Add the plane of interest to the **Lattice Planes** group.
2. With your plane's row selected, click the Actions button and choose: **Add Copy** from its drop-down menu.
3. Choose a distinctive colour for the second plane.
4. Using each plane's **Move** button to display a position popover, adjust the positions of the two planes so they define either side of the slab you require.
5. Choose: **Transform > Make Slab**. All atoms above and below the planes are now hidden, revealing an oriented slab of atoms.




Creating a crystal slab. Left: positionning two parallel lattice planes to define the intended top and bottom edges of the slab. Right: after choosing the Make Slab command.

## Controlling Atom Visibility

CrystalMaker allows you to hide atoms by site, by element symbol—or by molecule (if your Atoms Inspector has been configured to group atoms by molecule). This can be a useful way of "seeing the wood for the trees", or simply identifying a group of sites by flashing them on or off.

**Missing Polyhedra?** "Solid" polyhedra cannot be plotted if any of the constituent atoms are hidden (or lie outside the current plot range).

### To hide all atoms of the same site:

1. Display the Atoms Inspector.
2. Locate the site row and do one of the following:
   - Uncheck the "**Vis**" checkbox, *or*
   - Right-click on the row and choose: **Toggle Visibility** from the contextual menu that appears.

   The structure is replotted with all atoms on this site hidden.

### To hide all atoms of the same element:

1. Display the Atoms Inspector.
2. Locate the corresponding *element row* (which will have a disclosure triangle in front of it) and do one of the following:
   - Uncheck the "**Vis**" checkbox, *or*
   - Right-click on the row and choose: **Toggle Visibility** from the contextual menu that appears.

   The structure is replotted with all atoms with this element type hidden.

### To hide individual atoms:

1. Select the atoms to hide, e.g., using the Arrow, Lasso or Polygon tools.
2. Do one of the following:
   - Right-click in the Graphics Pane and choose: **Hide Selection**.
   - Choose: **Transform** > **Atom Range** > **Hide Selection**.

**Zap 'em:** You can quickly hide individual atoms by clicking on them with the Zapper tool.

## Symmetry-Related Atoms & Bonds

You can select all atoms or bonds that are related by symmetry in your crystal, using commands on the **Extend Selection** menu:

### To select atoms related by symmetry to the current selection:

- Right-click in the Graphics Pane and choose: **Extend Selection > Symmetry-Related Atoms** (or choose: **Edit > Select > Symmetry-Related Atoms**).

### To select bonds related by symmetry to the current selection:

- Right-click in the Graphics Pane and choose: **Extend Selection > Symmetry-Related Bonds** (or choose: **Edit > Select > Symmetry-Related Bonds**).

## Controlling Molecular Visibility

Whilst you can easily select individual molecules and hide them, you can also toggle their visilbities on or off using the Atoms Inspector, if its "Group by Molecule" option is set (**Actions > Group List > By Molecule**). Atoms are then divided amongst the different molecule types and you can use the corresponding *molecule row* (with a disclosure triangle) to hide all molecules of a particular type.

Chapter 11

# Transformation

This chapter outlines the ways in which you can transform a crystal structure, by applying one of various kinds of unit cell transformations: changing the shape or size of a unit cell, moving its origin, or defining a new, "surface cell", projected onto a lattice plane.

We also describe "crystal engineering" tools, which allow you to insert new atoms into a crystal or molecular structure, place molecules inside crystals, insert space in the lattice, duplicate, detach or delete atoms and change atom types.

## Discarding Symmetry

When working with crystal lattices, you need to take into account symmetry operations. A simple operation, such as moving an atom, might have unintended consequences, as additional atoms are generated by the symmetry elements inside the unit cell. To prevent this from happening, you can use the **Transform > Discard Symmetry** command. This will convert your structure to *P* 1 symmetry, adding new sites as required to preserve the contents of the unit cell.

For many of the operations described in the following chapter, CrystalMaker will automatically discard symmetry, leaving you free to transform your lattice or move atoms freely within the unit cell.

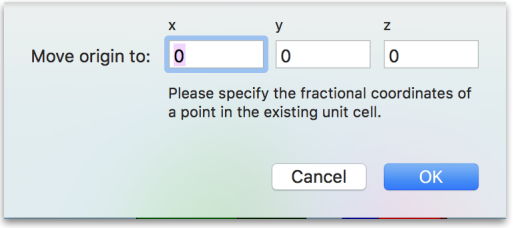
## Unit Cell Transformations

CrystalMaker lets you take an existing unit cell and transform it into a different-shaped (and possibly different-sized) cell, defined by a new set of unit cell ("basis") vectors.

You might, perhaps, wish to change the lattice type, from a centred, to a primitive lattice. If you regularly work with crystal surfaces, you might find it more convenient to work with a unit cell which has two of its three edges lying parallel to a plane of interest. To illustrate twin domains, you may need to generate a mirror image of your structure. Finally, there is the option to transform the unit cell into a larger, "supercell": an integral multiple of the existing cell dimensions.

## Move Origin

Sometimes you may wish to move the unit cell, relative to the structure. Perhaps you want to have a particular atom at the origin, or you need to have the origin at a symmetry point. You can opt to move the origin to your chosen position, using the **Move Origin** command.



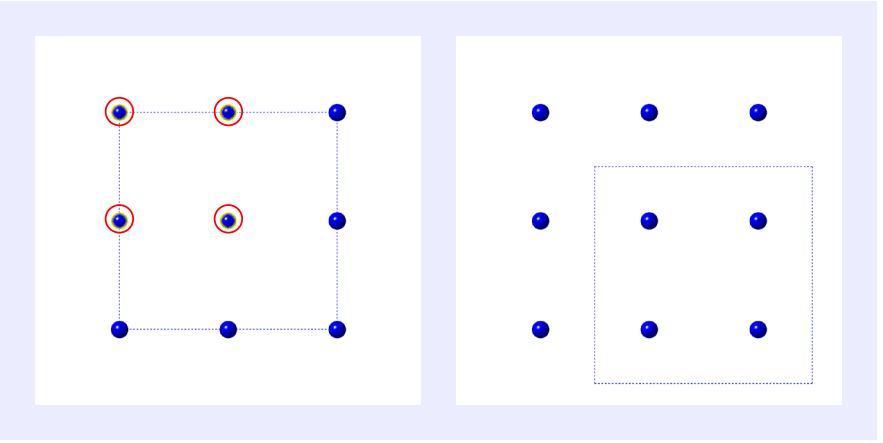

The Move Origin sheet.

### To move the origin to a specific point:

1. Choose: **Transform** > **Unit Cell** > **Move Origin**. The Move Origin window appears.
2. Enter the *fractional* coordinates of the point which should become the origin.
3. Click the **OK** button to replot.

### To move the origin to a specific atom or centre of selection:

1. Select the atom (e.g., by clicking on it with the Arrow tool), or a group of atoms if you require the *centroid* of selection.
2. Choose: **Transform** > **Unit Cell** > **Move Origin**. The Move Origin window appears, with the fractional coordinates of the selected atom (or the centroid, if more than one atom is selected) shown in the editing fields.
3. Click **OK** to replot the structure.

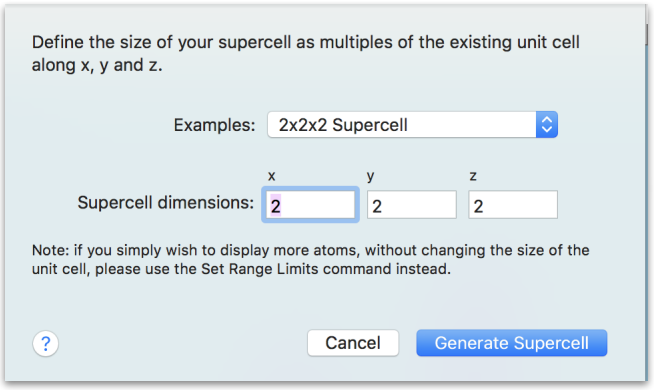


The Move Origin command in action. Four atoms are selected (red rings, on left) After using the Move Origin command (right) the origin has been shifted to the former centre of selection.

## Generate Supercell

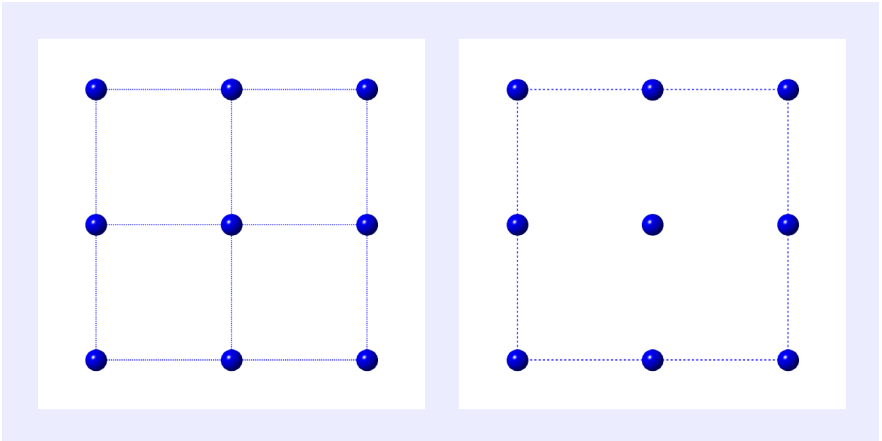
If you have an existing crystal structure and you wish to use a *larger* unit cell, you can specify the relative size of the new unit cell, with respect to the old cell. This can be useful when investigating order/disorder relations and/or creating a structure as a prelude to simulating "superlattice" reflexions in diffraction simulations.

The Supercell sheet.




**Set Range:** If you only want to display more atoms, use the **Transform > Set Range** command instead. That will let you display as many unit cells (or fractions of a unit cell) as you wish—without changing the size of the unit cell. Only use the Supercell option if you really want to create a larger unit cell.

A 2 x 2 block of unit cells transformed into a Supercell (right). The atoms are unchanged, but the new unit cell is larger.



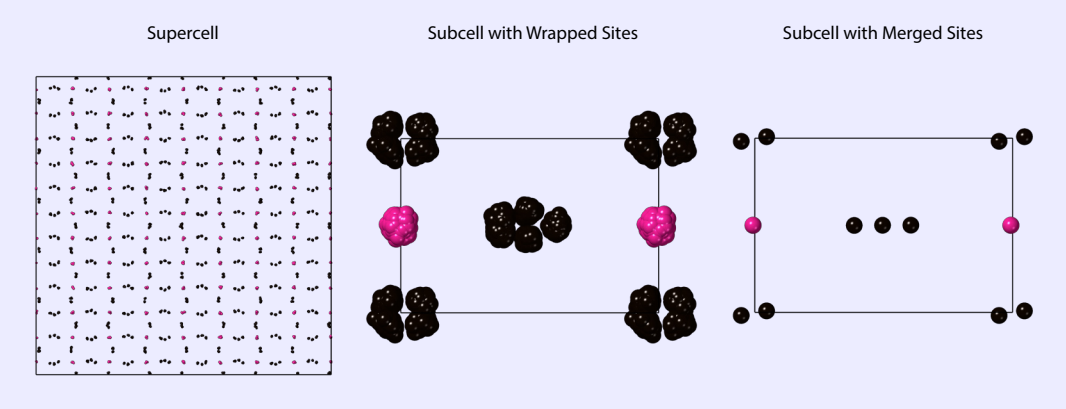
**Log Output:** When transforming a unit cell, CrystalMaker will print the transformation and reverse transformation matrices in the current document's Output Log.

## Collapse Supercell

If you have a supercell, you can opt to "collapse" it, by specifying the number of subcells that will result. For example, if you had a 2 x 2 x 2 supercell, you can collapse it back down to the original subcell (which has one eighth the volume of the supercell).

In collapsing the supercell, CrystalMaker "wraps" all sites back into the subcell. This is useful for quickly visualizing the output of a modelling calculation, allowing you to see the variation in atomic positions.

This command also gives you the option of merging all sites (with the same principal element symbol!) which lie within a specified maximum distance—as found within the subcell. This is useful for reconstructing an average structure.




A supercell (left) can be collapsed into its subcell showing a range of "wrapped" atomic positions (centre) or an averaged structure, merging sites within a specific distance (right).

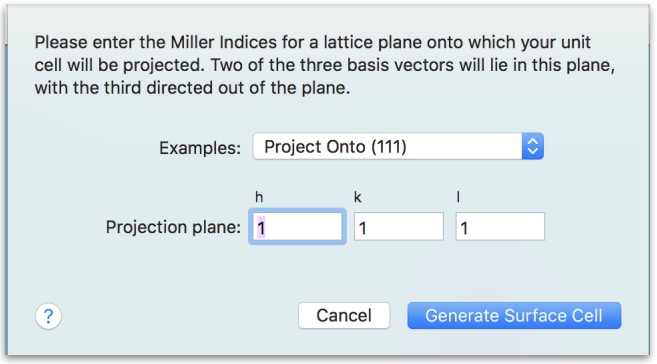
## Projection onto a Lattice Plane

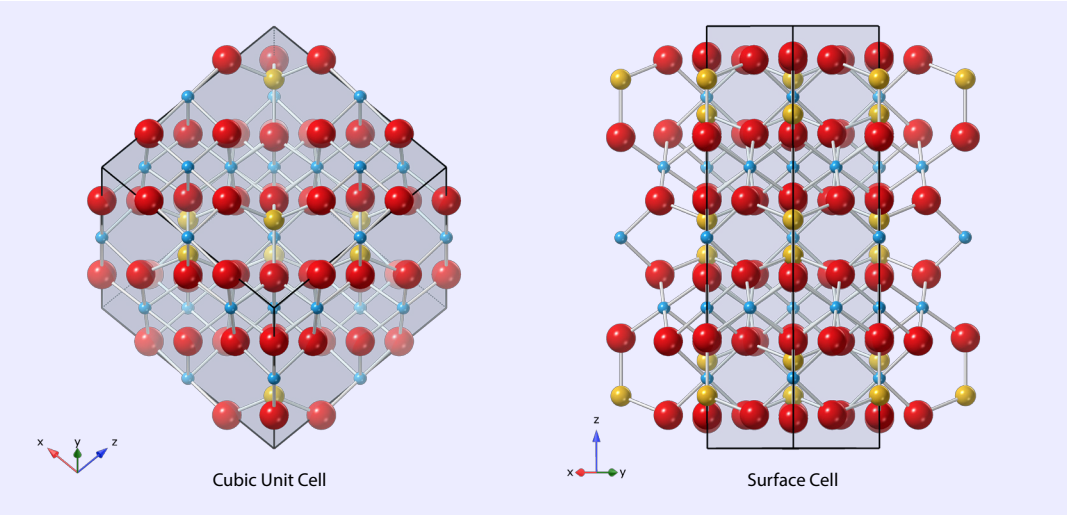
An alternative transformation is to define a new unit cell where two of the three basis vectors lie within a specified lattice plane. We call this a "lattice plane projection". This is useful in surface studies, as it makes it easy to display precise ranges of atoms parallel to a given surface.

To create a Lattice Plane Projection, one must specify the Miller Indices of the plane, and CrystalMaker will define a new unit cell, with the *x*- and *y*- axes lying in the plane, and the *z*-axis directed out of the plane. Where possible, the new unit cell is a *Primitive* cell.

Please note that because a *primitive* unit cell is being defined, there is no guarantee that the new *z*-axis is *perpendicular* to the lattice plane, although (unlike earlier versions of the program) CrystalMaker will try to find a lattice vector parallel to the plane normal as its *z*-axis.

The Project Onto Lattice Plane sheet.




Creating a surface cell for spinel. Left: the cubic unit cell (left) has been tilted to make a set of {111} planes horizontal. Right: a surface cell, with its *x*- and *y*-axes parallel to the (former) (111) planes.

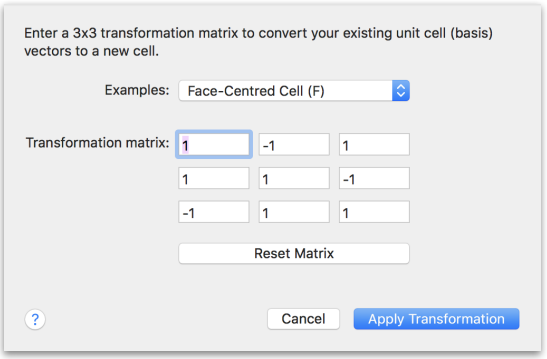
## General Transformation

You can enter a transformation matrix, ($m_{ij}$), that relates the new unit cell (basis) vectors, to those of the existing cell. Thus,

$$\begin{pmatrix} a' \\ b' \\ c' \end{pmatrix} = \begin{pmatrix} m_{11} & m_{12} & m_{13} \\ m_{21} & m_{22} & m_{23} \\ m_{31} & m_{32} & m_{33} \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix}$$

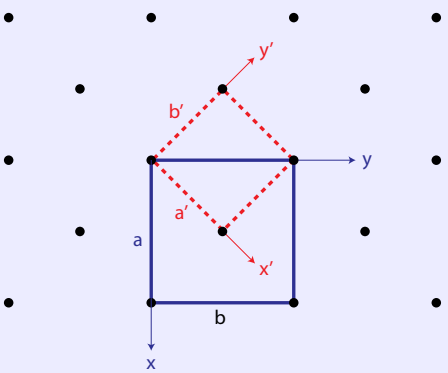
Where $\{a, b, c\}$ are the unit cell vectors of your existing cell (i.e., the existing basis vectors), and $\{a', b', c'\}$ are the unit cell vectors for the new unit cell (i.e., your new basis vectors).

The General Transformation sheet.




### Transformation Example: C to P Lattice

Consider a C-face centred cell, with unit cell vectors $\{a, b, c\}$. Lattice points are found at the corners of the unit cell, and at {½, ½, 0}. This unit cell is drawn in blue in the diagram below. We'll transform this C cell to a Primitive cell, as shown by the dashed red lines below:-




If the new axial vectors for our Primitive cell are $\{a', b', c'\}$, then we can summarize the orientation relationship in vector terms:

$\mathbf{a}' = \frac{1}{2}\,\mathbf{a} + \frac{1}{2}\,\mathbf{b}$

$\mathbf{b}' = -\frac{1}{2}\,\mathbf{a} + \frac{1}{2}\,\mathbf{b}$

$\mathbf{c}' = \mathbf{c}$

In matrix terms, this becomes:

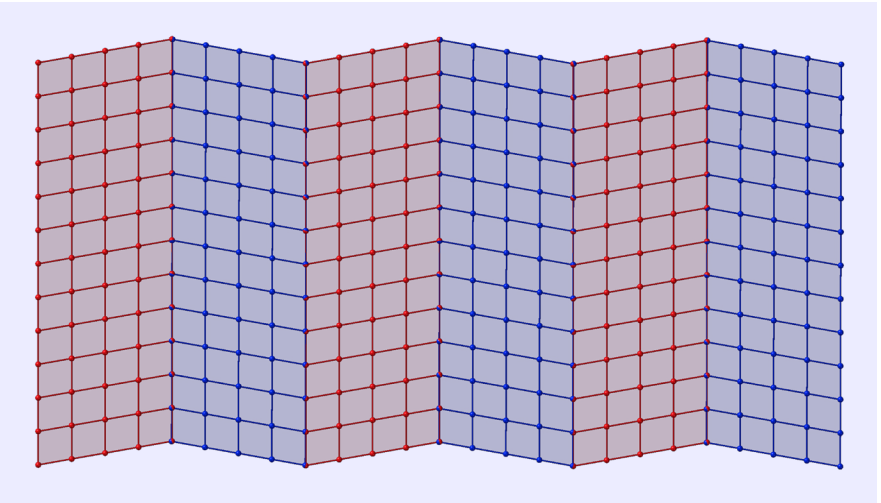
$$\begin{pmatrix} a' \\ b' \\ c' \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ -\frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix}$$

The coefficients of the 3x3 matrix should be entered into the "transformation matrix" fields of the Transform Cell sheet.

## Mirror Image

The **Transform > Unit Cell > Mirror Image** command lets you generate a reflection of the lattice. If you have duplicated your structure, you can build up a model of a twinned crystal, using one or more mirror images.

CrystalMaker will reflect the lattice in the (100) plane, but despite the reflection, the unit cell axes will remain right-handed, by changing the β angle (e.g., β changes from obtuse to acute).



Polysynthetic (repeated lamella) twinning.

This illustration was generated by creating copies of a simple lattice, then reflecting half the copies and moving them horizontally.

## Crystal Engineering

Whilst you can change the lattice type and basis vectors, the underlying structure is unchanged. If you wish to interactively edit your structure, CrystalMaker provides convenient "crystal engineering" tools: letting you detach, move, rotate, duplicate or delete groups of atoms; insert space in the crystal; and place an existing molecule into the lattice.

### Moving an Atom

You can drag atoms or edit their coordinates via a dialog.

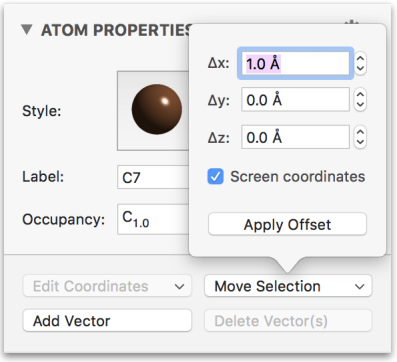
#### To change an atom's position with the mouse:

- Click-and-drag the atom with the Arrow tool.

#### To edit an atom's coordinates directly:

1. Select the atom(s) you wish to edit.
2. Ensure the Selection Inspector is visible, then click the Move Selection button in the Atom Properties group:

The Move Selection popover.



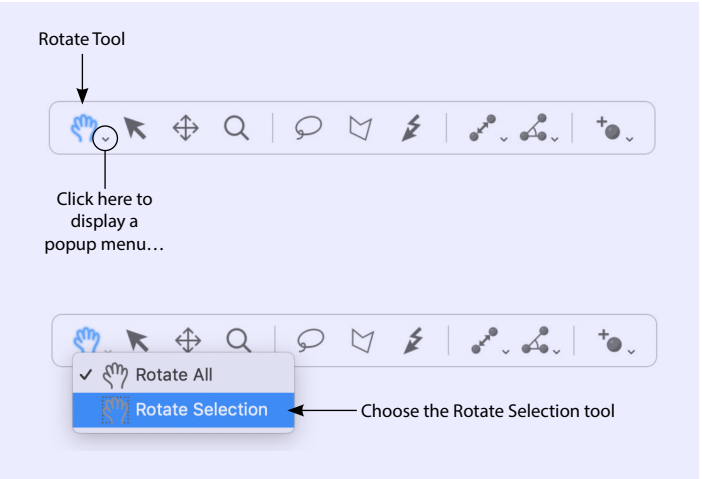

3. Use the Screen Coordinates checkbox to specify whether your offset is relative to the screen, or is in structure coordinates (i.e., fractional coordinates for crystals).
4. Enter your new values in the xyz text fields, then click **Apply Offset** to continue.

> **Discarding Symmetry:** Please bear in mind that directly editing atomic positions in crystal will result in the crystal symmetry being discarded (reset to *P* 1).

## Rotating an Atom

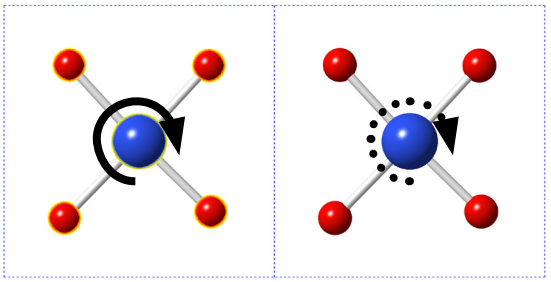
To rotate a selection, you must use the Rotate Selection tool, which is available from the Rotate tool's popup menu in the Tool Strip.

Locating the Rotate Selection tool from the Rotate tool's popup menu in the tool strip.




With the Rotate Selection tool active, you can click-and-drag with the mouse to rotate any selected atoms relative to the rest of the strutcure. Alternatively, you can use the Rotation popover in the toolbar. (*Note that, for lattice-tiling reasons, some rotations may not be possible if your selection extends beyond one unit cell.)*

Rotating a selection in one unit cell causes the corresponding atoms in other unit cells to rotate.

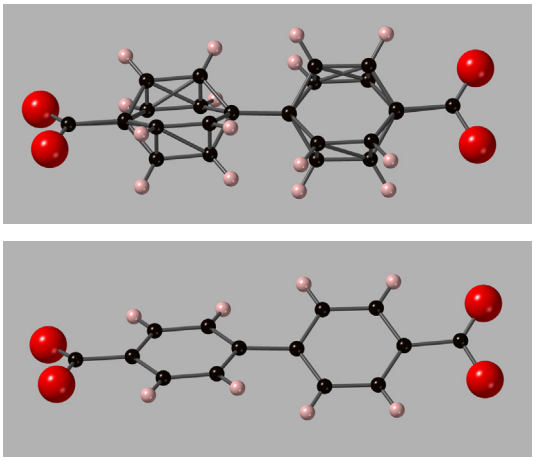


## Merging Atoms

If you are working with a disordered structure, you may find that a given site is split into two or more sites of fractional occupancy. If you wish to show the ideal structure, you will need to combine these separate sites into a single, merged site.

### To merge atoms:

1. Select the atoms to be merged.
2. Right-click in the Graphics Pane and choose: **Transform Selection > Merge** (or choose: **Transform > Selection Merge**).



Merging atoms in a disordered molecule (top) to give an idealized version (bottom).

## Adding new Atoms to a Crystal or Molecule

CrystalMaker lets you add new atoms into an existing structure using the Add Atom tool, in combination with its Atoms Popover. One can specify the type of atom to be added, and then simply click to add the atom. (Note that, for a crystal structure, the symmetry will be reduced to *P* 1—you will be prompted to confirm this—and the new atom will be tiled into other unit cells.)

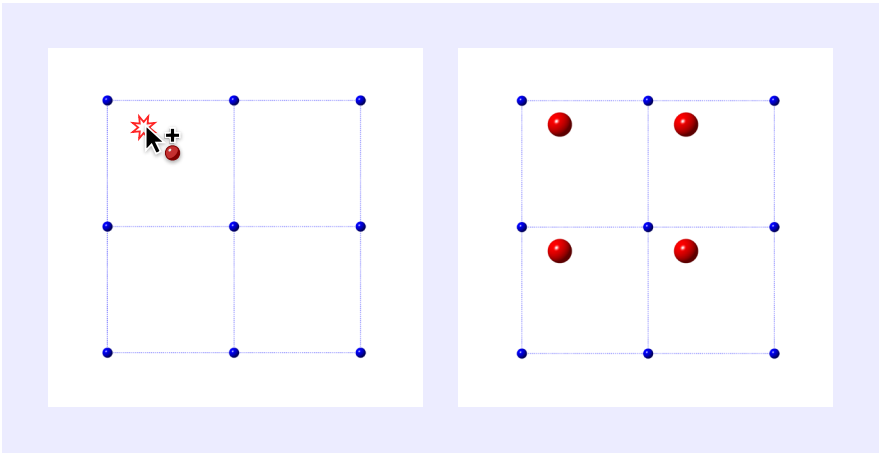
The Atoms Popover provides a series of shortcut buttons for commonly-used element types. This can be easily customized as follows:

- Click the **Sets** popup menu button and choose a new element set (e.g., Organics, Silicates, Halides…).
- Click and hold any preset button, then choose a new element symbol (or "blank", to clear the button) from the popup menu that appears.

### To add a new atom:

1. Choose the **Add Atom** tool from the Tool Strip.
2. Select the type of atom you wish to add from the Atom Picker palette.
3. Click in the Graphics window where you wish to insert your atom.

   Note: to adjust the height of newly-added atoms you may need to rotate the model and reposition the atom (select and drag with the **Arrow** tool).



Using the Add Atom tool to insert a single oxygen atom (red) into a unit cell. The original structure is shown on the left; the new structure, with auto-tiled oxygen atoms is shown on the right.

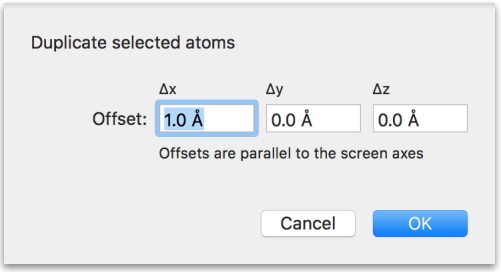
## Duplicating Atoms

You can easily take part of an existing crystal or molecule and duplicate it. In the case of a crystal structure, the duplicated atoms are tiled, so as to preserve the lattice symmetry. The space group will be reduced to *P* 1.

### To duplicate atoms:

1. Select the atoms to be duplicated (click with the Arrow tool; **shift**-click to select more than one atom, or use the Lasso or Polygon tools).
2. Do one of the following:
   - Right-click in the Graphics Pane to display a contextual menu and choose: **Transform Selection > Duplicate;**
   - Choose **Transform > Selection > Duplicate** from the main menu.
3. Specify an offset for the duplicated atoms (if required) then click the **OK** button to continue.

The Duplicate Selection sheet.




**Mouse-Driven Duplication:** You can also duplicate a selection by holding down the **option/alt** key as you click-and-drag a selection.

## Deleting Atoms

In the same way that atoms can be *added* to an existing structure, atoms can also be removed (deleted) from the structure. Note that for crystal structures, all *symmetry-related atoms* will be deleted; if you only require one atom (per unit cell) to be deleted, you should use the **Transform > Discard Symmetry** command before you try to delete any atoms in a crystal.

### To delete atoms in your structure:

1. Select the atoms to be deleted.
2. Do one of the following:
   - Right-click in the Graphics Pane and choose: **Selection > Delete**;
   - Press the **Delete** key on your keyboard.

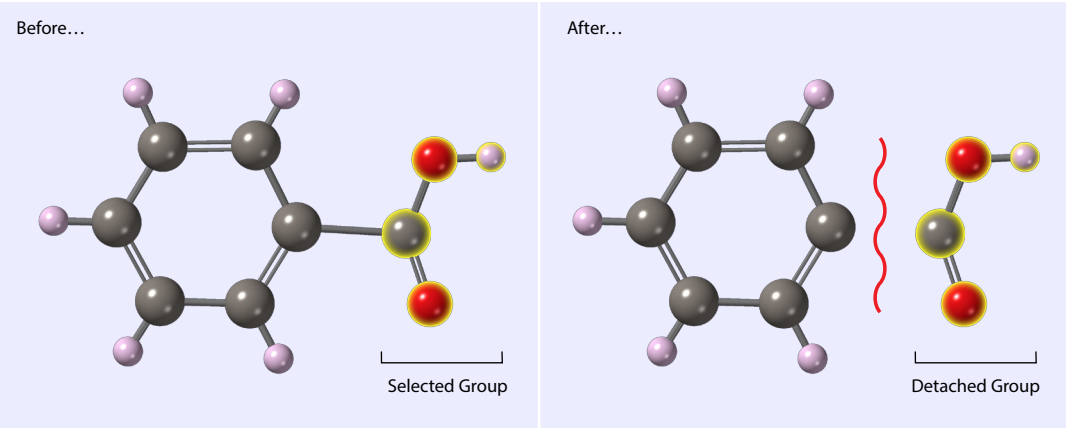
## Detaching a Group of Atoms

If you need to move a group of atoms, you can optionally detach ("unbond") them from the rest of the structure first.

### To detach atoms:

1. Select the atoms to be detached.
2. Do one of the following:
   - Right-click in the Graphics Pane to display a contextual menu and choose: **Selection > Detach**.
   - Choose: **Transform > Selection > Detach** from the main menu.

   Any bonds between the selected atoms and the rest of the structure are removed.



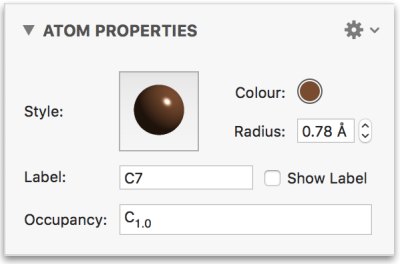

Detaching a selected group from its host structure (left) yields two fragments (right).

## Changing an Atom's Type

It is possible to change the atom types of selected atoms, without having to edit the entire structure. This makes it possible to create defect structure, e.g., with a Ge atom replacing a Si atom. (Note that if you change an atom's type in a crystal structure, this is likely to break any space group symmetry, and the structure will be reset to $P\,1$ symmetry.)

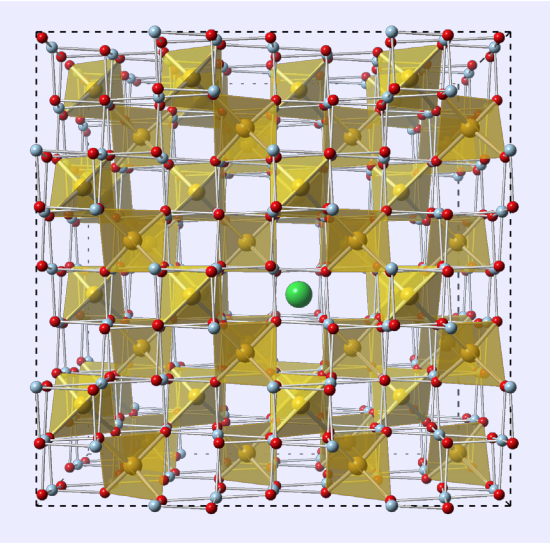
### To change an atom type:

1. Select the atom(s) whose type is to be changed.
2. Ensure the Selection Inspector is visible (**View > Inspector > Selection**), then inspect the atom properties you wish to change:




The Atom Properties group of the Selection Inspector.

3. Enter a new occupancy (e.g., type a new element symbol). Press the tab or return keys to update the structure (the colour and radius fields will be updated to match the primary element symbol in your site occupancy).
4. If required, define a new label, colour and radius. (Remember to press the tab or enter keys to update the structure.)



Visualizing a dopant atom (green) in a crystal structure. The Selection Inspector was used to replace a magnesium (yellow) atom with a strontium (green) atom.

## Inserting Space in a Lattice

CrystalMaker can insert a block of empty space, parallel to a displayed Lattice Plane, with a width specified by you. Your new structure will have a larger unit cell (although you can also specify a negative width, to close up an existing space), and CrystalMaker will automatically shift existing atoms for you.

### To insert (or remove) space in a lattice:

1. Use the Planes Inspector to display a lattice plane in your structure.
2. Use the **Plane Position** slider to move the lattice plane to where you wish to insert space.
3. Click: **Insert Space**. You will be prompted to discard symmetry, followed by a dialog requesting the total width of the block of space to be inserted. If you wish to *remove* space, then you should enter a *negative* amount here.
4. Click the **OK** button to continue. CrystalMaker will insert a block of space centred on the lattice plane position, i.e., half width on each side.

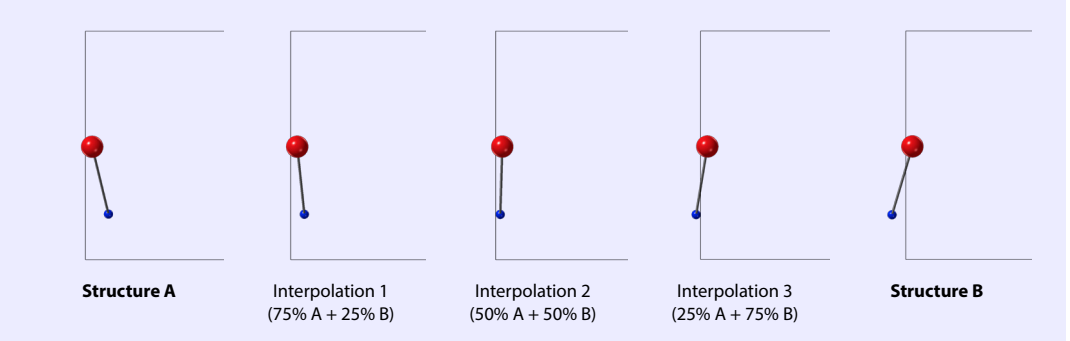
Important Caveats:

1. For best results, work with a single unit cell. Otherwise, if the lattice plane spans more than one unit cell the command may give unpredictable results.

2. Ensure that your lattice plane is parallel to one or more cell edges (e.g., a (100) plane). If the lattice plane is inclined with respect to all cell edges (e.g., a (111) plane) you will get unpredictable results.

## Interpolating Structures

Interpolation is an invaluable tool when visualizing structural behaviour: it allows you to smooth the behaviour, resulting in a more professional-looking display. It also offers a seamless guide to the eye that makes it easier to follow "jerky" atomic motions—thereby reinforcing visual understanding of subtle structural behaviour.




Interpolating three structures between two end-members, "Structure A" and "Structure B".

You can choose to interpolate between all structures in the Structures List, or between just a pair of selected structures:-

### To interpolate between just two structures:

Do the following:

1. Select two structures in the Structures List (e.g., by command-clicking on them).
2. Choose: **Edit > Interpolate Selected Structures** (or right-click in the Structures List and choose: **Interpolate Selected Structures**).
3. Specify how many structures to add using the Interpolate sheet that appears, then click the **OK** button to continue.

### To interpolate between all structures:

Do the following:

1. Ensure that only one structure is visible (selected in the Structures List).
2. Choose: **Edit > Interpolate Structures** (or right-click in the Structures List and choose: **Interpolate Structures**).
3. Specify how many structures to add using the Interpolate sheet that appears, then click the **OK** button to continue.

Having added interpolated structures to your list, you will probably want to use the **Synchronize** command to ensure the atom visibilities match (but see note below about phase transitions, where a change in space groups may cause synchronization to fail in some—but not all—cases).

### Interpolation Requirements

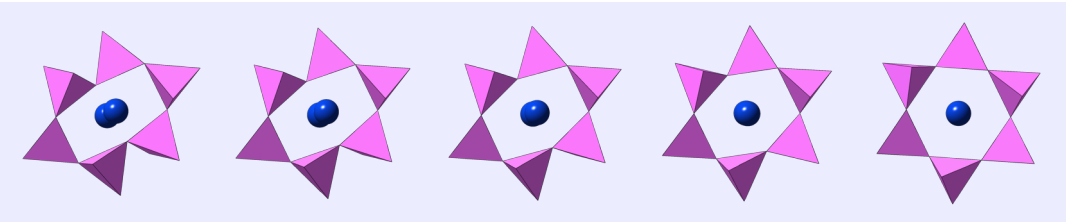
For interpolation between two structures to work, the structures must be directly comparable. They must have the same number of atoms (or, for a crystal, the same number of atoms in the unit cell), and those atoms should have a direct correspondence: their atom or site labels should match.

If your sequence includes crystals with different space groups, the process of matching atoms becomes more complicated. If is of course an essential prerequisite that structures have the same number of atoms in the unit cell. If their space groups differ, CrystalMaker will generate interpolated structures using the space group '*P* 1', so as to ensure the best chance of matching sites which might otherwise have different multiplicities and/or labels.

**Phase Transitions:** If your crystals have different space groups and CrystalMaker has to reduce symmetry, there is a chance the Synchronize command will fail if newly-generated sites (in the interpolated structures) have different site labels to the parent sites. In these circumstances it might be better to edit the high-symmetry structures, applying the same space group symmetry as the low-symmetry structures (and additional sites as required) so as to ensure continuity across a transition sequence.

## Synchronizing Structures

If you have a multi-structure document, you can use the **Synchronize** command to apply settings from the primary-selected structure) to all other structures in your document's Structures List. This includes scale, model type, atom colours, styles, visibilities, range, etc.



Atom-level synchronization lets you map the visible atoms in one structure (such as an arbitrary cluster) to atoms in all the other structures, thereby letting you animate the results, without having to individually hide atoms in each structure.

### To synchronize multiple structures:

1. Choose: **Transform > Synchronize**. The Sychronize dialog appears.
2. Click the **OK** button to continue.

The Synchronize dialog gives you two options:-

- **Atom-Level Synchronization.** Here, the program performs an atom-by-atom comparison (within a given search radius), attempting to track each individual atom and ensure its attributes are maintained across the entire sequence. This lets you synchronize a selected region in a larger structure, perhaps with custom atom and bond styles, and apply this to multiple structures.
- **Synchronized Bond Specifications.** You also have the option of resetting the bonding in all structures to match that in the template (current) structure. Bond specifications from the template structure are copied to the other structures. This works well if the structures are similar and correspond to similar temperatures and pressures. However, because bond lengths can change with pressure and temperature, bond specifications that work well for the source structure, may become inappropriate for other structures.

**Matching Labels:** Please note that atoms can only be synchronized if they have the same labels in source and destination structures! For example, if structure A has sites "T1", "T2" and "O1", and structure B has sites "T3", "T4" and "O2", no atom-by-atom synchronization can take place.

### Synchronizing Atoms Colours and/or Radii

You can use the **Actions** menu of the Atoms Inspector to apply the current structure's colours or radii to all other structures in the same document. You also have the option of applying default colours or radii to these structures.

### Synchronizing Specific Model or Rendering Settings

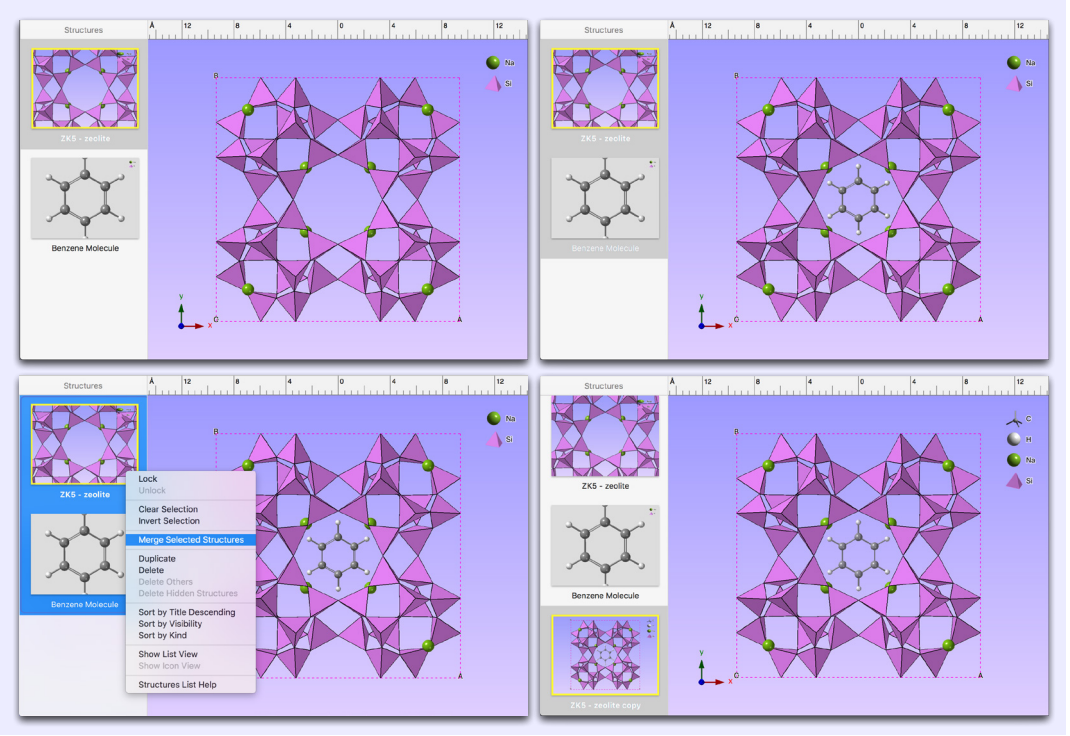
If you require fine-scale control over Model and Rendering settings, you can use the Model or Rendering Inspectors to propagate changes for specific model and rendering attributes. For example:-

#### To synchronize the background colour:

1. Display the Rendering Inspector.
2. Open the Background group.
3. Right-click in the group to display a contextual menu.
4. Choose: **Apply to All Structures**.

## Merging Multiple Structures

CrystalMaker X gives you the option of working with multiple structures in the same window, or merging separate structures into a single, composite structure.




Merging separate structures in the same window. Top Left: a molecule has been loaded as a separate structures into a document containing a zeolite cage. Top Right: the molecule is made visible by command-clicking its Structures List icon to add it to the current display. Bottom Left: right-clicking in the Structures List brings up a contextual menu with the option to merge the structures. In this case the molecule is to be merged into the primary selection: the zeolite crystal. Bottom right: after merging a new crystal structure has been created, being a composite of the original zeolite with the inserted molecule.

### Why Keep Structures Separate?

Working with separate structures in the same document is a great way to explore molecular docking, for example: you can keep your host structure (e.g., a crystal lattice) separate from the inserted structure (e.g., your molecule); you can apply different model types to the different structures, lock one structure and rotate or move another structure—and generally have more degrees of freedom than if you were simply working with selected atoms in a single structure.

**Working with Multiple Structures**: For more information about how to load multiple structures into the same window, including locking and unlocking structures and making more than one structure visible, please see *Chapter 4: Document Window*.

### Merging Structures Into One

CrystalMaker X does also let you merge *multiple* structures into a *single* crystal or molecular structure. This might allow you to take a molecule and position it within a crystal lattice, or to insert a block of atoms into a gap between crystal layers and hence build an intercalated structure—perhaps as input to an energy-modelling program which expects a single structure, rather than a list of separate structures.

In order to use this command, you need to understand how the multiple structures will be merged:-

- The Primary Selected Structure (as indicated by the yellow rectangular highlight in the Structures List) will serve as the *host structure*. If this is a crystal, then the final, merged structure will be a crystal; otherwise it will be a molecule.
- Any *visible* atoms from other structures will be inserted into the host structure.

**Added Flexibility**: Note that, unlike the "Place Molecule" command—used by CrystalMaker 9 and earlier—the new Merge Structures option is much more powerful, letting you combine more than two structures, and giving the option of crystal output, rather than molecule output.

#### To merge multiple structures:

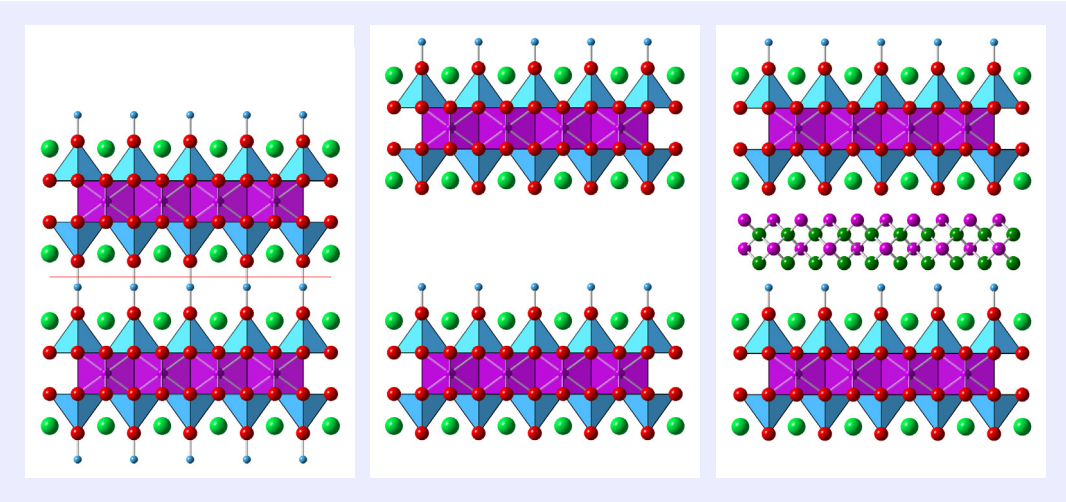
1. Display the Structures List (e.g., by clicking its button in the toolbar).
2. If necessary, add any structures to your document's Structures List by dragging-and-dropping their icons into the list, or by using the **File > Add to Window** submenu.
3. Ensure that all structures to be merged are visible. Either **command**-click (Mac) or **control**-click (Windows) on individual thumbnails to toggle their visibility.
4. Make your intended host structure the primary selection. To do this, simply click on its (selected) thumbnail so that a yellow rectangular highlight is shown.
5. Right-click in the Structures List and choose: **Merge Selected Structures** (or choose: **Edit > Merge Structures**). An alert will appear, explaining the plan of action and, if accepted, a new, merged structure will be added to the Structures List.
6. You can now safely remove any other structures by dragging their thumbnails out of the Structures List, or by right-clicking on them and choosing the **Delete** command.

## Creating an Intercalated Structure

CrystalMaker lets you design a new structure comprising layers of atoms from one structure, interspersed with layers from another structure. The best way to do this is to start with two separate structures in the same document, insert space in one structure, then use the **Merge Structures** command to insert a block of atoms from a second structure.

### Steps to create an intercalated structure:

1. Load two structures into the same document.
2. Designate one structure as your host structure: this should have two of its unit cell vectors in the plane of interest, so you may need to create a "surface cell".
3. Create a block of atoms from the second, "guest", structure, to be inserted into the host structure.
4. Use the **Insert Space** command to create a block of empty space in the host structure, large enough to hold a block of atoms from the guest structure.
5. Make both structure visible.
6. Lockthe host structure and manipulate your guest structure so that its block of atoms fits within the empty space.
7. Use the Merge Structures command to merge the block of atoms from the guest structure into the empty space you've created in the host structure.

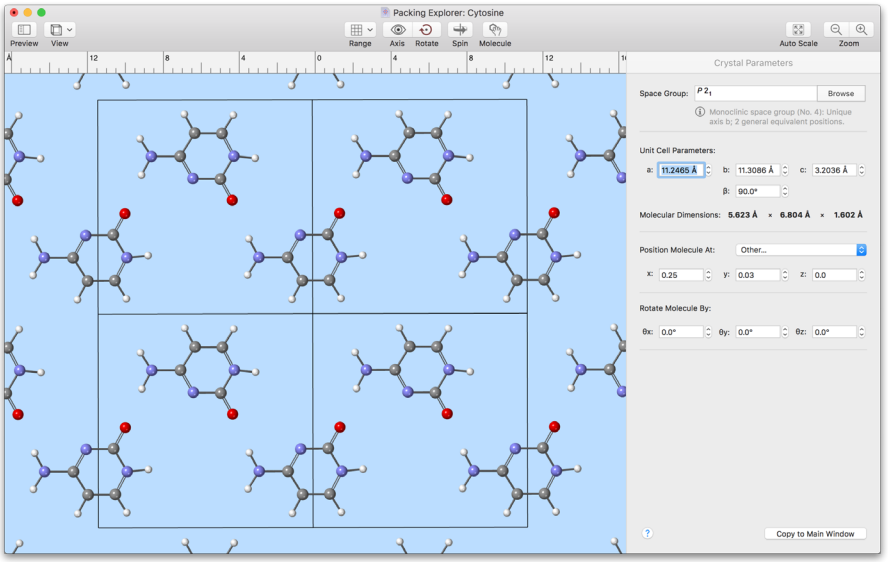


Using the Lattice Plane to define an insertion point in a crystal lattice (left). The resulting space (centre) provides room for the insertion of a block of new material (right).

## Converting a Molecule to a Crystal

By converting a "molecule" to a "crystal", you gain the ability to extend your structure through tiling—and hence, the ability to simulate diffraction properties.

The Packing Explorer window.




CrystalMaker X features a special Packing Explorer window which lets you experiment with different ways of packing a molecule in three dimensions. The window includes an inspector (on the right-hand side) with controls to let you:

- Specify the symmetry (space group) of the new lattice.
- Adjust the unit cell parameters.
- Reposition the molecule within the new unit cell.
- Rotate the molecule relative to the crystallographic axes.

A button in the Explorer's toolbar lets you toggle between rotating the crystal or rotating the molecule. Other controls let you specify a view direction, auto-rotate, zoom or auto-scale.

### To display the Packing Explorer:

1. Open any molecular structure.
2. Choose: **Transform > Molecule to Crystal**.

### To rotate the new crystal:

Do one of the following:

- Click-and-drag the structure with the mouse or trackpad.
- Click the toolbar's **Orient** button and choose a new view direction.
- Click the toolbar's **Rotate** button and use the popover to adjust the orientation.

### To change the orientation of the molecule:

Do one of the following:

- Select the **Molecule** button in the toolbar, then click-and-drag the mouse.
- Enter one or more rotation angles for the molecule using the **Rotate Molecule By** fields on the right-hand side of the window.

### To reposition the molecule:

Do one of the following:

- Choose a preset location using the **Position Molecule At** popup menu.
- Use the **x**, **y** and **z** fields to define the position of the molecule's centroid.

### To adjust cell parameters:

- Use the **Unit Cell Parameters** fields.

### To save your changes:

- Click **Copy to Main Window**. Your new crystal is added—as a separate structure—to your document window (together with your original molecule).

## Converting a Crystal to a Molecule

CrystalMaker lets you convert an existing, periodic crystal structure, to an aperiodic "molecule" (**Transform > Crystal to Molecule**). Your end result will look identical, but the unit cell and symmetry will have been discarded and any hidden atoms lost. Note that the original crystal remains as a separate structure in the Structures List.

Chapter 12

# Measurement

This chapter describes ways in which you can measure your structure: distances and angles on screen, or between atoms. We include ways of visualizing coordination environments, via bond searches, cluster display, and representation via custom, large-scale polyhedra. You can also visualize lattice planes or crystal surfaces, and measure angles between different planes or planar structures.

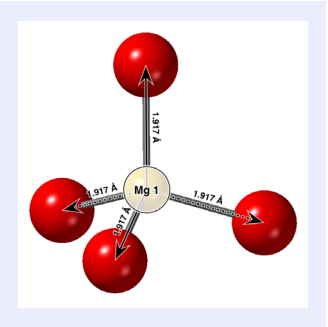
## Identifying Atoms & Polyhedra

You can find information about atoms and polyhedra using the Arrow tool, either in the form of on-screen overlays, or via the Selection Inspector.

### Atom Overlays

CrystalMaker's **Arrow** tool isn't just for selection: it also provides real-time identification of atoms and bond lengths (space permitting) as you move the mouse across the screen.

Hovering over an atom with the Arrow tool displays the atom label and its bond distances.

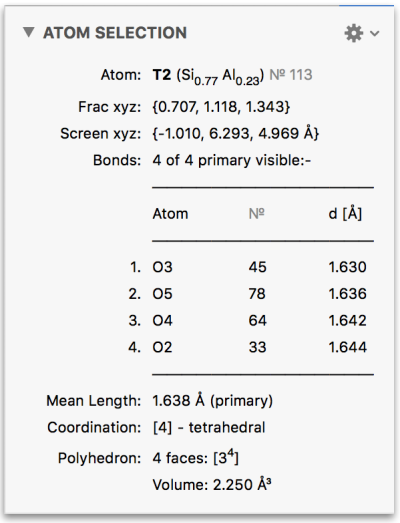


## Atom Selection

If you select an *individual* atom, detailed information about that atom will be displayed in the **Atom Selection** group of the Selection Inspector. Information includes:

- Site occupancy.
- Structural coordinates (these are the fractional coordinates, for a crystal; or the original orthogonal coordinates, for a molecule).
- Screen coordinates (orthogonal coordinates relative to the *screen* axes)
- Bonds to the selected atom (atom information and bond lengths)
- Mean bond length
- Coordination number
- Polyhedral information (including polyhedral volume and number of faces).

Information about a selected atom displayed in the Selection Inspector.




To display more information, use the actions popup (cog icon), which lets you print information about atoms, bonding (neighbours and their distances) and bond angles in the Output Log.

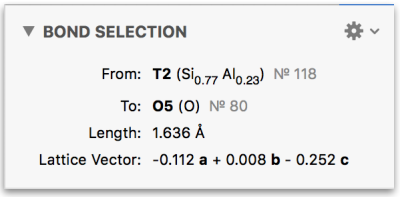
### Show in Atoms Inspector

You can reveal the selected atom in the Atoms Inspector using the Show in Atoms Inspector button on the Actions menu. This is useful for crystals, as it allows you to edit the corresponding *site*. For example, you might wish to change radius and colour information for *all* atoms with this site— rather than just the specific selected atom.

## Bond Selection

Unlike earlier versions of the program, CrystalMaker X lets you select bonds, so you can change their styles and colouring. As for selected atoms, a selected bond's details are displayed at the top of the Selection Inspector:

Information about a selected bond is displayed in the Selection Inspector.




Information includes:

- End-member atoms (labels, site occupancies and atom numbers).
- Bond length.
- Lattice vector (in the form U**a** + V**b** + W**c**, where a, b and c are the axial vectors).

For more information, see the Actions popup menu which lets you reveal the corresponding bond specification (if any) in the Bonds Inspector, and print a summary of the bond in the Output Log.

## Measuring Distances and Angles

CrystalMaker lets you measure distances and angles on screen, between clicked atoms or polyhedra, or between planes, via the Angle Calculator, the Distance Explorer, or output to a text file.

### Distance Tool (Distance Group)

This measures distances in the *plane of the screen*, giving a real-time distance display until you anchor the measurement with a second click.

**Tool Groups:** The Distance tool isn't shown in the default Tool Strip. Instead, related tools are grouped under the same icon and you can switch functionality by clicking the popup menu (the downwards pointing arrow to the right of the icon).

### Bond Distance Tool (Distance Group)

This measures the *three-dimensional distance* between the centres of two clicked atoms or polyhedra. To use this tool, simply click on two atoms in succession and the distance between them is displayed.

Note that this tool offers a "rollover" mode, which works in two ways:

- If you move the mouse over an *existing* bond, its distance is shown (and vanishes when you move the mouse away); click on the bond to highlight it and "freeze" your measurement.
- Alternatively, click an atom to start measuring (the atom will become highlighted), then as you move the mouse over different atoms, their distances from the clicked atom will be shown. Click on the second atom to freeze the distance measurement (your frozen measurement will vanish if you update the plot or click elsewhere).

**Rotate and Measure:** Unlike earlier versions of the program, you can now rotate and scale your structure without losing your distance or angle measurements!

### Detailed Output

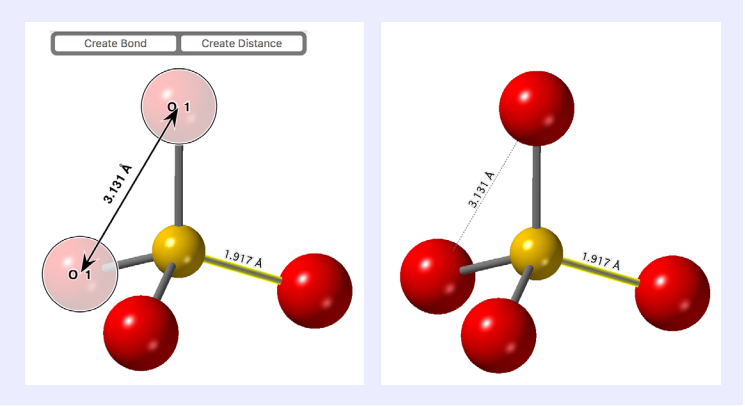
In addition to the screen overlay display, the Bond Distance tool prints more-detailed information in the document window's Output Log:-

- Bond *vector* and its *magnitude*. (Error propagation is used if the structure includes error information for coordinates.)
- *Projected bond distance* (in the plane of the screen). This may be useful to electron microscopists, used to working with two-dimensional *projections* of the three-dimensional structure.

### Preserving Distance Measurements

You have two options for preserving distance measurements. If you are measuring an existing bond, you can simply turn on that bond's label. To do this, simply select the bond and enable the **Show Label** checkbox in the **Bond Properties** group of the Selection Inspector.

If there is no bond between the two atoms, you can create a new "measurement" between them. This is actually a *secondary bond* (which, as with all secondary bonds, is ignored for the purposes of coordination and molecular detection) showing a default dotted line style with a label.




Clicking on two atoms with the Bond Distance tool (left) gives you the option of preserving the measurement (right).

## Angle Tool (Angle Group)

This measures the included angle, in the *plane of the plot*, between three clicked points. If you shift-click with this tool, you can preserve existing angle measurements (although these will be erased if you resize the screen). A summary of the angle measurement is printed to the Output Log.

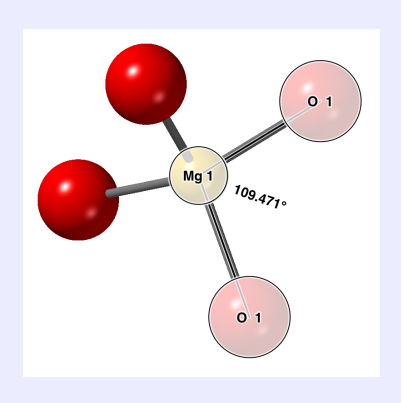
## Bond Angle Tool (Angle Group)

The "bond angle" is the included angle, in three-dimensions, between the centres of three clicked atoms or polyhedra. Bond *vector* information (as well as the included angle) is printed in the Output Log for this measurement.

As with the Bond Distance tool, the Bond Angle tool provides rollover modes. You can use the tool in two ways:

- Simply position the mouse between three *bonded* atoms in the same structure (without clicking) and the included angle between the closest pair of bonds is shown. The angle display is updated as you move the mouse.
- Alternatively, you can simply click on three atoms in succession (which do not need to be bonded) and see their included angle displayed. Note that after your two clicks you can "rollover" to display the bond angle to any third atom under the mouse.

As with the Bond Distance tool, you can rotate and scale your structure without losing your measurement.

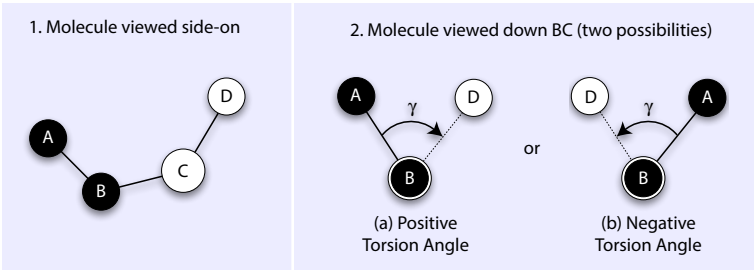


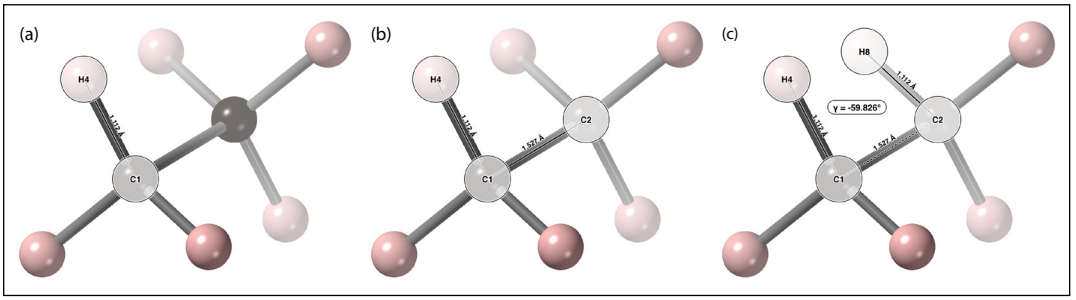

Measuring the included angle between three atoms using the Bond Angle tool.

## Torsion Angle Tool (Angle Group)

You can measure a torsion angle by clicking on four atoms with the Torsion Angle tool. Consider a molecule with four atoms, ABCD. The atoms define two planes, ABC and BCD, which intersect along the BC bond direction. The angle between these planes is the torsion angle, γ, the sign of which depends on the relative orientation of AB and CD, as illustrated below.

Torsion Angle sign convention.




Torsion angle measurements in CrystalMaker. (a) Clicking on the first atom results in a distance rollover to a second atom. (b) Clicking on a second atom provides an angle rollover to the third atom. (c) Clicking on the third atom and moving the mouse results in a torsion-angle rollover to the fourth atom.

**Haptic Feedback:** Mac users with force-touch trackpads can enjoy haptic feedback when they use the Arrow, Bond Distance/Angle and Torsion Angle tools: the trackpad vibrates when you position the cursor over an atom or bond, thereby making it easier to locate your measurement targets.

To enable haptic feedback, open your System Preferences panel, navigate to the Trackpad pane and turn on the "Force Click and haptic feedback" checkbox.

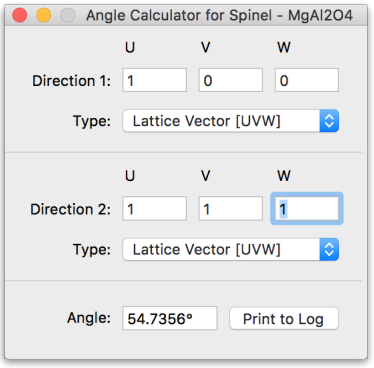
# Calculating Angles

As an alternative to interactive measurement, you can calculate angles between any pair of directions, using the Angle Calculator. Angles between molecules (or, rather, angles between their *best-fit planes*) can also be calculated.

## Angles Between Planes and Vectors

CrystalMaker allows you to measure angles between lattice planes and/or vectors, by entering their indices into the Angle Calculator (**Calculate > Angle Calculator**) and setting their types (Lattice Vector *or* Plane Normal) using the popup menus.

The Angle Calculator.




For distances and angles between *displayed* lattice planes, please see the section on Lattice Planes later in this chapter.

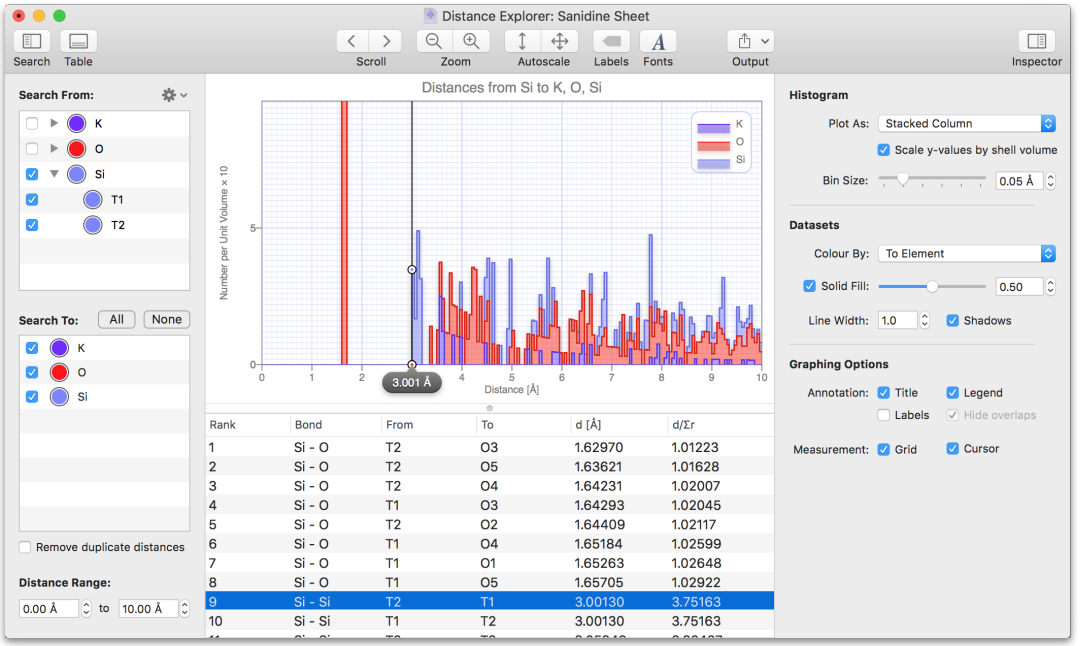
## Angles Between Molecules

If you are working with a molecular *crystal*, you can readily calculate the angles between a pair of molecules: simply select at least one atom in each of the molecules to be measured, then choose the **Calculate > Angles Between Molecules** command. CrystalMaker calculates the best-fit lattice plane through each molecule, and the resulting inter-planar angle. The results are printed in the Output Log.

# The Distance Explorer

Whilst you can measure inter-atomic distances using the screen tools, CrystalMaker provides a more powerful way of getting an overview of the distance *distributions* in your structure. The Distance Explorer window (**Calculate > Explore Distances**) provides a colourful histogram of distributions between any combination of chemical elements or sites in your structure. This is effectively a "pair distribution function", which you can customize to learn more about potential bonding patterns and coordination environments.

This window lets you search distances to atoms from a specified element or site. You can specify a distance range for searching, and view the results as a table and a graph (histogram).




The Distance Explorer window, showing data for a silicate structure. One distance result has been selected in the list (blue highlight row) and the corresponding position in the histogram is indicated by the vertical black cursor line.

## Distance Explorer Layout

The window includes a toolbar, below which there are three vertical panes, from left-to-right:

- Search Pane (left): lets you define your search criteria.
- Display Pane (middle): split into a graphical view and a table view.
- Inspector Pane (right): lets you customize the graph display.

## Starting a Search

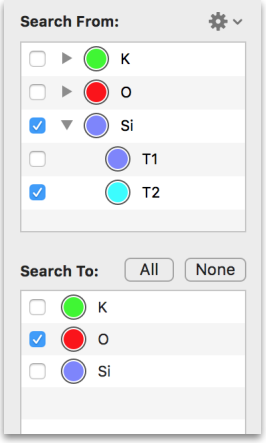
You can specify a site label, or opt to search every site that shares a specified element symbol.

### To search from all sites with a specific element type:

1. Ensure that your distance range is appropriate (refer to the **Range** fields).
2. Select the element symbol in the **Search From** list. A search will begin immediately. (You can cancel this, if required, by pressing the **escape** key.)

### To search from a specific site:

1. Ensure that your distance range is appropriate (refer to the **Range** fields).
2. Locate the site's element symbol in the **Search From** list, then click the element's disclosure triangle to reveal all sites with this element.
2. Select the corresponding site label to execute a site search.




Searching for distances from a specific site (T2) to O.

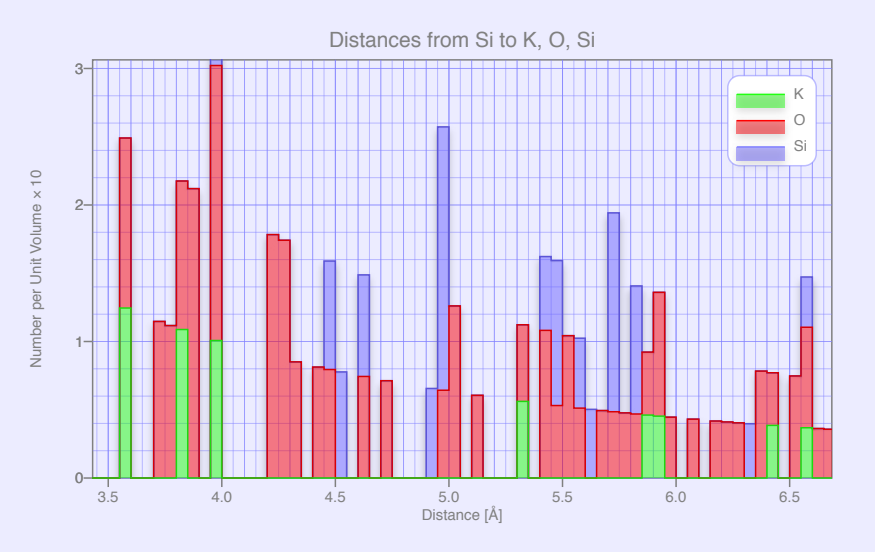
### Fine-Tuning Your Search.

You can quickly execute a search by entering a new value in one of the two **Range** fields, and then pressing the **return** or **enter** keys. Alternatively, press the **Search** button to execute a new search. If your search is taking too long, you can cancel it by pressing the escape key. Any results gathered will be presented.

## Exploring the Histogram

You data are shown graphically, in the form of a histogram at the top of the display pane. You can use multi-touch to *zoom* and *scroll* this graph. Clicking in the graph reveals a vertical cursor, which can be dragged to different parts of the graph to measure distances.

You can use multi-touch to scroll and zoom your graph. The results can be copied to the clipboard or exported as vector artwork.




You can set the bin size (sampling interval—the width of the histogram columns) and change other display options, using the Inspector on the right of the screen. Options include:

### Display Modes

You can switch between one of four display modes:-

- Stacked Column (as illustrated above)
- Column
- Stacked Area
- Area

### Colouring Options

CrystalMaker provides four colouring options for the graph:-

- **None** - a greyscale display
- **From Atom/Site** - coloured according to the "from atom" in your "Search From" list.
- **From Element** - coloured according to the element colour in your "Search

From" list.

- **To Element** (the default option) - coloured according to the element colour in "Search To" list.

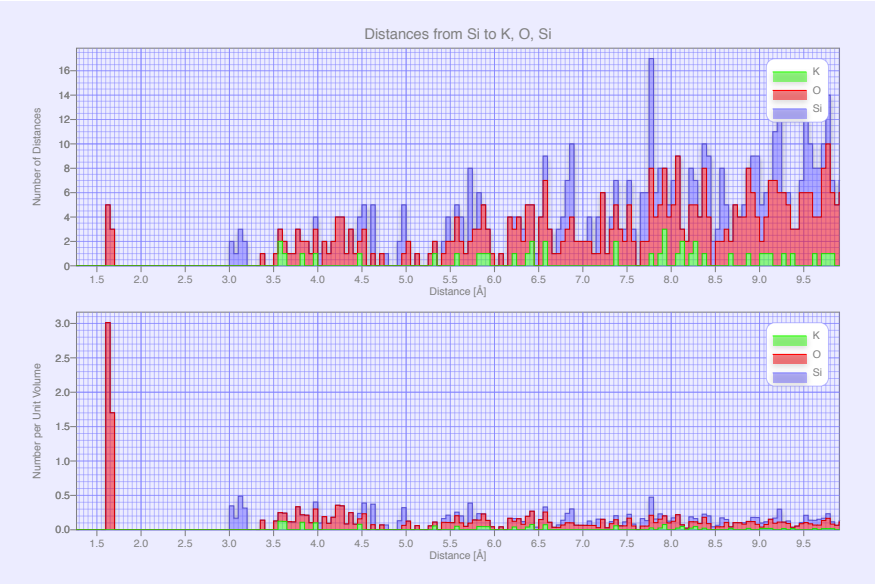
Colouring by "To Element" is a quick and easy way to identify bond distance ranges for a given site. For example, in an organic crystal, searching for bonds around a carbon site, you might find a Hydrogen peak around 0.9 Å, a Carbon peak around 1.3 Å or possibly Oxygen or Nitrogen peaks at 1.2 Å or 1.4 Å, respectively.

**Colourful Searching:** You can change the colours of all the elements and/or sites in the "From" and "To" lists by clicking their colour buttons!

## Correct for shell volume

The histogram represents a series of concentric shells (like "onion skins"). The wider the bond search, the greater the volume of the outer shells, and hence the greater the likelihood of finding bonds within the shell.

CrystalMaker lets you correct for the increasing shell volume, by dividing the absolute number of bonds found in each shell, by the volume of that shell. This then gives something resembling a Pair Distribution Function, with greater prominence given to bonds as shorter distances.




The effect of shell volume: both histograms show the same data, but the lower one has been corrected for shell volume.

### Graph Labels

You can opt to display labels for each histogram bin. The labels currently show the absolute number of bonds found for each bin. Note that these will change as you change the bin size! Please note also that, if you have specified an "Element" search, then the number of bonds includes bonds for each of the different sites with that element symbol.

## Tabular output

Your bond data are also presented in tabular form, at the bottom of the screen. This data browser lets you scroll and sort the results by column header:-

- Bond. This describes the element-pair combination used for the search entry. For example, if you've opted to search an organic crystal by the element carbon, then you might find a range of element-pair combinations such as "C-H", "C-O", "C-N" and so on. When the list is sorted by "bond", you will find bonds in order of increasing bond distance for a particular bond.
- **From**. This is the site label for the first of the two atoms in the bond result. If you've chosen to search from only one site, then this "From" site will be the same for all results. However, if you opted to search "by element", then this column will contain a range of site labels, corresponding to the element symbol used in the search.
- **To**. This is the site label for the second of the two atoms in the Bond result.
- **d [Å]**. This is the distance, in Ångstrom units, between the "From" and "To" atoms.
- Error value (σ [Å]). If your structure contains error values for the cell parameters and/or the fractional coordinates, then CrystalMaker will calculate errors in the bond distances and display these in this column.
- d/Σr. This is the ratio of the bond distance, to the sum of the radii for the "From" and "To" atoms. Assuming that your radii are correctly set, then this value should be close to 1.

**Double-Click the List:** You can identify the corresponding histogram peak by double-clicking a row in the list—or vice versa.

## Saving the Results

The **Output** button in the Explorer window's toolbar lets you save your results in one of five ways:

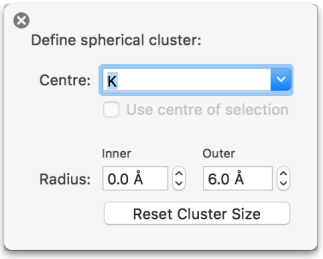
- Copy graphics to the clipboard;
- Export graphics to a vector graphics file (PDF on Mac);
- Print graphics;
- Export graph data to a text file (an x-column, plus a column for every coloured dataset) for use in an external charting program;
- Export all distances to a text file.

Alternatively, you can right-click in the histogram to **Copy** or **Export** the graph, or simply drag-and-drop the graph into another program.

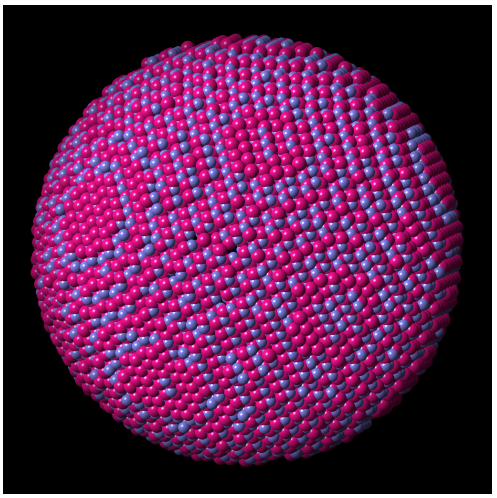
## Displaying a Coordination Sphere

You may prefer to investigate nearest-neighbour coordination environments graphically. The **Cluster** button in the toolbar (**Transform > Atom Range > Define Cluster**) lets you display all atoms that lie within a defined distance range (shell) from a specified central atom. Note that this interface gives a live output, allowing you to control your cluster size interactively.

Defining a spherical cluster using the Cluster popover.




A 50 Å cluster in GaN.



Note that if you are using a polyhedral plot and your cluster radius is too small, it may not be possible to draw a complete polyhedron and you may end up with a blank window.

**Select Nearest Neighbours:** Another way of showing local clusters is to use the **Edit > Select > Nearest Neighbours** command. This can be used iteratively, to select 1st, 2nd, 3rd, etc. nearest neighbours. You could use this command in combination with the Selection Inspector to show different coordination shells around a central site.

## Generating Coordination Data

The **File > Export Data** submenu provides various options for saving information about your structure's bonding in a text file (file extension "**.txt**") which can be edited using any text or word processor. You can opt to have the coordinates of atoms and their bonded neighbours saved, or specify a comprehensive listing of coordinates, distances and angles (regardless of whether or not bonds have been defined).

### 1. Coordinates

The **Export Data > Coordinates** command is the simplest output option, saving a text file with fractional and/or orthogonal coordinates for all visible atoms.

### 2. Visible Coordination

The **Export Data > Visible Coordination** command is more powerful, saving the coordinates of all atoms that are currently displayed on screen, but arranged in coordination groups with bond distances. Each atom entry is followed by a list of its bonded neighbours, with distances. This provides a convenient summary of currently-displayed bonding.

### 3. Crystal Coordination

If you have a crystal structure, chances are, some atoms won't show their full complement of bonds because their neighbours lie outside the current plot range. In this case, the **Export Data > Visible Coordination** command won't list the full coordination data either…

Instead, you can use the **Export Data > Crystal Coordination** command. This will give a systematic listing of the contents of one unit cell—irrespective of the current plot range—with complete bond data. Thus, each atom in the unit cell is summarized, with all of its bonded neighbours (some of which may lie outside the unit cell), plus bond distances and a summary of the atom's coordination number.

### 4. Distances & Angles

So far we've discussed commands for saving details of atomic coordinates and distances derived from your *existing* bond specifications. But what if you haven't defined any bonds yet?

The **File > Export > Distances & Angles** command provides a detailed summary of all distances and angles for every site in a structure, out to a predefined maximum distance. This gives a comprehensive summary of the coordination states in your structure, without you having to manually define bonds or coordination searches.

The format of the file is described in more detail in *Chapter 14: Data Import/Export*.

# Cavity Finder

CrystalMaker lets you automatically locate the positions and sizes of cavities within a low-density crystal structure. The **Calculate > Cavities** command prompts for the minimum cavity size of interest and will then proceed to locate cavities in the crystal. For each cavity, the program calculates the maximum sphere size that can fit—using your current space-filling radii. Detailed results are printed in the Output Log.

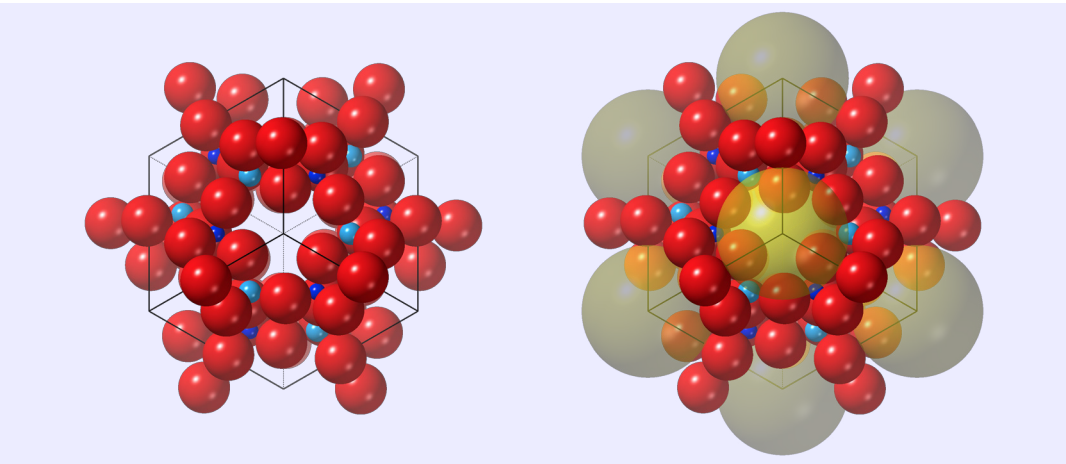
## Treat Hidden Sites as Voids

You can choose to treat hidden sites as voids (N.B., by "hidden sites", we refer to sites whose visibilities have been disabled, using the "**vis**" checkboxes in the Atoms Inspector; individually-hidden atoms—or atoms which are not visible by virtue of them being outside the current plot range—are not considered as being "hidden sites").

## Visualizing Cavities

You can optionally have the program add an appropriately-sized, translucent sphere at each cavity position. (This works best when you display a space-filling model.)

**Cavities not Interstices:** this command is designed for low-density framework structures such as zeolites, not for high-density structures such as oxides or metals (whose voids—or "interstices" —are typically too small for guest atoms)..



Using the Cavity Finder to locate and visualize voids in the crystal structure of sodalite (left). The located voids are represented by translucent spheres with the appropriate cavity-sized radii (right).

## Visualizing Custom Polyhedral Geometries

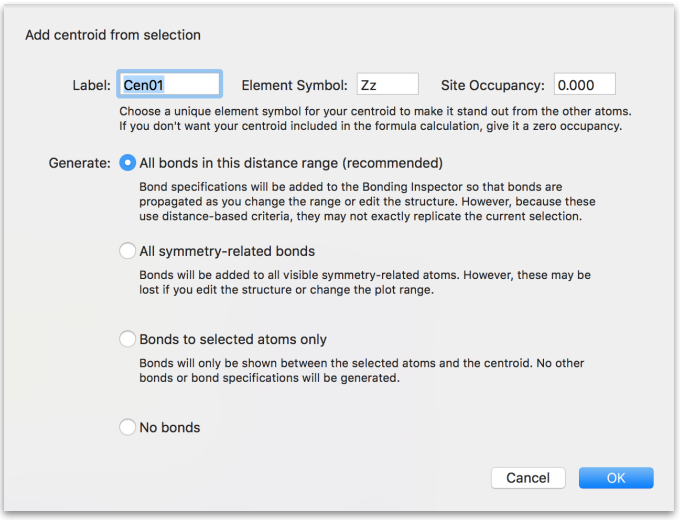
CrystalMaker allows you to display coordination polyhedra, on the basis of maximum bond distances from a target atom. This works very well in most cases, but does require that you know the explicit distance range—and also restricts you to *radial* coordination clusters. Visualizing a non-radial arrangement, e.g., part of a zeolite channel is more difficult.

An alternative method is to tell the program where to build a polyhedron, and from which (vertex) atoms. This generates a new site at the centroid of an existing atom selection, with bonds generated between the centroid and the vertex atoms. The presence of these bonds then allows you to display a polyhedron.

### To generate a polyhedron from three or more selected atoms:

1. Select the atoms you wish to appear as the vertices of your polyhedron (e.g., shift-click with the Arrow tool to select multiple atoms).
2. Right-click in the Graphics Pane and choose: **Transform Selection > Add Centroid Atom** (or choose: **Transform > Selection > Add Centroid Atom** from the main menu). A sheet appears with various options (discussed below).
3. Choose a unique label and a distinctive element symbol for the (dummy) centroid atom that CrystalMaker will generate for you.
4. Click **OK** to generate the centroid atom and its bonds.

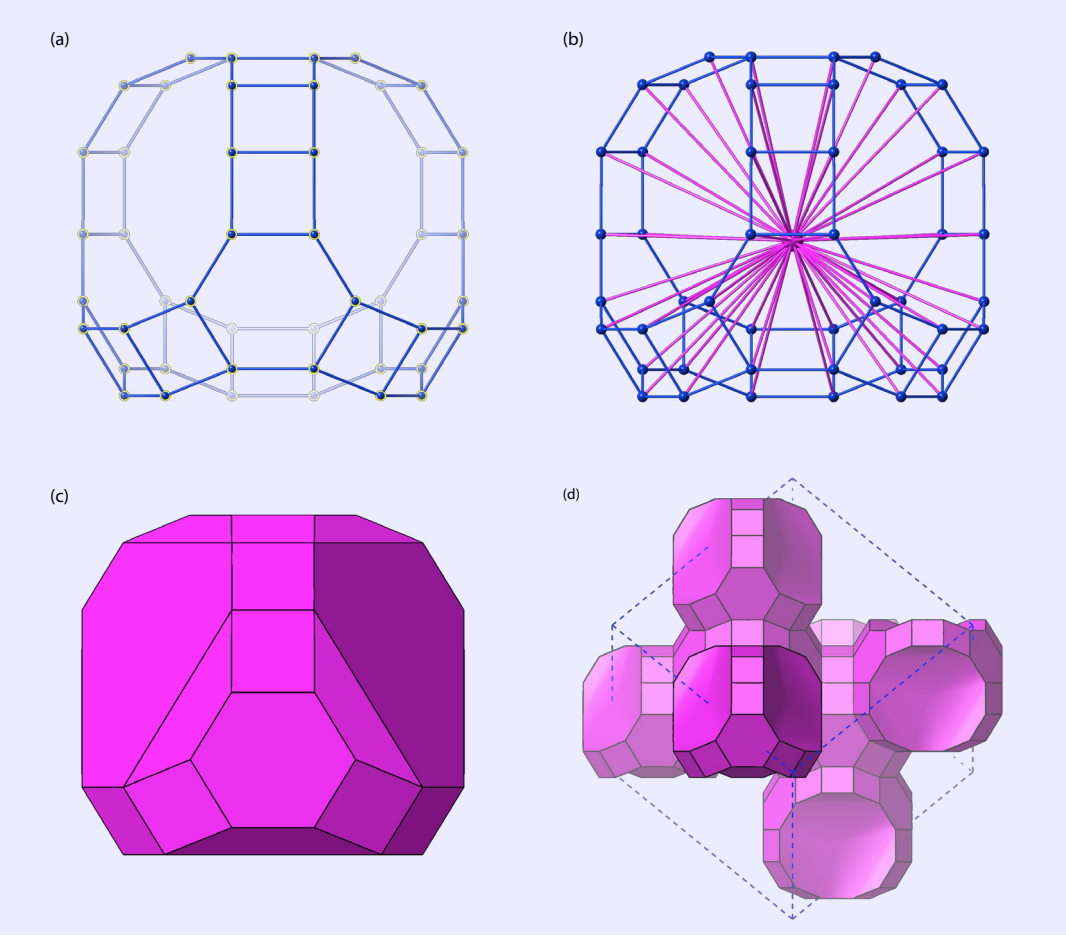
The Add Centroid Atom sheet.



## Radial Bonding Specifications

The default, bonding option, **All bonds in this distance range** generates appropriate global bond specifications, based on the selected distance range and, as a result, polyhedra will be preserved as your plot range changes.

For example, if you wish to represent an aluminosilicate "cage" in a zeolite using a "solid polyhedron", you can simply select the Al/Si cage atoms and choose the **Make Polyhedron** command. The default option analyses the range of bond distances from the cage atoms to the cage centroid, and generates global bond specifications which will propagate this polyhedron throughout the plot range.




The Make Polyhedron command in action. (a) A cavity selected. (b) The result of choosing the "All bonds in this distance range" option to generate a centroid atom. (c) The corresponding polyhedron. (d) Changing the plot range generates additional polyhedra—here they have been rendered as *concave* polyhedra.

## Symmetry-Related Bonds

If you need to visualize a non-radial bonding environment, e.g., a zeolite channel, then the default "radial" bond generation algorithm may result in unintended bonds being generated. In these cases you may prefer to choose the **All symmetry-related bonds** option instead—but note that this is only appropriate for the current plot range, and may be reset if you choose to extend the plot range and hence regenerate the crystal lattice.

You can choose whether or not to display any symmetry-related sites; whether bonds should be generated from the centroid atom to the selected vertex atoms—and whether this bonding should be "cloned" over all symmetry-related sites.

**Use Dummy Element Symbols:** If you are adding a "dummy atom" so you can generate a large polyhedron, it's worth specifying a "dummy" element symbol (such as the default "Zz" used by CrystalMaker). This makes it easier to distinguish between real and dummy atoms in your extended structure—but please remember to set the site occupancy to zero for any dummy atoms. This will ensure that the calculated chemical formula and density remain correct.

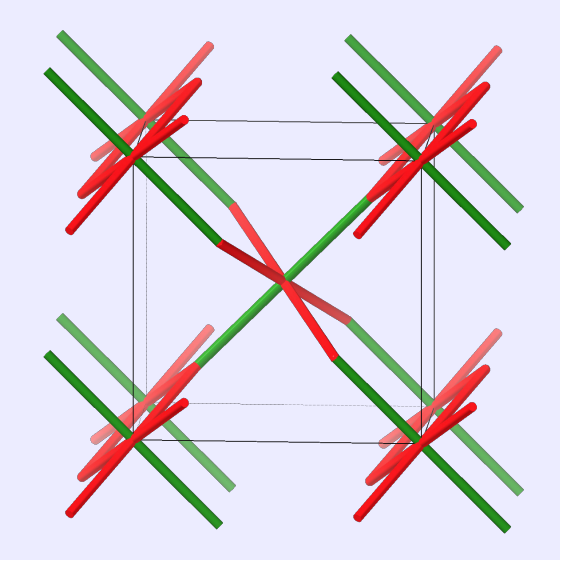
## Symmetry-Related Bonds

Whilst CrystalMaker's bond-generation algorithm searches on the basis of element pairs within an isotropic distance range, you can use the **Symmetry-Related Bonds** command to select any bonds related by symmetry to an existing, selected bond.

### To show bonds related by symmetry:

1. Select a bond (e.g., by clicking on it with the Arrow tool).
2. Choose: **Edit > Select > Symmetry-Related Bonds**.

For example, in the case of rutile, there are two sets of Ti–O bonds, with subtly-different bond distances (1.95 and 1.98 Å). Selecting the symmetry-related bonds allows one to colour code them, and hence distinguish them from other bonds in the structure.



Two sets of symmetry-related bonds in rutile, colour-coded red and green.

**SYSTRE:** CrystalMaker can import connectivity information from SYSTRE files, including symmetry-related bonding. Such bonding can be propagated throughout an extended crystal lattice, thanks to CrystalMaker's addition of dummy atoms at the centres of specific bonds, thereby preserving symmetry relationships as the plot range is increased.

## Measuring Planes and Vectors

CrystalMaker allows you to display any number of lattice planes slicing through a structure. A plane can also be used to slice away part of a structure, to reveal a surface, as detailed in the previous chapter.

### To display a best-fit line through points:

1. Select the atoms through which your line should pass.
2. Choose **Calculate > Line Through Points**. The best-fit orientation is calculated, and its details are printed in the Output Log.

### To display a best-fit plane through points:

1. Select the atoms through which your plane should pass.
2. Choose **Calculate > Plane Through Points**. The best-fit orientation is calculated and a new lattice plane added in the Lattice Planes group of the Model Inspector. The fit results are printed in the Output Log.

### To display the distance from a point to a plane:

1. Select the atom(s) whose distances you wish to measure.
2. Choose **Calculate > Distance From Plane**. The distances are printed in the Output Log. Note that if you have multiple planes, distances are reported for each visible plane.

### To calculate the angle between two lattice planes:

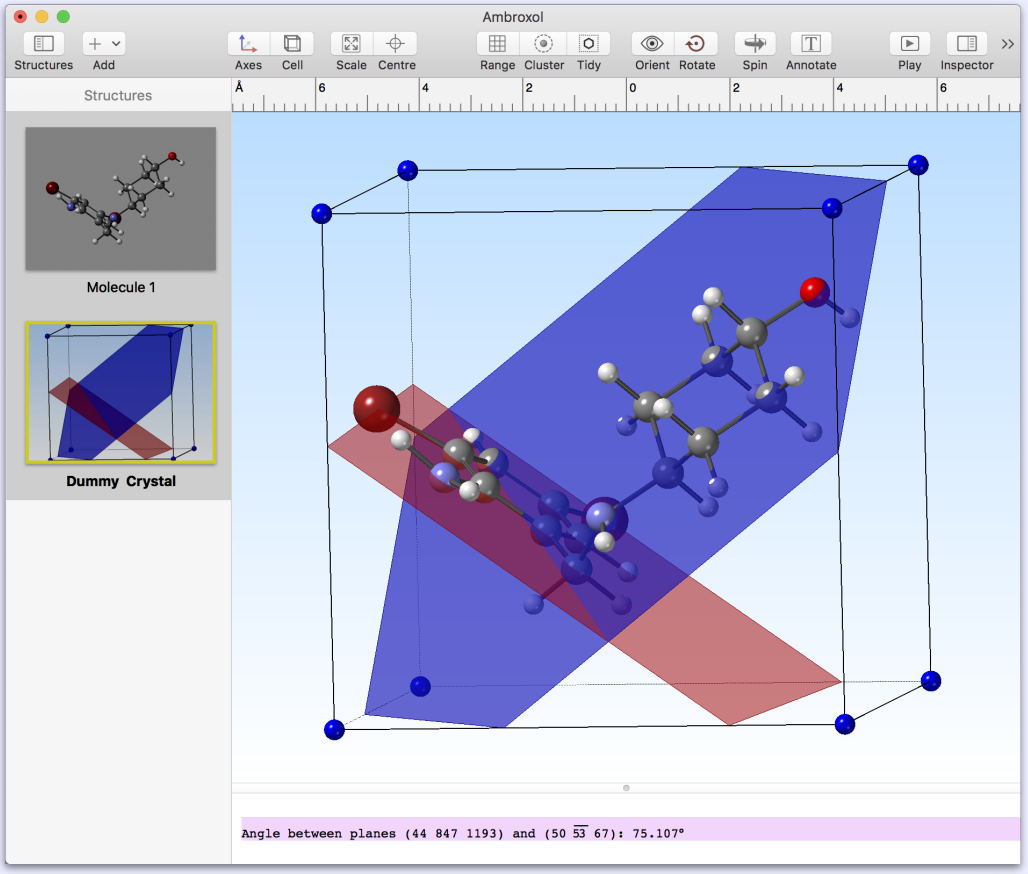
1. Ensure the planes are visible on screen (refer to the **Lattice Planes** group of the Model Inspector).
2. Choose: **Calculate > Angle Between Planes**. The included angles between all combinations of visible lattice planes are printed in the Output Log.

## Working with Planes in Molecules

CrystalMaker can only visualize lattice planes for *crystal* structures, as an underlying *unit cell* is required. If your structure is a "molecule", without any crystallographic data, you will not be able to visualize lattice planes.

You can still calculate the best-fit plane through points in a molecule: the fit results (including the vector components of the plane normal, and a point on the plane) are printed in the window Log.

One workaround is to convert your molecule to a "crystal", using the Molecule to Crystal command. Another option is to add a separate (dummy) crystal to the window containing your molecule and make both the dummy crystal and the molecule visible; you can then calculate the best-fit plane through points in your molecule and have it displayed relative to the dummy crystal—as illustrated below.




Calculating the angle between two planes in a molecule—here displayed with a dummy crystal, which provides the reference for the lattice planes. The dummy crystal is the primary selection (yellow highlight in the Structures List), and the planes were fit through points in the molecule (which remains a separate structure). The angle between the two planes has been printed in the Log at the bottom of the window.

# Ring Finder

CrystalMaker allows you to select a ring passing through a selected atom, and it can also list detailed information about each and every ring passing through that atom.

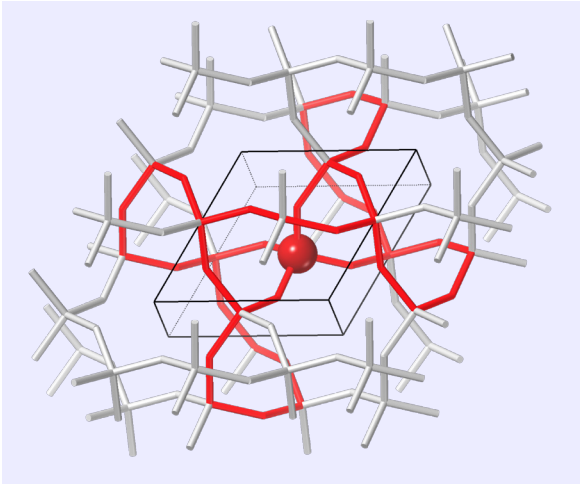
### To select all atoms in a ring:

1. Select one atom in the ring.
2. Right-click in the Graphics pane and choose: **Extend Selection > Ring**.

The (smallest) ring containing the selected atom then has all its atoms selected. Details of the selected ring are printed in the window's Output Log.

## Ring Data

The **Calculate > Rings Through Atom** command provides an exhaustive list of all rings that pass through the selected atom—out to the maximum extent of the plot range. Each ring is a closed path (e.g., , A → B → C → D → E → F → A that doesn't cross over itself (i.e., no "figure of eight" paths are allowed) .



Part of the quartz structure, showing all rings passing through the central silicon atom (red sphere).

For each ring found, CrystalMaker lists:-

- Complete ring circuit (atom label and number) from start to finish.
- The Miller Indices of the best-fit plane passing through the ring atoms.
- The location of the ring centroid.

Such information can be useful when working with low-density three-dimensional frameworks (such as tectosilicates), where ring size and density can be used to characterize the framework structure.

## Formula and Density

CrystalMaker keeps track of the chemical formula of your structure and displays the results in the Info panel, at the bottom of the Info Inspector (**View > Inspector > Info**). Two formulae are actually shown:

- **Chemical Formula.** The formula for an ideal crystal or molecule with all atoms shown.
- **Display Formula.** The formula corresponding to all visible atoms on the screen for the current structure.

If your structure is a crystal structure, then the calculated density is also shown, together with the cell volume and site density (numbers of sites—irrespective of occupancy—per cubic Ångstrøm).

The Info panel at the bottom of the Info Inspector, showing chemical formulae, density and other data for a crystal structure.

| | |
|---|---|
| **Structure Type:** | Crystal |
| **Chemical Formula:** | $K_{2.6}\ Na_{1.4}\ Al_4\ Si_{12}\ O_{32}$ |
| **Display Formula:** | $K_{1.3}\ Na_{0.7}\ Al_2\ Si_6\ O_{24}$ |
| **Spacegroup:** | *C* 2/*m* |
| **Crystal System:** | Monoclinic |
| **a:** | 8.5580 Å |
| **b:** | 12.9970 Å |
| **c:** | 7.1790 Å |
| **β:** | 116.070° |
| **Asymmetric Unit:** | 8 sites |
| **Unit Cell:** | 52 sites per unit cell |
| **Site Density:** | 0.0725 sites/Å³ |
| **Visible Atoms:** | 34 |
| **Cell Volume:** | 717.266 Å³ |
| **Density:** | 2.5254 g/cm³ |

**Unknown Density?** If the Info Pane displays "Unknown" for your density, this is because CrystalMaker was unable to calculate the mass of one or more elements in your structure. This is probably because you used an unconventional element symbol for one of your sites.

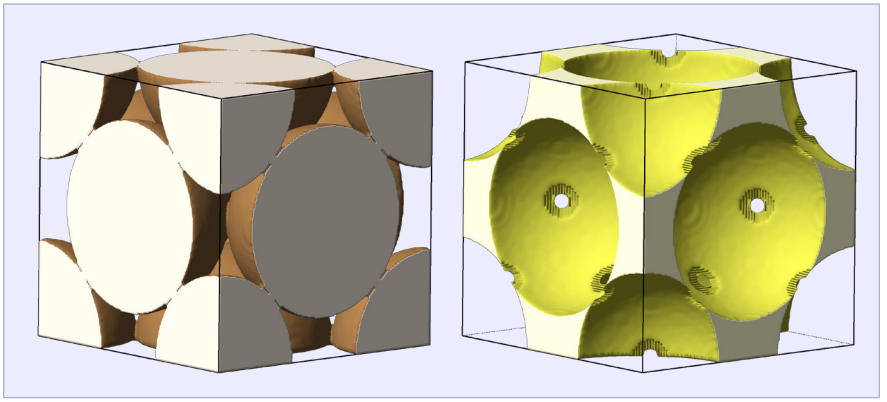
Please use conventional element symbols wherever possible; don't try to indicate disorder by using something like "Al/Si" as an element symbol. Instead, enter a meaningful site occupancy such as "Al0.5 Si0.5" for the site; this will then ensure that:

- Density is calculated correctly.
- Formulæ are shown.
- You can find your structure when you search by formula.

If you do need to use a dummy element symbol—e.g., for a centroid site—ensure that its site occupancy is set to zero. That way, it won't be included in any formula or density calculations.

## Porosity

CrystalMaker lets you calculate the porosity of any crystal structure as the percentage of free space. You can also visualize the free—or filled—space, as a porosity map: a volumetric dataset which can be plotted as a 3D surface. Porosity maps are useful for understanding diffusion pathways, and can be managed—together with other volumetric data—in the **Volumetric Data** group of the Model Inspector.



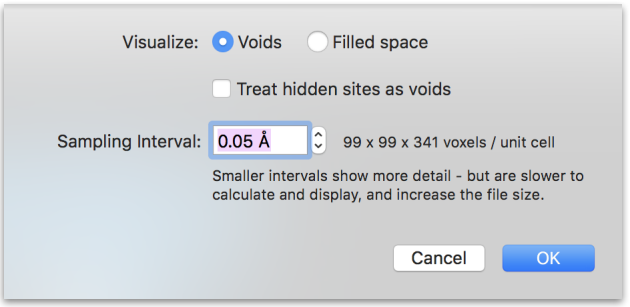
Porosity maps for one unit cell of copper. Left: filled space; right: void space.

### To calculate the porosity value:

- Choose: **Calculate > Porosity**. The amount of filled space and amount of void space are printed in the current window's Output Log.

### To visualize porosity in 3D:

1. Choose: **Calculate > Volumetric Data > Porosity Map**.
2. In the sheet/dialog that appears, use the radio buttons to specify whether you wish to visualize **Voids** or **Filled Space** (the latter is essentially a "Space Filling Surface"). You can also opt to treat any hidden atoms (within the current plot range) as voids.




The Porosity Map sheet.

3. Specify a sampling interval: this defines how many "voxels" (volumetric elements -

miniature unit-cell-shaped "building bricks") will be used for the calculation. The finer the sampling interval, the more voxels will be generated, and the greater the level of detail—but at the expense of memory (and time).

4 Click the **OK** button to continue.

### To change the way your porosity map is displayed:

1 Show the Model Inspector (e.g., **View > Inspector > Model**).

2 Select your porosity map in the **Volumetric Data** group.

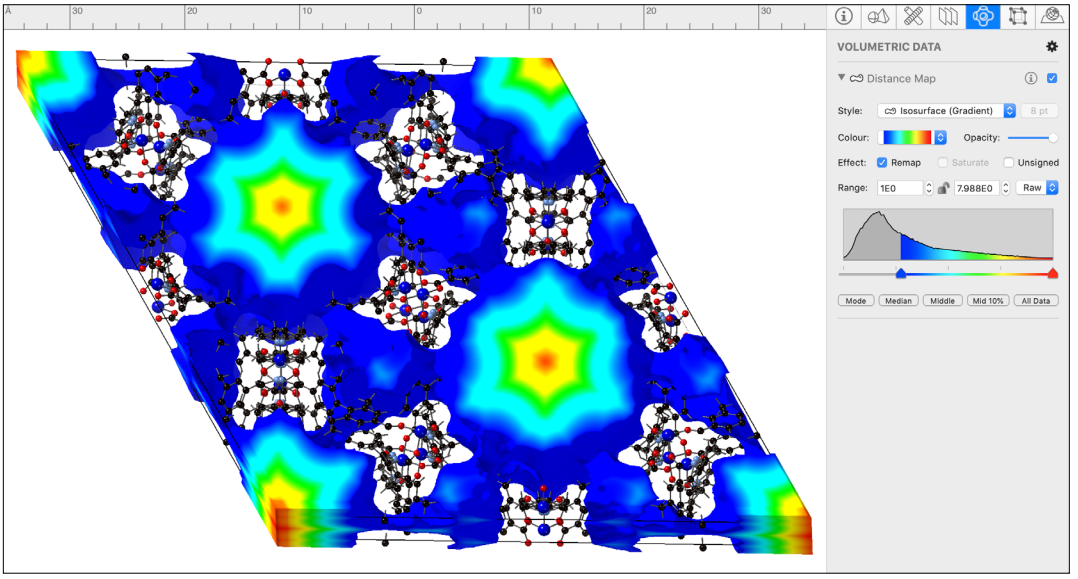
3 Use the **Type** popup in the list row to choose an appropriate display (hint: the **Isosurface** (Colour) option works well).

4 If required, set the opacity for your display.

**Beware File Sizes:** Volumetric datasets can easily become massive: with millions of points. Such large datasets can slow down program operations and increase file sizes—so please take care to ensure that the sampling interval is not too fine.

## Distance Maps

Distance maps are ideal for understanding the layout of cavities and channels within framework structures. Unlike a "Porosity" map (where "voxels" are either filled or unfilled), a distance map lets you visualize how close a point is from the surface of the nearest atom—and you can dynamically change the map by adjusting the Range slider in the Volume Inspector.



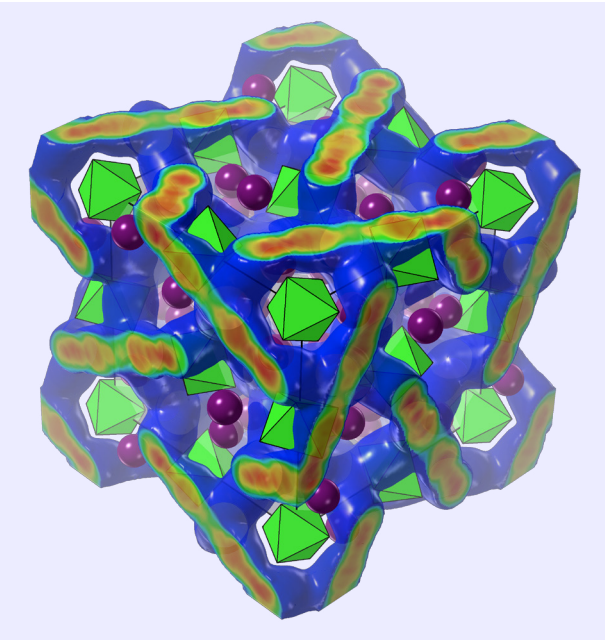

Editing a distance map for a MOF structure. The filled areas represent regions of the structure that lie more than 1 Å from the surface of the framework. These values are adjusted using the histogram interface in the Volume Inspector on the right.

When constructing a distance map, CrystalMaker calculates the distance from each volume element ("voxel") to the *surface* of the nearest atom. (You can specify whether to use the existing radii, or *Van-der-Waals* radii in this calculation.) You can then use the Range controls (text fields and slider) in the Volume Inspector to reveal possible diffusion pathways for atoms of a particular size or greater.

**Set Your Minimum Radius:** You can use the text fields in the Volume Inspector to precisely set the minimum and maximum sizes you are interested in. Note that you can switch between relative (percentage) or raw (absolute) values, using the popup menu to the right of the range fields. For a distance map, the raw values are in Ångstrøm units.

## Atom Density

The "Atom Density" map help you to visualize disordered atom distributions, e.g., resulting from diffusion and/or thermal motions. This is particularly useful if you have "collapsed" a large supercell, resulting in multiple atoms (each with fractional occupancy) becoming "wrapped" onto each other, with varying amounts of offset.



Lithium-ion density in a lanthanum zirconolate (data courtesy of Martin Dove, Queen Mary University of London).

CrystalMaker generates a porosity-style map, but instead of each volume element (or "voxel") being marked as "empty" or "filled", they have numeric values which depend on how many atoms lie at the corresponding point. In many ways, this representation is clearer than a space-filling model, as it lets you see the clustering of atoms, and focus on areas of greater atom density (especially when viewed as a "Point Cloud").

Note that atom density maps are really only suitable for structures with significant amounts of positional disorder; for an ordered structure, an atom density map will look like a space-filling model, or a porosity map with the "filled space" option set.

### To visualize atom density in 3D:

1. Choose: **Calculate > Volumetric Data > Atom Density Map**.
2. In the sheet/dialog that appears, choose whether to treat any hidden atoms (within the current plot range) as voids and specify a sampling interval.
3. Click the **OK** button to continue.

## Surface Maps

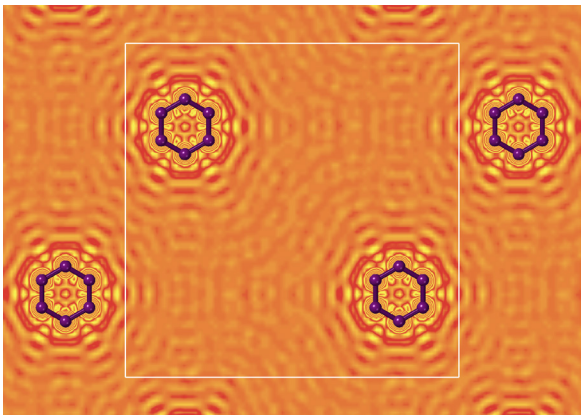
If you are interested in the *filled space* in your structure, you can visualize it as one of three kinds of "surface map":-

- Space-Filling Surface
- Van-der-Waals Surface
- Solvent-Excluded Surface

These surface types are described in more detail in *Chapter 7: Models*, in the context of the Surface Overlay. However, you can achieve greater flexibility (albeit only for crystals) by creating a "one-off" surface as a Volumetric Dataset. Because the surface does not change as you change atom visibilities, you can control which atoms should be inside the surface. You can also opt to make your surface *periodic* (compared to the "aperiodic" surface overlay), and you can use the Volume Inspector to change the way that the surface is displayed

## Electron Density

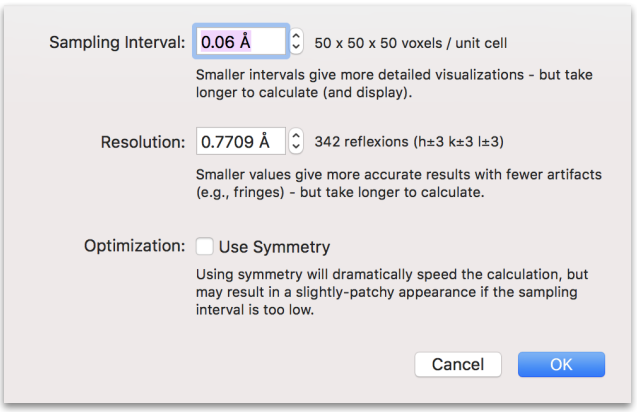
CrystalMaker can simulate electron density in your crystal using tabulated atomic scattering factors for all elements. This "atomistic" model assumes that atoms are spherical, with electron distributions summarized by the shape of the atomic scattering factor. Because crystal structure refinements follow a similar process—albeit in reverse (going from a computed electron density map to a final structure)—this makes for a useful comparison with the results of any external electron density calculations, e.g., from energy modelling programs.



Electron density contours, visualized for a molecular crystal. Here, the density has been projected onto a lattice plane and an orange gradient used to emphasize the contour levels.

### To visualize electron density in 3D:

1 Choose: **Calculate > Volumetric Data > Electron Density Map**. The Electron Density sheet appears.




The Electron Density sheet.

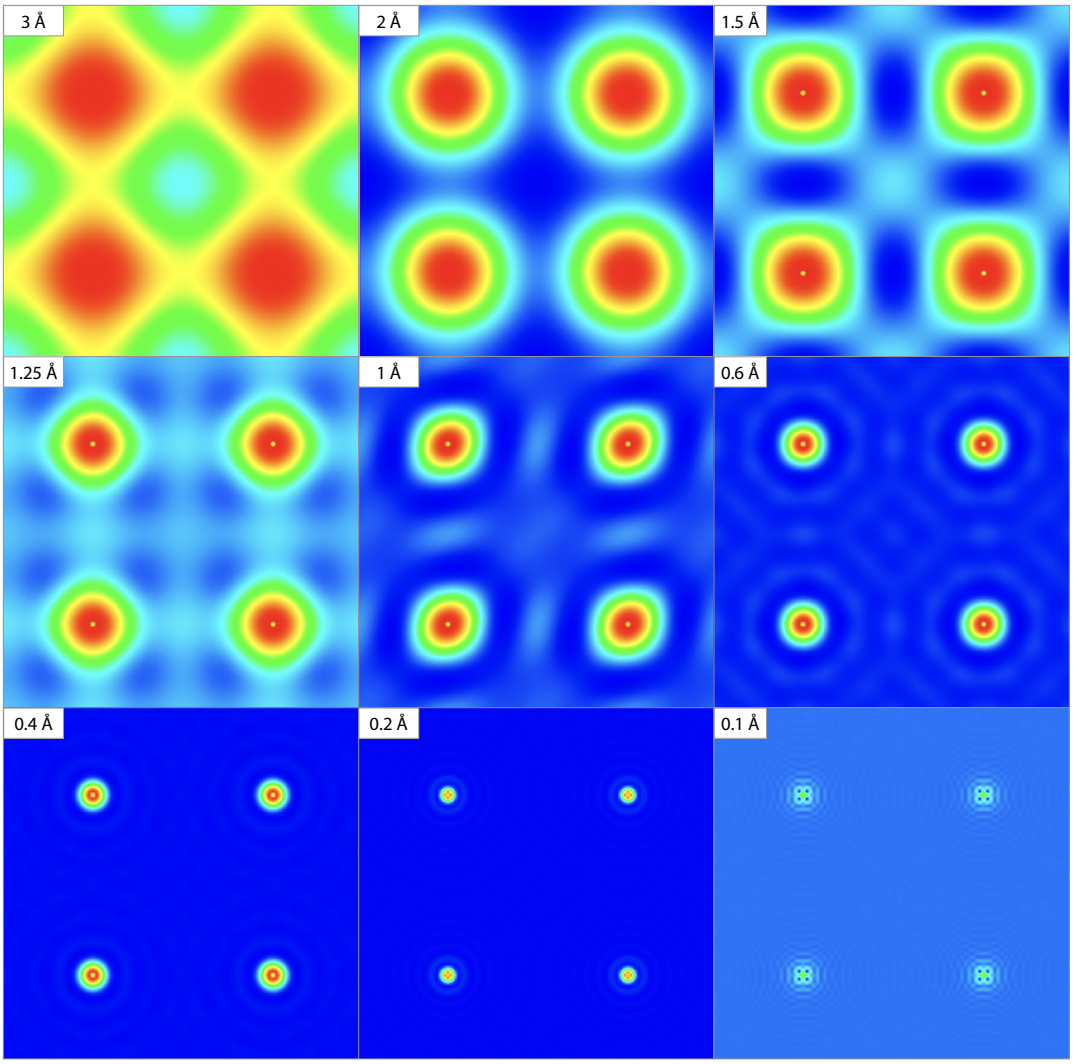
2 In the sheet/dialog that appears, specify a sampling interval: this defines how many "voxels" will be used for the calculation.

3 Specify the resolution to be used. This defines the minimum d-spacing to be used in the calculation. Lower values give more precise results, but take considerably

longer. Higher values can cause "ripples" to appear in the electron density map.

4. If your crystal has symmetry, you can speed up your calculation by specifying that symmetry should be used. This reduces the number of calculations required—but can cause a slightly uneven look if the sampling interval is too low. For final output, turn this option off.

5. Click the **OK** button to continue.




Electron density projections for a primitive cubic lattice (atoms 3 Å apart), showing the effect of increasing the resolution from 3 Å (separate atoms barely resolvable) down to a fraction of an Ångstrom. Note the prominent fringes which become weaker as the resolution increases to 0.2 Å. Note that at 0.1 Å we start to see moiré effects due to limited sampling ("aliasing"); these could be avoided by increasing the number of voxels used (i.e., reducing the sampling interval).

### To change the way your electron density map is displayed

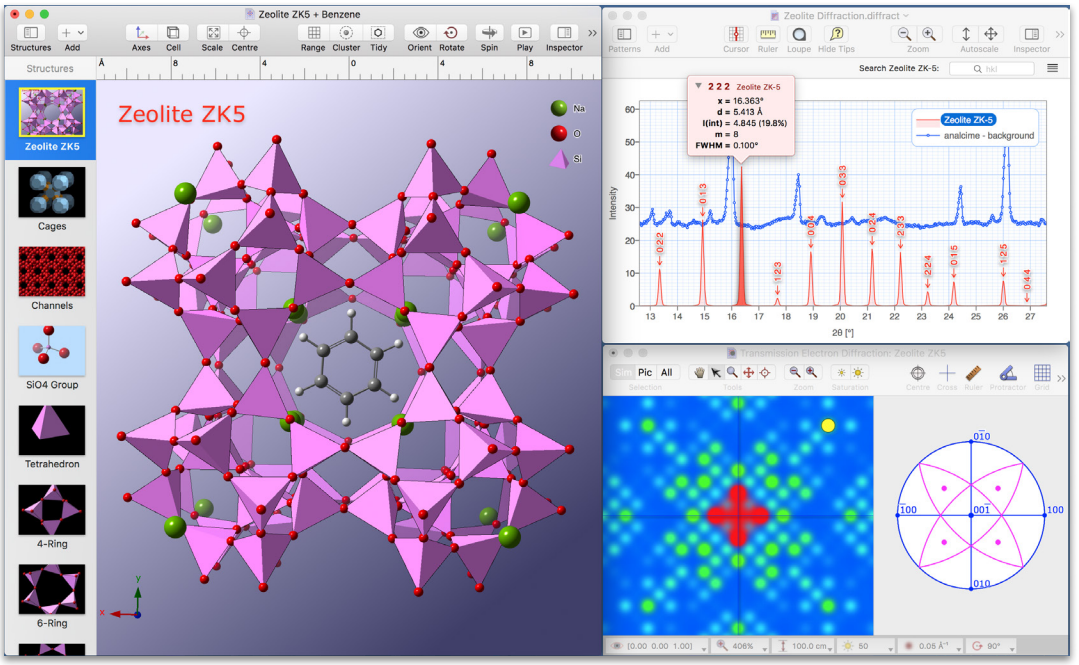
1. Show the Volume Inspector (e.g., **View** > **Inspector** > **Volume**).
2. Select your electron density map in the **Volumetric Data** group.
3. Use the **Type** popup in the list row to choose an appropriate display (hint: the **Lattice Plane Section** option works well).
4. If required, set the opacity for your display.

**Slicing Through Data:** If you have opted to project your electron density onto lattice planes, you can use the Lattice Planes group of the Volume Inspector to move any plane through the structure, so as to visualize the changing electron density. You can also add more planes, to get a better view of the variation in electron density.

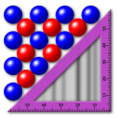
## Diffraction Patterns

If you have installed the companion programs CrystalDiffract® 6 or SingleCrystal™ 4, you will be able to use any displayed crystal to simulate its diffraction pattern.

**Modular Software.** We have made our software modular so you need only purchase the tools you require. This also allows us to design better products that are easier to use—instead of having one gargantuan "Jack of All Trades" program. Both CrystalDiffract and SingleCrystal operate in a free "Demo" mode until unlocked by a licence code (for which licence fees are charged).




The "CrystalMaker Office": CrystalMaker (left) works with CrystalDiffract (top right) and SingleCrystal (bottom right).



## CrystalDiffract®

CrystalDiffract is a program for simulating and measuring x-ray, neutron and electron powder diffraction patterns. You can visualize multiple patterns in the same window, combine them into simulated mixtures, and compare them with observed data: an ideal way of characterizing the results of synthesis experiments.

CrystalDiffract offers real-time control over sample and equipment parameters. You can vary cell parameters to see how peaks split with phase transitions, adjust site occupancies, particle size, strain, preferred orientation, peak width, profile type and even wavelength. It is designed to help you undertand the fundamental constraints on the diffraction process, letting you conduct "what if" experiments—from the comfort of your computer.

### To simulate a powder diffraction pattern directly from CrystalMaker:

Do one of the following:

- Choose: **Calculate > Powder Diffraction > New Pattern** to add a new powder pattern to an *existing* CrystalDiffract 6 window. If you want to show the pattern in a new CrystalDiffract window, please open a new window in CrystalDiffract *before* you execute this command.
- Choose: **Calculate > Powder Diffraction > Replace Pattern** to replace the uppermost diffraction pattern in the *frontmost* CrystalDiffract window. This is a good way of editing a structure and seeing the effect on its diffraction pattern.

## Live Powder Diffraction

The "Live Powder Diffraction" mode lets you relate changes in your crystal structure to its diffraction properties. CrystalMaker establishes a link between the current window and the *frontmost* window in CrystalDiffract. Thereafter, any changes you make to the *primary-selected structure* in CrystalMaker will trigger an update of the *frontmost* diffraction pattern in CrystalDiffract.

For example, you might want to see what happens when you move or rotate atoms in the unit cell; you will see the corresponding powder pattern update in real time. Alternatively, you might animate a sequence of structures through a phase transition and see how the powder peaks split.

### To start Live Powder Diffraction:

- Choose: **Calculate > Powder Diffraction > Enable Live Diffraction**.

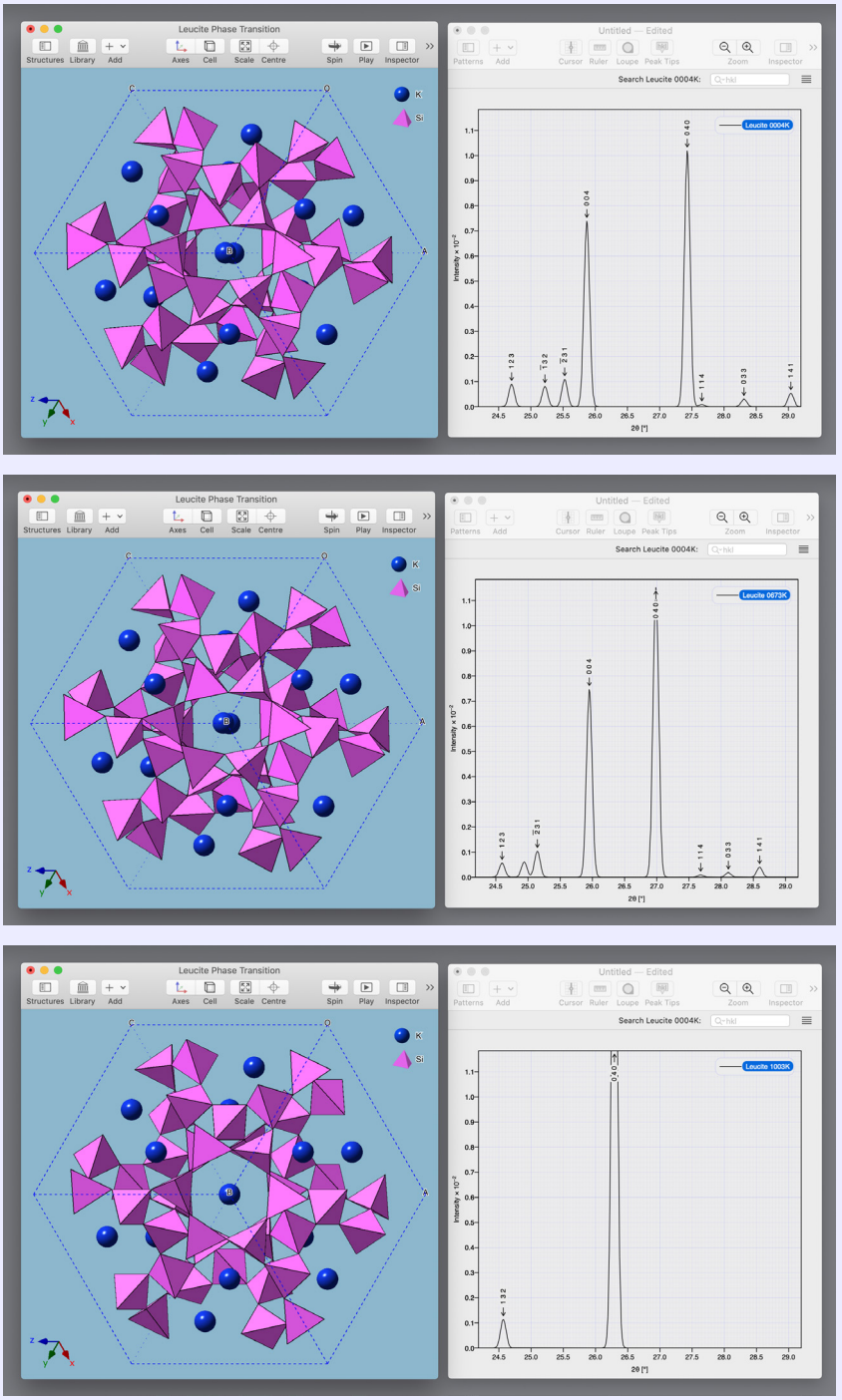
### To cancel Live Powder Diffraction:

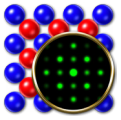
- Choose: **Calculate > Powder Diffraction > Disable Live Diffraction**.

**Update CrystalDiffract.** Please note that the new "Replace Pattern" command and the "Live Powder Diffraction" mode require CrystalDiffract 6.8 or later.

Live Powder Diffraction in progress. The CrystalMaker window (left) is animating a sequence of structures, so that the effect on the powder diffraction pattern (right) can be seen.

Here we have the crystal structures of the feldspathoid mineral, leucite, measured at 4K (top), 673K (middle) and 1003K (bottom). There is a tetragonal to cubic phase transition between the middle and last structure, associated with a convergence of sets of diffraction peaks.





## SingleCrystal™

SingleCrystal is an award-winning program for simulating and measuring x-ray, neutron and transmission electron microscope diffraction (TEM) patterns from single crystals. It features a range of experimental geometries, including the Precession technique, Laue front, back and cylinder geometries, and TEM, as well as reciprocal lattice display.

SingleCrystal provides high-resolution simulated diffraction patterns, with the option of overlaying these above images of observed patterns, for characterization. TEM users will appreciate our unique Grid tool, which allows easy auto-indexing of diffraction patterns. SingleCrystal also offers stereographic projections of planes, vectors and their traces.

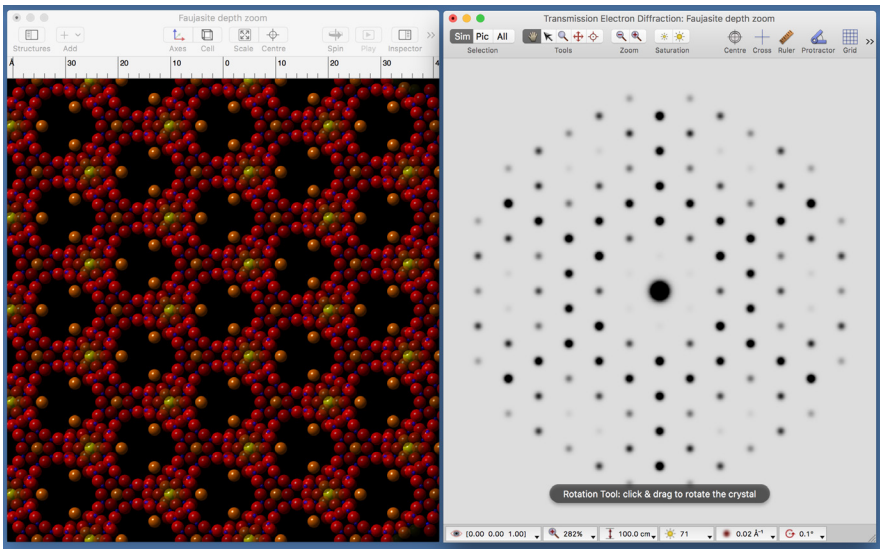
As with CrystalDiffract 6, SingleCrystal 4 can read from CrystalMaker X files. However, it is more convenient to share structural information directly from CrystalMaker, thereby taking advantage of "Live Rotation" mode.

### To simulate a single-crystal diffraction pattern directly from CrystalMaker:

- Choose: **Calculate > Single-Crystal Diffraction > New Pattern** to display a single-crystal diffraction pattern (e.g., TEM or X-ray Laue) in a new window in SingleCrystal 4 (if installed).

## Live Rotation

CrystalMaker gives you the option of linking a structure with its simulated single-crystal diffraction pattern, so that rotating one causes the other to rotate; we call this "Live Rotation".




Live Rotation Mode: linking CrystalMaker (left) with the corresponding diffraction pattern in SingleCrystal (right).

For example, you might rotate a crystal structure in CrystalMaker, and observe the corresponding diffraction pattern rotating in SingleCrystal. Alternatively, you could switch to SingleCrystal, rotate the diffraction pattern (or the stereographic projection), then observe the corresponding structure rotating in CrystalMaker.

Live Rotation requires that you have the original structure open in CrystalMaker, and have established a link with SingleCrystal, as summarized below:

#### To rotate a structure and pattern simultaneously:

1. Ensure that **Live Rotation** is enabled (**Calculate > Single-Crystal Diffraction > Enable Live Rotation**).
2. Choose **Calculate > Single-Crystal Diffraction > New Pattern** to simulate a diffraction pattern for your structure.
3. You can now rotate the crystal structure in CrystalMaker and see the diffraction pattern rotate in SingleCrystal (and vice versa).

#### Live Rotation with a Saved Diffraction Pattern

So far we have discussed simulating a *new* diffraction pattern, directly from a CrystalMaker structure, and creating a link via Live Rotation mode. However, suppose you *already* have a diffraction pattern, created in an earlier session, which has been saved as a SingleCrystal "session file". How does one get Live Rotation to work for this pre-existing pattern? The answer is to open the two files (the session file, in SingleCrystal; and the crystal structure, in CrystalMaker), and then link them using CrystalMaker's **Calculate > Single-Crystal Diffraction > Enable Live Rotation** command.

#### To cancel Live Rotation

- Choose: **Calculate > Single-Crystal Diffraction > Disable Live Rotation**.

### Live Intensity Mode

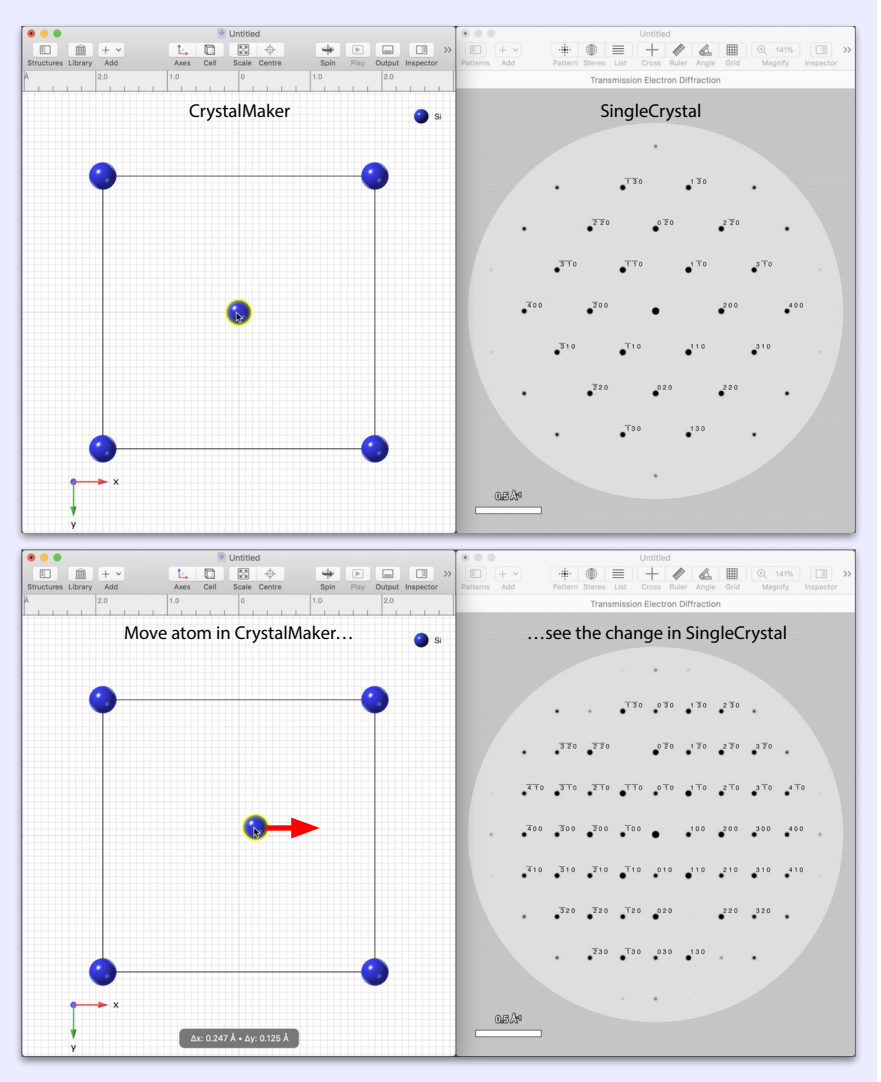
SingleCrystal's equivalent of CrystalDiffract's "Live Diffraction Mode" is called "Live Intensity Mode" . With this mode in effect, editing the crystal structure in CrystalMaker—including interactive atom movement/rotation—immediately causes the corresponding single-crystal diffraction pattern to be updated, in SingleCrystal.

#### To start Live Intensity Mode:

- Choose: **Calculate > Single-Crystal Diffraction > Enable Live Intensities**.

#### To cancel Live Powder Diffraction:

- Choose: **Calculate > Single-Crystal Diffraction > Disable Live Intensities**.




Live Intensity Mode in action. Simulating diffraction from a body-centred lattice (top); moving the central atom causes previously-hidden reflexions to appear (bottom).

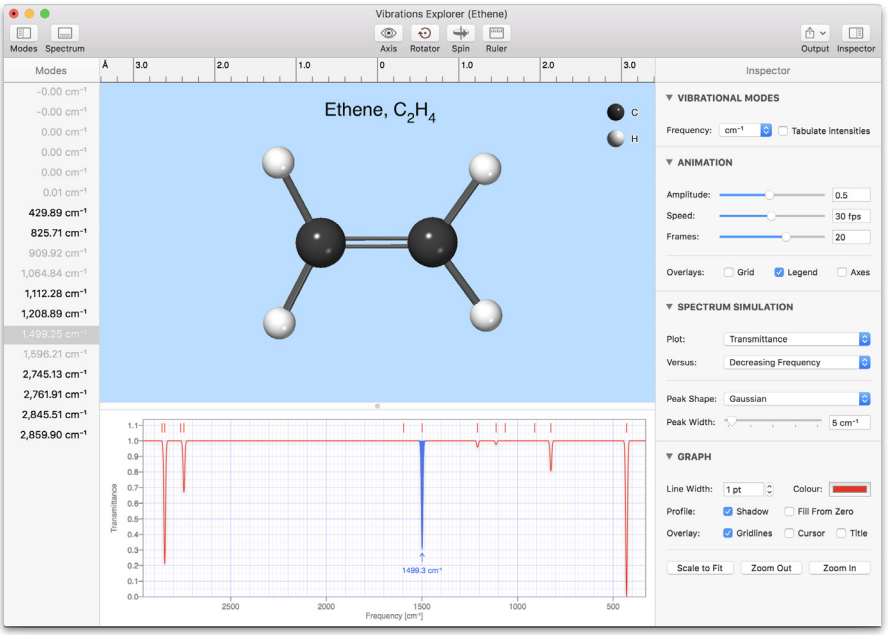
## Vibrational Spectra

The Vibrations Explorer displays all possible vibrational modes for a molecule, their calculated frequencies (in your choice of units), and their infra-red intensities—as a simulated IR spectrum. The spectrum can be customized to show transmittance or absorbance, with an increasing or decreasing *x*-axis. The peak shape and width can be adjusted, together with other display parameters.

> **Missing Peaks?** Note that whilst all possible vibrational modes—including the six zero-frequency translational modes—are included in the Modes list, some of these may be Raman-active modes which won't appear in an infra red spectrum.

You can also visualize individual vibrational modes, as rotatable animations. These can be exported as videos for use in teaching or research.

Visualizing the vibrational behaviour of ethene.




### To show the Vibrations Explorer:

1. Open a molecular structure in CrystalMaker.
2. Ensure the structure is fully-relaxed (use the **Relax** command if necessary).
3. Click the toolbar **Vibrations** button or choose: **Calculate > Vibrational Frequences**.

### To choose a vibrational mode:

Do one of the following:

- Select a mode frequency from the **Modes** list.
- Double-click a peak in the Infra Red spectrum.

### To rotate the animation:

Do one of the following:

- Click-and-drag the animating molecule with the mouse or trackpad.
- Click the toolbar's **Rotator** button and use the Rotator panel to adjust the molecule's orientation.

### To edit the animation:

1. Locate the Inspector on the right-hand side of the window (if this is not visible, click the **Inspector** button in the window's toolbar).
2. Locate the **Animation** group, then use the slider controls to adjust the amplitude, speed (frames-per-second) and quality (number of frames per animation cycle).

### To save an animation:

- Click the **Output** button and choose: **Vibrations Movie**.

### To save the infra red spectrum:

Do one of the following:

- Drag-and-drop the infra red spectrum into a graphics program.
- Click the **Output** button and choose: **Spectrum Image**.

### To save a list of vibrations in a text file:

- Click the **Output** button and choose: **Vibrations List**.

#### Vibrational Spectra: Tips and Caveats

The IR spectrum shown in the Vibrations Explorer is not designed to be an exact facsimile of an experimental spectrum. Instead, it shows calculated vibrational frequencies, based on the atomic positions and bonding in the molecule, and the potentials used in CrystalMaker's modelling calculations.

For such modelling calculations, a general rule of thumb is that calculated frequencies should be within approximately 10% of the true result. If your frequencies don't look right, try relaxing the structure first.

A good test of a correctly-relaxed molecule is the absence of any negative-frequency modes; you should see six (approximately-)zero-frequency modes, with a total of $3n$ modes in total, where $n$ is the number of atoms in the molecule.

Chapter 13

# Graphics & Video

This chapter describes ways in which you can extract graphics—via the clipboard; to a file on disc; and direct to print—and how to specify the size, resolution and format of this output. The chapter also covers creating a self-contained 3D model, which can be shared with dedicated 3D graphics programs, viewed in iBooks on your Mac or iPad, or printed on a 3D printer.

## Graphic Formats

CrystalMaker X provides pixel- or vector-based graphics.

- Pixel Graphics ("bitmaps") comprise hundreds or thousands of individual pixels—just like the screen image. Pixel images have the highest-quality with photo-realism; however they are not scaleable. Pixel images can be saved in a wide variety of formats, including JPEG, TIFF, PNG and BMP.
- Vector Graphics contains hundreds if not thousands of individual triangles, rather than pixels. They can be scaled using vector drawing packages such as *Adobe Illustrator,* but do not provide fine-scale photo-realism, are incredibly slow to generate and produce massive output files.

Whilst some users may instinctively feel that vector graphics provides the best quality, the reality is that high-resolution pixel graphics offers superior output—better photo realism—with smaller file sizes. One must also appreciate that the massive size of vector graphics files generated by photo-realistic programs such as CrystalMaker X means that whilst the graphics can be scaled, they are not readily amenable to editing—and will likely overload any graphics program.

### Graphics with Transparent Backgrounds

CrystalMaker exports graphics using your chosen background. This could be a solid colour, a gradient, or a background picture. If you prefer not to have a background, choose a PNG or TIFF format and specify a transparent background.

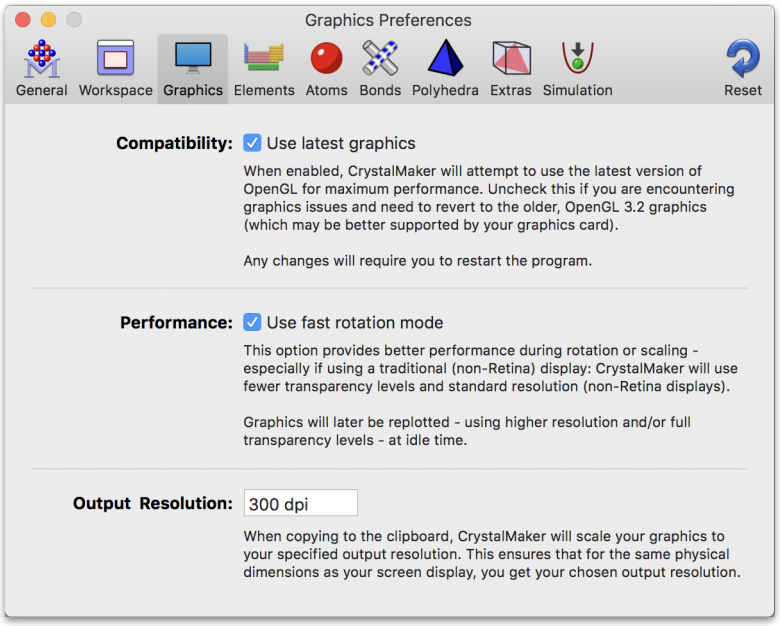
## Exporting an Image

You can copy graphics to other programs via the clipboard, or a graphics file. You have control over the output size and resolution, as well as its format. Note that the *aspect ratio* of the output (i.e., the ratio of the horizontal to vertical dimensions) will be the same as your on-screen image. You may wish to resize the Graphics window before you copy or export a graphic, to ensure that your structure fits snugly.

### Output Resolution

You can specify the nominal *resolution* of your graphics output using the **Graphics** pane of the Preferences panel. The default output resolution is 300 dpi, but please note that this is only a nominal resolution: most graphics programs will allow you to resize graphics and will adjust the resolution accordingly (e.g., 100 pixels at 300 dpi is twice the width of 100 pixels at 600 dpi).

The Graphics pane of the Preferences panel.




### Copying Graphics to the Clipboard

If the Graphics Pane is focused (i.e., you have clicked there recently) you can copy its image to the clipboard using the **Edit > Copy** command. CrystalMaker generates an output image at the same physical size as your on-screen image, but at the (generally) higher resolution specified in your preferences.

- *For example, if your Graphics Pane is 720 pixels wide on a 72 dpi screen, it occupies 10 inches of screen space; exporting this at 144 dpi would result in a 10-inch wide graphic with 1440 pixels.*

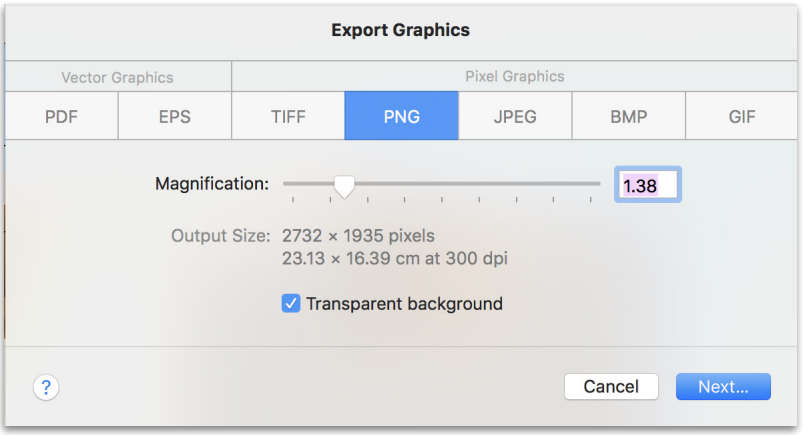
## Exporting a Graphics File

You can export your graphics to a wide choice of graphics file formats, including JPEG, TIFF, BMP and PNG.

CrystalMaker saves JPEG graphics using a high-quality compression scheme; these files can be read by other computer platforms and are ideal for distributing high quality graphics over the internet.

### To save pixel graphics in a file:

1 Choose **File > Export Graphics > 2D Graphics**. The Export Graphics sheet appears:




The Export Graphics sheet showing export to a PNG file with transparent background.

2 Choose a graphics format by clicking on its button.

3 For Pixel Graphics, use the **Magnification** slider or text field to adjust the output size. Note that CrystalMaker provides a default output size which is designed to match the physical dimensions of the Graphics Pane, albeit with your default output resolution.

4 If using TIFF or PNG formats, you can optionally specify a **Transparent Background**.

5 Click the **Next** button to continue.

6 Use the file navigation dialog to specify a filename, a location, and a file format, then click the **Save** button.

**Use Pixel Graphics Not Vector Graphics.** We strongly recommend that you stick to Pixel Graphics for your image export. This may come as a surprise to traditionalists, but simply put, Pixel Graphics are better: they allow much better rendering of photo-realistic detail than clunky polygon-based Vector Graphics. Furthermore, the memory requirements are much lower (even with very-high-resolution images). Chances are, your Vector Graphics will result in such massive files that few, if any, third-party programs will be able to read them.

### Exporting other Graphics

You can also export an image of the simulated infra-red spectrum from the Vibrations Explorer. This can be done in one of three ways:

- Drag-and-drop the spectrum into another graphics program (Mac);
- Right-click the spectrum and choose the **Copy** or **Export** commands.
- Click the toolbar **Output** button and choose: **Spectrum Image**.

## Exporting a 3D Model

CrystalMaker lets you create a 3D "print" of your structure, via an STL file. You can also save a self-contained three-dimensional COLLADA model, which can be opened in other programs or embedded in "iBooks" for macOS or iOS.

### COLLADA 3D Files

COLLADA (collaborative design activity) is a file format for sharing three-dimensional models. It is an open-standard XML-based format, with file extension "`.dae`"(digital asset exchange). The format is managed by a non-profit consortium, the Khronos Group, and has been adopted by ISO as a publicly-available specification, ISO/PAS 17506.

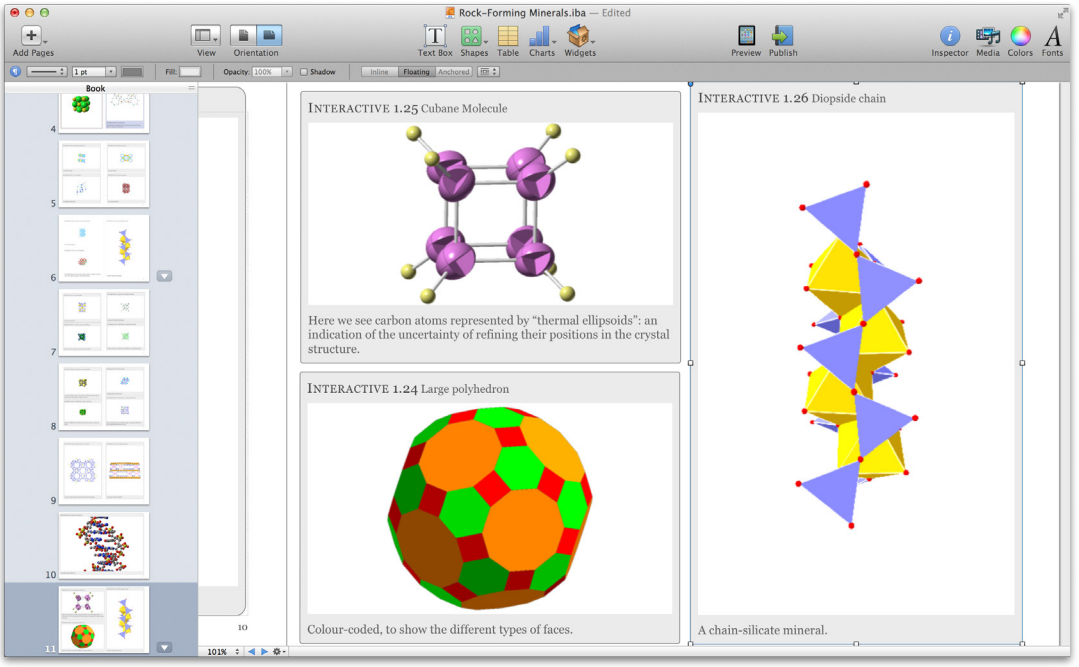
#### To export a COLLADA file:

1. Choose: **File** > **Export** > **COLLADA 3D File**.
2. Use the file navigation dialog to your output filename and location.

#### To view a COLLADA file on your iPad or iPhone:

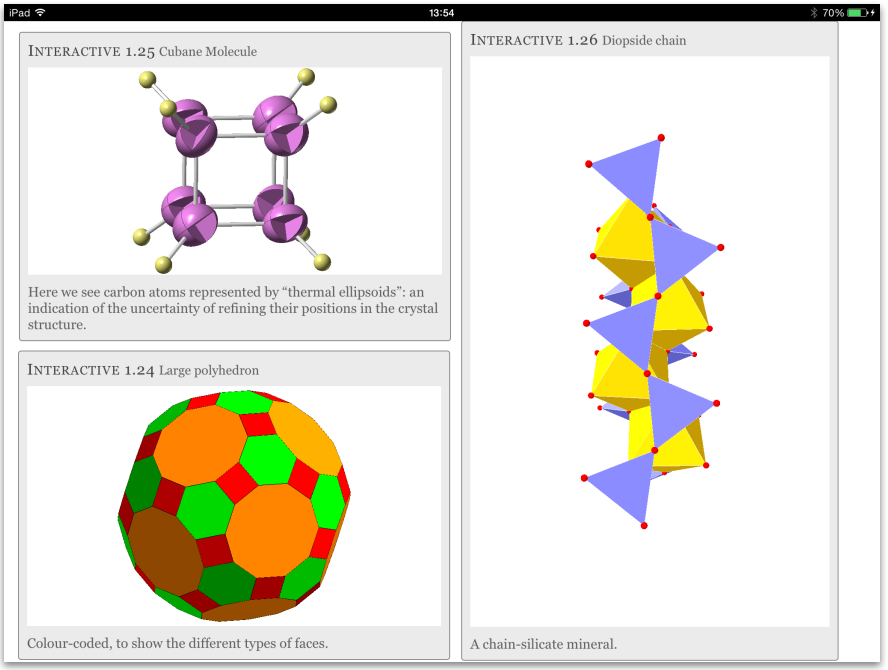
1. Open a new, or existing, *iBooks* project using *iBooks Author* (a free download from the Apple *App Store*).
2. Drag your CrystalMaker COLLADA file into the project.
3. Connect your iPad or iPhone to your Mac.
4. Launch *iBooks* on your iPad or iPhone.
5. Click the **Preview** button in the *iBooks* toolbar on your Mac. Your iBook is copied to the iPad and will open at the current page.

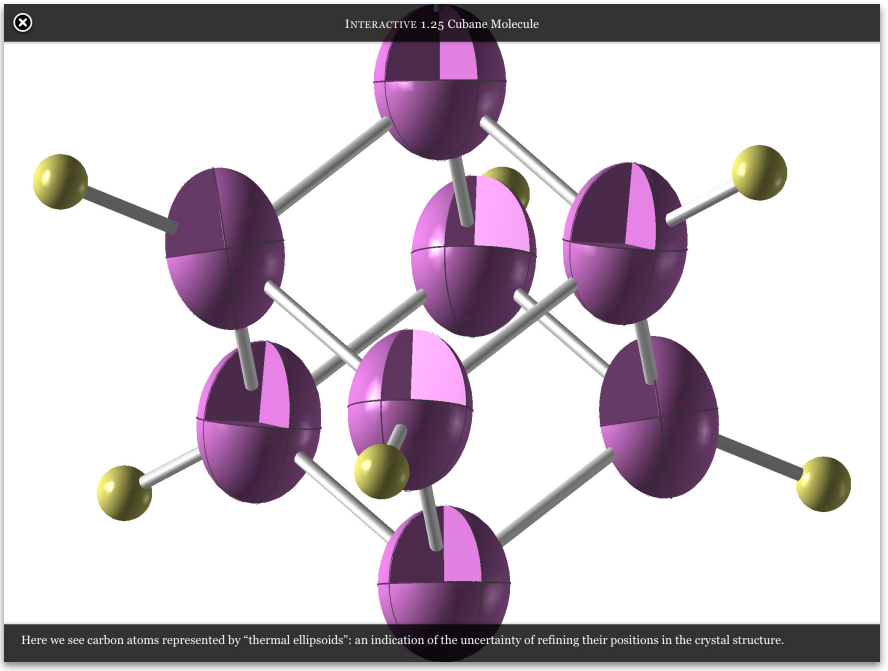
   Mac users can manipulate COLLADA files directly, using the Preview application. Windows users may need to download a third-party application (e.g., the free *Blender* program).




CrystalMaker-generated COLLADA models in iBooks Author

The resulting iBook page, as viewed on an iPad. These images are fully-rotatable 3D models which can be zoomed by touching them, and rotated by sliding a finger across the screen.






A CrystalMaker-generated COLLADA 3D model shown zoomed to full-screen on an iPad. Touching the centre of the screen hides the black information bars, and the image can be freely rotated by sliding a finger horizontally or vertically across the screen.

### STL Files for 3D Printing

CrystalMaker lets you output your structure as a binary STL file, suitable for most 3D printers. However, the format does not currently include colour or rendering information, so is not really suitable for standalone 3D models.

#### To export an STL file:

1. Choose: **File > Export Graphics > STL 3D File**.
2. Use the file navigation dialog to your output filename and location.

### Other 3D Formats

COLLADA is designed as an inter-change format, which means that it is widely supported by 3D modelling programs (e.g., the free "*Blender*" application) and can readily be converted to third-party formats including ray-tracing programs and 3D printer formats.

## Printing

Printing from CrystalMaker X is straightforward and uses the standard Mac or Windows print dialog. The resolution used for printing is the same default **Output Resolution** setting used for copying or exporting graphics, which you can edit in the **Graphics** pane of the Preferences panel.

# Video Export

CrystalMaker lets you save three kinds of video:

- Rotation (for any displayed structure)
- Animation (for a multi-structure document)
- Vibration (for a selected vibrational mode in the Vibrations Explorer)

## Video Options

CrystalMaker X works different on Mac and Windows versions. Mac users get the best-quality "H.264" video codec (the *de facto* standard), saved as QuickTime video—with a slider control to lower the quality, if you need smaller output.

Unfortuntely, video on Windows is not as well integrated as on the Mac, and this codec is not included in Microsoft's AVI for Windows. This means that Windows users will need to do a little preparation, as described below.

### Setting up Video for Windows

Whilst the Mac version can take advantage of built-in support for the highest-quality (H.264) video codecs, this is not possible on Windows. Instead, CrystalMaker for Windows lets you choose from one of a number of available codecs. These include the special **MotionJpegVideoEncoderWPF**, which offers Motion JPEG encoding.

You may wish to download an H.264 codec, which offers better performance and compression—and should match the Mac version for overall quality. This **x264vfw** codec is available from the following website:-

`https://sourceforge.net/projects/x264vfw/`

*Please note that this is a third-party website and we are unable to take any responsibility for the content or the results of any resources downloaded from this site.*

Once you have downloaded and installed the x264vfw codec you should be able to select it, by name, from CrystalMaker's Video Codecs dialog.

### Setting the Frame Size

By default, video is recorded using the same dimensions as your Graphics Pane. However, you can specify a scale when you export the video, so that a smaller video frame can be used (e.g., you might want to have your output 50% of the screen size).

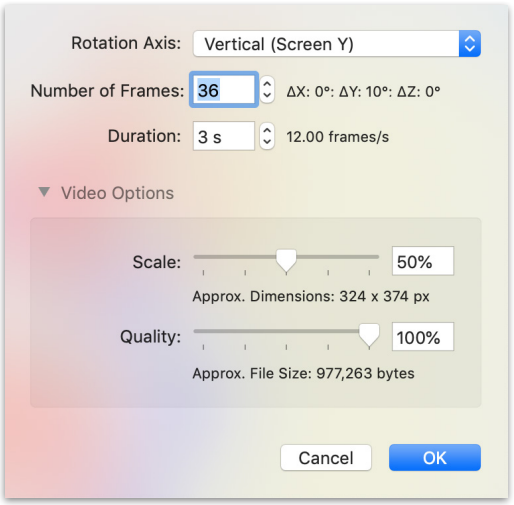
## Rotation Movies

If you are giving a presentation and wish to illustrate a particular structure, why limit yourself to a static—and two-dimensional—image? A much better option would be to embed a rotating "model" of your structure in your *Powerpoint* or *Keynote* presentation…

The easiest way of doing this is to let CrystalMaker generate a "Rotation Movie" for you: saving a series of images—each corresponding to a view at a different angle—in a self-contained video file. You simply need to specify a rotation axis, the number of frames required, and how long you want the rotation to last.

### To save a video of a rotating structure:

1 Choose: **File > Export Video > Rotation Movie**. The Rotation Movie sheet appears.




The Rotation Movie sheet, showing video scale and quality options (Mac).

2 Specify the rotation axis: vertical, horizontal—or whichever rotation axis was last used by the **Spin** command.

3 Specify how many frames should be saved, and how long the movie should last.

4 If you want to customize the output size and/or quality level, click the **Video Options** disclosure control to reveal its controls: a **Scale** slider and text control and (for Mac users) a **Quality** slider and text control. An *approximate* file size will be computed.

5 Click **OK** to continue. CrystalMaker will now generate the requisite frames, and save them in a movie.

## Animation Movies

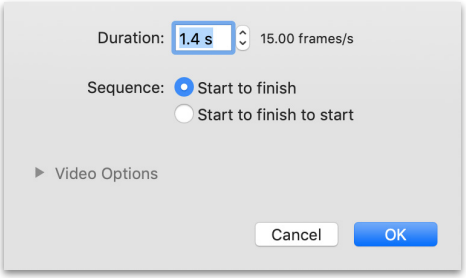
If you are working with a sequence of structures you can *synchronize* them and animate them within CrystalMaker. You can export the result as an "Animation Movie", which provides a self-contained animation outside the program.

### To record an animation as a video:

1. Start by ensuring that you have either synchronized your sequence (if all structures are related), or at the very least, specified the same scale.

   (A good way of doing the latter is to explicitly set a scale for one structure using the **Transform > Scale & Centre > Set Scale** command and ensure that the **Apply to all structures** checkbox is set.)

2. Choose: **File > Export Video > Animation Movie**. The Animation Movie sheet appears:




The Animation Movie sheet. The video output options are hidden here.

3. Specify the movie duration or the frame rate (the two are connected, as the number of frames is fixed: this is the number of structure views in your Structures List).

4. Specify a **Sequence** option, either **unidirectional** (from start-to-finish), or **bidirectional** (from start-to-finish and back to start).

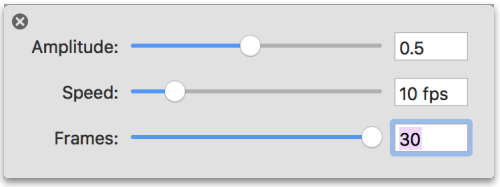
   *(The "bidirectional" option is intended for use with programs that have a "loop" command, but lack a "loop back-and-forth" option.)*

5. If you want to customize the output size and/or quality level, click the **Video Options** disclosure control to reveal its controls: a **Scale** slider and text control and (for Mac users) a **Quality** slider and text control. An *approximate* file size will be computed.

6. Click **OK** to continue. CrystalMaker will now generate the requisite frames, and save them in a movie.

## Vibration Movies

The Vibrations Explorer window animates any selected vibrational mode. You can control the orientation of the molecule being animated and also the quality of the animation: its speed and the number of frames (steps). These settings—available via the Animation popover in the window's titlebar—are automatically applied to any video you generate in this window.




The Animation popover in the Vibrations Explorer.

### To export an vibrational animation as a movie:

1. Click the **Output** button in the window toolbar to display a popup menu.
2. Choose: **Vibration Movie** and specify a filename and location in the navigation dialog that appears.

Chapter 14

# Data Import/Export

CrystalMaker can read structural and volumetric data from a very-wide range of data files. In most cases, the program can auto-detect the file format. This means you can simply drag-and-drop one data files into the program for instant display with bonds and polyhedra automatically generated for you. This chapter summarizes the formats that are supported, and also includes some notes about the various (non-structural) data output options.

## Input/Output Options

You can import and export data using a wide range of file formats. Files can generally be opened using **File > Open** command, or by dragging-and-dropping their icons onto the CrystalMaker application icon.

CrystalMaker relies on the file extension in order to determine what type of file is being used. In the following table we summarize the file formats supported, and their recognised file extensions.

In some cases, different formats claim the same file extension (e.g, STRUPLO, ATOMS, TOPAS all claim ".str"—which, in hindsight, seems a rather poor choice of file extension). In these cases, CrystalMaker has to "sniff" the file, opening it up and performing diagnostic tests, in order to decide which format must be used.

If, for some reason, you are unable to open a file, you can force CrystalMaker to treat the file as being in a specific format, by using the **File > Open File With Format** submenu.

### Structural Data File Formats

CrystalMaker X can load crystal or molecular data from the file formats listed below. Note that many of these are multi-structure formats, and some include volumetric data.

| | File Format | Required Filename/Extension | Import | Export |
|---|---|---|---|---|
| 1. | ATOMS | *.str, *.atoms | ✓ | |
| 2. | CASTEP Cell | *.cell | ✓ | ✓ |
| 3. | CASTEP Output | *.castep | ✓ | |
| 4. | CASTEP Volumetric | *.chdiff_fmt, *.den_fmt, *.elf_fmt | ✓ | |
| 5. | CCL | *.ccl | ✓ | |
| 6. | Chem3D Cartesian | *.chem3d | ✓ | ✓ |
| 7. | CIF | *.cif | ✓ | ✓ |
| 8. | CrystalMaker X Document | *.cmdx | ✓ | ✓ |
| 9. | CrystalMaker 7–9 Crystal | *.cmdf | ✓ | |
| 10. | CrystalMaker 7–9 Molecule | *.cmmf | ✓ | |
| 11. | CrystalMaker Text | *.cmtx | ✓ | ✓ |
| 12. | CSSR | *.cssr, *.xr | ✓ | |
| 13. | Gaussian CUBE | *.cube | ✓ | |
| 14. | DL_POLY Config | *.dlpoly, CONFIG | ✓ | ✓ |
| 15. | DL_POLY Revcon | *.dlpoly, REVCON | ✓ | |
| 16. | DL_POLY History | *.dlpoly, HISTORY | ✓ | |
| 17. | DMol3 “CAR” file | *.dmol, *.car | ✓ | ✓ |
| 18. | DMol3 “ARC” trajectory file | *.dmol, *.arc | ✓ | |
| 19. | FDAT (CCSD) | *.fdat | ✓ | |
| 20. | GROMACS | *.gromacs, *.gro | ✓ | |
| 21. | GSAS | *.gsas, *.exp | ✓ | |
| 22. | GULP | *.gulp, *.out, *.got | ✓ | |
| 23. | ICSD | *.icsd | ✓ | |
| 24. | LAMMPS dump | *.lammps, *.dump | ✓ | |
| 25. | Molfile | *.mol | ✓ | |
| 26. | PDB | *.pdb | ✓ | ✓ |
| 27. | RMCProfile | *.rmc6f | ✓ | ✓ |
| 28. | SDfile | *.sdf | ✓ | |
| 29. | SHELX | *.shelx, *.shlx, *.res | ✓ | |
| 30. | STRUPLO | *.struplo, *.str | ✓ | |
| 31. | SYSTRE | *.systre, *.cgd | ✓ | |
| 32. | TOPAS | *.topas, *.str | ✓ | |
| 33. | VASP Volumetric | *.elk, *.chg, *.chgar | ✓ | |
| 34. | VASP Structure | *.vasp, *.contcar, *.poscar | ✓ | ✓ |
| 35. | VASP Trajectory | *.vasp, *.xdatcar | ✓ | |
| 36. | VESTA | *.vesta | ✓ | |
| 37. | WIEN2k Structure | *.wien2k, *.w2k, *.struct | ✓ | |
| 38. | XCrysDen Structure | *.xsf | ✓ | |
| 39. | XCrySDen Animation | *.axsf | ✓ | |
| 40. | XYZ | *.xyz | ✓ | ✓ |

## Automatic Bond Generation

CrystalMaker is set to automatically generate bonds when it reads in a non-native text file. This option can be turned off using the **Automatically Generate Bonds** checkbox in the **General** pane of the Preferences panel.

## Unique Site Labels

Some file formats used in modelling (e.g., CASTEP, DL_POLY, GULP) may not specify unique site labels, instead presenting an element symbol for each site. Rather than end up with thousands of unlabelled sites, CrystalMaker will generate unique site labels by appending the atom number. However, if custom site labels have been entered for these formats (i.e., not merely an element symbol) these will be respected.

## Other Data Files

In addition to these structure file formats, CrystalMaker can handle a variety of other data formats:

| | File Format | Description | Import | Export |
|---|---|---|---|---|
| 1. | Elements | Element radii and colours | ✓ | ✓ |
| 2. | Voxel | Volumetric data tiled along xyz | ✓ | ✓ |
| 3. | DENS | Volumetric data with symmetry information | ✓ | |
| 4. | GRD | Volumetric data tiled along xyz | ✓ | ✓ |
| 5. | 3ED | "Aperiodic" volumetric data (xyz range 0–1) | ✓ | |
| 6. | Coordinates | Coordinates for all visible atoms | | ✓ |
| 7. | Visible Coordination | Coordination data for visible atoms | | ✓ |
| 8. | Crystal Coordination | Coordination data for one unit cell | | ✓ |
| 9. | HTML Structure | Table of structural data, suitable for the web | | ✓ |
| 10. | Distances & Angles | Coordinates, distances & angles for each site | | ✓ |
| 11. | Vibrations List | Vibrational modes, frequencies & eigenvectors | | ✓ |

## 3ED

This is an "aperiodic" 3D volumetric data format that can be opened by CrystalMaker (if files have the requisite ".3ed" file extension) or loaded into an existing structure's Volumetric Data list.

These files contain no atoms, merely lists of data values corresponding to points within a structure. If opening such a file directly, CrystalMaker will generate a dummy structure (a primitive lattice with hidden atoms at the corners of the unit cell) and display the volumetric data.

Please note that the data format used is *identical* to the GRD format—with one important difference. "3ED" files are described as being "aperiodic", because they contain more data points than are required to *tile* the data into a periodic lattice. The data points extend into the next unit cell along each of the $x$, $y$ and $z$ axes, i.e., there are data points in the range $0 \leq xyz \leq 1$. By contrast, the GRD (and similar "Voxel" file) formats have data points in the range $0 \leq xyz < 1$.

For example, a "periodic" GRD file might save data values at $x = 0, 0.2, 0.4, 0.6, 0.8$. The corresponding 3ED file would have the same data values plus an additional point at $x = 1.0$.

When importing a 3ED file, CrystalMaker skips the (superfluous) data points in the second unit cell and generates periodic data.

The "3ED" format consists of:

- Title line.
- Unit cell parameters: $a$, $b$, $c$, $\alpha$, $\beta$, $\gamma$ (distances in Å; angles in degrees).
- Header line with three integers: $Nx$, $Ny$ and $Nz$. These are the numbers of data points along the unit cell's $x$, $y$ and $z$-edges, respectively—for the range 0 to 1.
- A series of floating-point numbers corresponding to the $Nx \,.\, Ny \,.\, Nz$ points.

The data points can be arranged on multiple lines if required, as long as they are arranged in the correct order: scanned along $z$, then along $y$, and finally along $x$ (i.e., $\Delta z > \Delta y > \Delta x$).

Part of a 3ED file (long lines have been truncated).

```
Electron Density data
10.0 10.0 10.0 90.0 90.0 90.0
104    104    233
 8.798907e+01     8.725596e+01     0.000000e+00     8.508385e+01   ...
 3.303827e+01     3.775127e+01     0.000000e+00     4.216966e+01   ...
...
```

# ATOMS

ATOMS is an old program for producing images of crystal structures, produced by Shape Software in the USA.

ATOMS has a proprietary (and undocumented) text format, which changes with program version. Two examples of differing ATOMS text formats are given below. Note that, for brevity, only the first part of each file is shown.

CrystalMaker will extract the essential structural data from the file, including the cell parameters, general equivalent positions and fractional coordinates of atoms in the asymmetric unit. CrystalMaker will also attempt to extract atom and bond colours, radii, bonding and polyhedral information.

When first displayed, a single unit cell is shown; you can use the **Transform > Set Range** command to expand the range of atoms shown. You may well wish to edit the atom colours, rendering and other settings too.

Part of an ATOMS text structure file, in "version 5.0" format.

```
ATUNIV2
VERS      5.00000
TITL   1000194
GNIN1  1 1 3 0 0 0 0 0 0 0
GNIN2  0 1 1 1 1 1 1 0 0 0
GNIN3  0 1 1 2 2 2 0 0 0 0
GNIN4  0 0 0 4 1 0 0 4 0 0
GNIN5  0 0 0 0 0 1 6 0 0 0
GNIN6  0 0 0 0 0 0 0 0 1 0
GNIN7  0 0 0 5 1 0 1 2 0 1
GNIN8  0 0 0 0 1 6 0 3 0
GNIN9  15 15 15 1 1 1 1 0 1 0
GNN10  0 0
SHADI  1 0 1 1 1 0 32
GNFP1    5.33200e+00   1.11300e+01   5.45500e+00   9.00000e+01   ...
GNFP2    8.16533e-01   4.08212e-01   4.08212e-01   0.00000e+00   ...
GNFP3    0.00000e+00   0.00000e+00   0.00000e+00   0.00000e+00   ...
   ...
```

Part of an ATOMS text structure file, in "version 4.9" format.

```
ATUNIV
Structure title goes here
   4.90000
     3     2     0     6     6     0     1     6     0
     0     1     0     0     1     1     0     0     1     0
     1     4     0     0     1     0     0     1     0     1
     0     2     2     0     0     0     1     1     1     0
     0     0     1     0     8    32     0     0     4     1
     0     0     4     0     0     0     2     0     0     0
  9.04534e-001 -3.01511e-001  3.01511e-001
  0.00000e+000  0.00000e+000  0.00000e+000
  0.00000e+000  0.00000e+000  0.00000e+000
  0.00000e+000  0.00000e+000  0.00000e+000  0.00000e+000  0.00000e+000
  0.00000e+000  0.00000e+000  0.00000e+000  0.00000e+000  0.00000e+000
  5.01745e-001  5.01745e-001  5.01745e-001  5.00000e-001  3.00000e+000
  4.00000e+001  0.00000e+000  0.00000e+000  4.50000e-001  1.20000e-001
  1.35000e+002  3.00000e+000  2.00000e-001  0.00000e+000  0.00000e+000
  0.00000e+000  0.00000e+000  0.00000e+000  0.00000e+000  0.00000e+000
     5     5    15     1     2     3
...
```

# CASTEP

CASTEP is a molecular dynamics program, developed by a group of British academics and originally funded by the UK Science & Technology Facilities Council (STFC).

## CASTEP Cell

Structure input for the program is in the form of a "Cell" file. This includes a list of all the atoms in the unit cell, cell parameters and symmetry elements. Because the symmetry elements may be "tweaked" to refer to Cartesian Axes, rather than crystallographic axes, CrystalMaker ignores these, and instead loads the complete set of atomic coordinates.

Part of a CASTEP "Cell" file.

```
%BLOCK LATTICE_CART
ang    # angstrom units
   5.700000000000000   0.000000000000000   0.000000000000000
   0.000000000000000   4.936300000000000   0.000000000000000
   0.000000000000000   0.000000000000000  10.800000000000001
%ENDBLOCK LATTICE_CART

%BLOCK POSITIONS_FRAC
Co   0.000000000000000   0.000000000000000   0.000000000000000
Co   0.000000000000000   0.000000000000000   0.500000000000000
Co   0.250000000000000   0.500000000000000   0.000000000000000
Co   0.250000000000000   0.500000000000000   0.500000000000000
Co   0.500000000000000   0.000000000000000   0.000000000000000
Co   0.500000000000000   0.000000000000000   0.500000000000000
Co   0.750000000000000   0.500000000000000   0.000000000000000
Co   0.750000000000000   0.500000000000000   0.500000000000000
Na   0.500000000000000   0.666666666666667   0.250000000000000
Na   0.000000000000000   0.333333333333333   0.750000000000000
Na   0.000000000000000   0.000000000000000   0.250000000000000
Na   0.500000000000000   0.000000000000000   0.750000000000000
O    0.000000000000000   0.333333333333333   0.090800000000000
O    0.000000000000000   0.333333333333333   0.409200000000000
O    0.250000000000000   0.166666666666667   0.590800000000000
O    0.250000000000000   0.166666666666667   0.909200000000000
O    0.250000000000000   0.833333333333333   0.090800000000000
O    0.250000000000000   0.833333333333333   0.409200000000000
O    0.500000000000000   0.666666666666667   0.590800000000000
O    0.500000000000000   0.666666666666667   0.909200000000000
O    0.500000000000000   0.333333333333333   0.090800000000000
O    0.500000000000000   0.333333333333333   0.409200000000000
O    0.750000000000000   0.166666666666667   0.590800000000000
O    0.750000000000000   0.166666666666667   0.909200000000000
O    0.750000000000000   0.833333333333333   0.090800000000000
O    0.750000000000000   0.833333333333333   0.409200000000000
O    0.000000000000000   0.666666666666667   0.590800000000000
O    0.000000000000000   0.666666666666667   0.909200000000000
%ENDBLOCK POSITIONS_FRAC

%BLOCK SPECIES_POT
O   2|1.5|12.86|16.537|18.375|20UU:21UU(qc=6.25)[2p4.75]
Na  2|1.3|1.3|1|11.8|13.6|15.3|20U=-2.07:30U=-0.105:21U=-1.06U=+0.25[]
Co  3|2.5|2.5|1.5|5.9|7.7|10|40UU:32UU:41UU{4s1.95,4p0.05}(qc=4)[]
%ENDBLOCK SPECIES_POT

symmetry_generate
```

## CASTEP Output

CASTEP simulations generate an output file that may contain multiple structures: the original structure, plus progressive stages of its relaxation. By visualizing the complete sequence as an animation, within CrystalMaker, one can better understand the trajectory of the simulation.

The file format is too complex and extensive to show here, and includes energies, potentials and other details beyond the scope of structure visualization.

## CASTEP Volumetric

The CASTEP program can generate separate files for charge density, electron localisation or charge differences. These files contain a series of points in space, measured at regular intervals within a unit cell; however, the underlying crystal structure is not included.

Such files can be visualized in CrystalMaker in one of two ways, either:

- By reading the file directly into the program as a "dummy crystal" (unit cell, but no atoms); or:
- By loading the volumetric data into the corresonding crystal, using the "+" button in the **Volumetric Data** group of the Model Inspector.

The start of a CASTEP electron density file (".den_fmt")

```
 BEGIN header

          Real Lattice(A)                Lattice parameters(A)    Cell Angles
   5.7317856   0.0000000   0.0000000     a =    5.731786  alpha =   90.000000
   0.0000000   4.9523644   0.0000000     b =    4.952364  beta  =   90.000000
   0.0000000   0.0000000  11.2359721     c =   11.235972  gamma =   90.000000

   2                              ! nspins
  64    60   125                  ! fine FFT grid along <a,b,c>
 END header: data is "<a b c> charge spin" in units of electrons/grid_point *
nu
 mber of grid_points

     1     1     1         5579.706779          -15.876545
     1     1     2         5083.049583          -16.933963
     1     1     3         4171.531704          -17.716965
     1     1     4         3135.650539          -16.281456
     1     1     5         2206.064061          -12.164877
     1     1     6         1466.481467           -7.112142
     1     1     7          938.484147           -2.863050
     1     1     8          576.584989           -0.409691
     1     1     9          326.881516            0.188664
     1     1    10          208.406153            0.368616
...
```

## CCL

The CCL format is a flexible format used for controlling least-squares refinement of crystal structures. The example below was generated at the Rutherford-Appleton Laboratory, England, for Rietveld profile refinement of neutron powder data.

These files have the general form indicated by the example below. A one-character "card" identifies the data; CrystalMaker reads the "A" (atom), "S" (symmetry) and "C" (cell parameter) cards. Any remaining cards are ignored. CrystalMaker can also import CCL files that contain spacegroup symbols on the "S" line—designated by the "GRUP" control card, e.g., `"S GRUP I M A 2".`

Example of a CCL file for tetragonal leucite. For clarity, some of the temperature factors have been removed from the listing.

```
N Leucite: (tetragonal form, I41/a, 100 deg C, run 2177)
Z
Z Atom coordinates:
Z Name    x          y          z          ITF            SITE
A K       0.36628    0.36535    0.11714    0.00000
A Al1     0.05816    0.39671    0.16544    0.00000        1.15898
A Al2     0.16851    0.61241    0.12795    0.00000        1.09160
A Al3     0.39327    0.64060    0.08633    0.00000        1.15535
A O1      0.13076    0.31362    0.11114    0.00000
A O2      0.09267    0.51045    0.13100    0.00000
A O3      0.14546    0.67899    0.22693    0.00000
A O4      0.13417    0.68387    0.03584    0.00000
A O5      0.28922    0.57730    0.12120    0.00000
A O6      0.48407    0.61753    0.16647    0.00000
Z
Z Temperature factors:
Z Name     type  B11        B22        B33        B23        B13        B12
T K        2    3.08227    3.60303    8.72175   -1.40161   -0.41780    0.41179
T Al1      2    2.31015    1.62830    2.09483   -0.07154   -0.57991   -0.03895
T Al2      2    2.61028    1.40379    1.68022    0.27654   -0.35900   -0.28226
T Al3      2    2.38851    1.59443    1.40649    0.22217    0.29850    0.37947
T O1       2    3.61923    1.97148    3.40467   -0.99642    0.62805    0.62841
...
Z
Z  Form factors.  1 ==> neutron scattering lengths
Z Name          b
F K        1    0.36700
F O        1    0.58050
F Al       1    0.34490
Z
Z  Cell parameters
C  13.08966  13.08966  13.75299    90.000    90.000    90.000
Z
Z  Symmetry elements: only the generators are required
S     1/2+X,1/2+Y,1/2+Z
S     -X,-Y,-Z
S     -X,1/2-Y,Z
S     3/4-Y,1/4+X,1/4+Z
Z
Z Some control parameters.
I NCYC 5 MCOR 0 PRIN 0 PRFO 0 PRPR 2 PRFC 2  BMIN 1.5 BMAX 3.2
Z
Z What to vary in the refinement.
L VARY ONLY SCAL 1 ALL BACK
L VARY A* C*  ZERO 1  PKCN 2  SIGM 2  SIGM 3 GAMM 2 GAMM 3
L VARY ALL XYZ
L VARY ALL BIJ
L VARY Al1 SITE Al2 SITE Al3 SITE
```

## Chem3D Cartesian

Chem3D is a molecular modelling package used on various computing systems. Its Cartesian file format is as basic as they get: a listing of orthogonal coordinates.

The first line of the file is the total number of atoms to be read. Subsequent lines contain the atom's element symbol, its number, and its orthogonal coordinates in Ångstrøm units.

CrystalMaker can import and export this file format. When importing a Chem3D file, CrystalMaker will attempt to auto-generate bonds, using the currently-set element radii, if the **Transform > Generate Bonds at File Import** option is set.

The first part of a Chem3D Cartesian file.

```
432
C  1     -9.394   -2.061   -7.164
C  2     -6.549   -2.402   -5.772
C  3     -6.549   -2.968   -3.433
C  4     -9.392   -0.253   -14.627
C  5     -9.393   -1.494   -9.503
C  6     -6.548   -0.594   -13.235
C  7     -6.548   -1.161   -10.896
C  8     -9.392    0.314   -16.966
C  9     -6.547   1 .214   -20.698
C 10     -6.547    0.647   -18.359
C 11     -9.401   -7.293   -8.431
C 12     -6.556   -7.634   -7.039
C 13     -6.556   -8.201   -4.7
…
```

If you export an existing *crystal* to Chem3D format, CrystalMaker generates orthogonal coordinates $\{x_o y_o z_o\}$ using the standard convention:-

- The new $x_o$-axis is parallel to the crystal's $x$-axis.
- The new $y_o$-axis lies in the crystal's $xy$ plane and is perpendicular to $x_o$.
- The new $z_o$-axis is perpendicular to $x_o$ and $y_o$.

# CIF

The Crystallographic Interchange File format is increasingly being used for data transfer. It has a complex format with new options being added all the time. CrystalMaker ignores most of the options, extracting the basic crystallographic information and site occupancies. A typical CIF file is listed on the next page.

CIF files consist of a number of control cards, each beginning with an underscore character, and sometimes grouped into a "loop" of multiple items. There are strict formatting rules for data entry and if you do need to edit a CIF file you should exercise great care. We should draw your attention to some of the following:

- Text strings which include spaces should be enclosed within single quotes (if the string fits on one line), or semicolons (for multiple lines of text).
- Each control card must have an associated data item: do not leave a blank.
- Do not insert blank lines within a list (the group of "looped" data items which begins "**loop_**").
- You *must* include a blank line *after* a list (looped data).

### Symmetry

Please note that CrystalMaker uses symmetry operators (general equivalent positions) in preference to any space group symbols included in the CIF file (there being no agreed standard on the format for text-based space group strings).

### Temperature Factors

CrystalMaker can read isotropic, $B_{ij}$ and $U_{ij}$ values from CIF files. If a file contains both isotropic and anisotropic temperature factors for a particular site, the anisotropic factors are used for display purposes.

### Error Information

CrystalMaker reads error values for cell parameters and fractional coordinates (the errors are generally given in brackets after each entry). Error values can be used by CrystalMaker for error propagation, when calculating bond distances on screen, or when exported in a Bond Data file.

### Multi-Structure Files

If your CIF file contains more than one structure CrystalMaker will add each structure to the document. This way you can easily animate your results.

### Multi-Part Files and Disorder

As with SHELX, the CIF format allows disordered structures to be modelled in terms of a series of alternative representations or "disorder groups" (equivalent to "parts" in SHELX terminology). Whilst other programs end up plotting a composite structure (thereby ignoring the separate parts), CrystalMaker provides the option of showing either the composite structure, or individual representations.

For example, a carbonate structure might have a $CO_3$ group (which is shaped like a helicopter rotor, with carbon in the centre and oxygens at the ends of the "rotor blades") in one of three possible orientations. Each orientation would have its atoms listed in the CIF file with their own `_atom_site_disorder_group` identification numbers, e.g., "1", "2" and "3". Other, ordered, atoms in the structure would have their "disorder group" as "0" (or left blank). Plotting the entire structure would show the three rotor orientations superimposed. However, at any instant in time, the correct structure would show just a single orientation: atoms from "group 0" plus one of the three possible orientations of the rotor, "group 1", "group 2" or "group 3". CrystalMaker would therefore show four structures in the Structures List:-

- Composite structure (ordered atoms in disorder group 0, plus disordered representations, e.g., disorder groups 0 - 3)
- Individual representation 1 (group 0 + group 1)
- Individual representation 2 (group 0 + group 2)
- Individual representation 3 (group 0 + group 3)

By default, the composite structure is shown, but individual representations can easily be selected by clicking on their thumbnails.

### Problems with your CIF?

The International Union of Crystallography (IUCr) maintains a free online CIF checker, which you can access at: `http://checkcif.iucr.org`. Please use this facility to verify your data *before* contacting us about any file import problems.

An example CIF file for the silicon diphosphate structure.

```
data_ICSD-8096

_audit_creation_date              95-08-03
_database_code_ICSD               '8096'
_chemical_name_systematic         'Silicon diphosphate - A IV'
_chemical_formula_structural      'Si P2 O7'

_publ_section_title
;
Refinement of the crystal structure of silicon diphosphate, Si P~2~
O~7~ AIV - a phase with six-coordinated silicon
;
_publ_author_name                 'Hesse, K F'
_journal_name_full                'Acta Crystal B (24,1968-38,1982)'
_journal_coden_ASTM               'ACBCA'
_journal_volume                   35
_journal_year                     1979
_journal_page_first               724
_journal_page_last                725

_cell_length_a                    4.713(1)
_cell_length_b                    11.987(2)
_cell_length_c                    7.628(2)
_cell_angle_alpha                 90
_cell_angle_beta                  91.2(2)
_cell_angle_gamma                 90
_cell_volume                      430.85

_symmetry_space_group_name_H-M    'P 1 21/n 1'
_symmetry_Int_Tables_number       14
_symmetry_cell_setting            monoclinic

loop_
_symmetry_equiv_pos_as_xyz
   'x,y,z'
   '1/2+x,1/2-y,1/2+z'
   '-x,-y,-z'
   '1/2-x,1/2+y,1/2-z'

loop_
_atom_site_label
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_attached_hydrogens
_atom_site_calc_flag
   Si4+1     4 e  0.21950(40)  0.85050(20)  0.34740(30)   1.000 0 d
   P5+1      4 e  0.79910(40)  0.51820(20)  0.19620(20)   1.000 0 d
   P5+2      4 e  0.72030(40)  0.69700(20)  0.44830(30)   1.000 0 d
   O2-1      4 e  0.70730(100) 0.57250(40)  0.37430(60)   1.000 0 d
   O2-2      4 e  0.08050(100) 0.46450(40)  0.23640(60)   1.000 0 d
   O2-3      4 e  0.57880(100) 0.43500(40)  0.14120(60)   1.000 0 d
   O2-4      4 e  0.83490(100) 0.61090(40)  0.06510(60)   1.000 0 d
   O2-5      4 e  0.62240(90)  0.68730(40)  0.63150(60)   1.000 0 d
   O2-6      4 e  0.02150(100) 0.73640(40)  0.43030(60)   1.000 0 d
   O2-7      4 e  0.51530(90)  0.76240(40)  0.33790(60)   1.000 0 d

_refine_ls_R_factor_all            0.05
```

# CSSR

These files are generated by the Daresbury Laboratory's crystallographic data base system. They have a very simple format that includes the unit cell parameters, spacegroup symbol, database information (ignored by CrystalMaker), and the fractional coordinates of atoms in the asymmetric unit.

An example CSSR file for a sulphur polymorph.

```
REFERENCE STRUCTURE =  1662   A,B,C =   8.442  13.025   9.356
   ALPHA,BETA,GAMMA =  90.000 124.980  90.000    SPGR = 13 P12/C1
   8   0 CODEN=    2091 SYMOPS=50038
  40     RFAC= 7.5 ERRFLAG=0 (C-C)ESD=0
   1 S1       .64720    .34530    .32360
   2 S2       .80970    .57940    .46960
   3 S3       .74570    .44300    .53160
   4 S4       .58390    .67660    .38390
   5 S5       .08120    .79790    .19990
   6 S6       .24230    .03130    .22050
   7 S7       .30670    .89380    .34990
   8 S8       .14820    .12750    .32930
```

## Gaussian CUBE

This file format originated with Gaussian, Inc., and combines volumetric data with crystallographic data. Files begin with a header that specifies the positions of atoms in the unit cell. This is then followed by an array of numbers corresponding to data points scanned across *x*, *y* and *z*.

CrystalMaker can read CUBE files in one of two ways, either:

- Directly, by opening the file as a new structure, in the usual way (e.g., **File > Open** command). The volumetric data are automatically added to the imported crystal.
- Indirectly, by importing the *volumetric dataset* from the CUBE file into an existing structure. This is accomplished using the Add (+) button in the **Volumetric Data** group of the Model Inspector.

Part of a Gaussian CUBE file, showing the header information (structure data), followed by the start of a list of volumetric data points.

```
guan-kp
charge density as extracted with castep2cube (unit: e/voxel, i.e.
sum(voxels)=number of electrons)
   10    0.000000    0.000000    0.000000
   73    0.227299   -0.131231    0.000000
   73    0.000000    0.262462    0.000000
   46    0.000000    0.000000    0.251963
    1    1.000000    3.856729   -0.330263   11.338357
    1    1.000000    2.214381   15.722368   11.338357
    1    1.000000    1.642348    3.505157   11.338357
    1    1.000000   14.151127    6.273737   11.338357
    1    1.000000   14.723160   -5.943474   11.338357
    1    1.000000   12.508780    9.118367   11.338357
    6    4.000000    0.000000   18.897261    0.000000
    7    5.000000    2.169264   -1.252425    0.000000
    7    5.000000   16.365507   -6.943781    0.000000
    7    5.000000   14.196244    8.196206    0.000000
  0.28385E-02  0.29295E-02  0.30923E-02  0.29086E-02  0.22264E-02  0.14747E-02
  0.91439E-03  0.54708E-03  0.32250E-03  0.18915E-03  0.11133E-03  0.65023E-04
  0.37561E-04  0.21681E-04  0.12819E-04  0.76004E-05  0.44375E-05  0.25387E-05
  0.15194E-05  0.93767E-06  0.59534E-06  0.39109E-06  0.31092E-06  0.31092E-06
  0.39109E-06  0.59534E-06  0.93767E-06  0.15194E-05  0.25387E-05  0.44375E-05
  0.76004E-05  0.12819E-04  0.21681E-04  0.37561E-04  0.65023E-04  0.11133E-03
  0.18915E-03  0.32250E-03  0.54708E-03  0.91439E-03  0.14747E-02  0.22264E-02
  0.29086E-02  0.30923E-02  0.29295E-02  0.28385E-02
...
```

## DENS Volumetric

This file format is used by programs such as MEED/PRIMA and their derivatives. It includes one or more volumetric datasets, expressed in terms of voxel coordinates, and using symmetry to reduce the overall file size. CrystalMaker can read up to 5 different datasets from the same DEN file.

CrystalMaker can read DEN files in one of two ways, either:

- Directly, by opening the file as a new structure, in the usual way (e.g., **File > Open** command). The volumetric data are automatically added to the imported crystal.
- Indirectly, by importing the volumetric dataset(s) from the DEN file into an existing structure. This is accomplished using the Add (+) button in the **Volumetric Datasets** group of the Model Inspector.

DEN files begin with an optional comment line, a title line, and the number of data lines. The data lines are followed by a set of unit cell parameters and are set of symmetry operators. These can include translations expressed as fractions, or as integers (the voxel numbers corresponding to the fractions (e.g., "32" in a 64-pixel grid denotes the fraction 1/2). The symmetry operators include a rotation matrix which, bizarrely, is written out in transpose form (e.g., $m_{11}$ $m_{21}$ $m_{31}$, $m_{12}$ $m_{22}$ $m_{32}$, $m_{13}$ $m_{23}$ $m_{33}$).

Part of a DEN file showing three rows of volumetric data (xyz voxel indices and two columns of data). The unit cell parameters are included, with symmetry operators below.

```
** This is a comment **
This is the title line
1234
    0    0    0    1.234000-03    0.100000e+00
    1    0    0    2.456000-03    0.200000e+00
    1    1    0    0.347500-03    0.300000e+00
    ...
   4.74950   4.75950  12.99500  90.00000  90.00000 120.00000
   64   64   64    6    1    3
    1    0    0    0    1    0    0    0    1    0    0    0
    0    1    0   -1   -1    0    0    0    1    0    0    0
   -1   -1    0    1    0    0    0    0    1    0    0    0
    1    0    0   -1   -1    0    0    0   -1    0    0   32
    0    1    0    1    0    0    0    0   -1    0    0   32
   -1   -1    0    0    1    0    0    0   -1    0    0   32
    0    0    0
   42   21   21
   21   42   42
```

# DL_POLY

These files are generated by the "DL_POLY" Molecular Dynamics program, funded by the UK Science & Technology Facilities Council (STFC).

## "Config" Files

This format is used to encode structural data prior to performing a DL_POLY simulation. It comprises a header with a title line, followed by unit cell parameters then the coordinates of atoms in the unit cell.

Part of a DL_POLY CONFIG file, showing the file header and the first set of atomic coordinates.

```
temperature
         0         3
       34.5717341191        0.0000000000        0.0000000000
        0.0000000000       34.9300000000        0.0000000000
        0.0000000000        0.0000000000       34.1200000000
Ba                 1
    -14.40488922        -17.46500000        -2.843333333
Ba                 2
    -14.40488922        -17.46500000         14.21666667
Ba                 3
    -14.40488922        -12.47500000        -2.843333333
Ba                 4
    -14.40488922        -12.47500000         14.21666667
Ba                 5
    -14.40488922        -7.485000000        -2.843333333
...
```

## "Revcon" Files

This is another input format used by the DL_POLY program. Superficially-similar to CONFIG, CrystalMaker can auto detect either format.

Part of a DL_POLY REVCON file—for the same structure as shown in the CONFIG example.

```
BaCO3 at room temperature
         2         3     50000    0.5000000000E-02
     37.703837784199      0.030387054865      0.040722897324
      0.029825062647     38.221410648370      0.058052279491
      0.040856112846      0.057214246029     37.990668308902
Ba                 1
    -15.40247823         18.98142930        -3.409467241
 -0.514663106260       1.18222095098      -1.97772315973
  -3574.56281934       4245.57400428       1375.52610695
Ba                 2
    -15.39770516        -18.96488519         15.64864132
 -0.752236817368      0.445815957438      -1.56274144185
  -2565.99802226      -4712.44663280      -2575.60931355
Ba                 3
    -15.44697676        -13.70314421        -3.339480823
 -0.491182477163     -0.205273990861E-01   1.41683478280
   4652.81947393      -181.545214457       1589.95050080
Ba                 4
    -15.39266387        -13.64576760         15.69599370
  0.266307863524     -0.270415376512     -0.711799346621
   429.667412152       3076.84351484       1154.67634113
...
```

## "History" Format

DL_POLY "History" files contain a comprehensive listing of atomic coordinates, velocities and forces—for each time step of a molecular dynamics simulation—and are therefore useful in understanding the motion of the atoms. However, these files can be huge; depending on your operating system, you may be limited to loading files with a maximum size of 4 GB.

> CrystalMaker can read old, fixed-format files (DL_POLY 3 and earlier), as well as the newer, DL_POLY 4 files, which have a more relaxed file format.

**Visualizing the Trajectory** When importing a History file, the individual structures are loaded in the same window, as separate View thumbnails. These can then be synchronized, animated, and exported as a movie. This is an ideal way for visualizing the progress of a simulation.

**Crystal or Molecule?** Structures could either be periodic, "crystal" structures, or aperiodic "molecule" structures, depending on the Periodic Boundary Condition flag "**imcon**", as found in the second line of the file.

**Orientation & Bonding** When presented with a crystal structure, CrystalMaker derives an orientation matrix to relate the given orthogonal coordinates of atoms, to their fractional (crystallographic) equivalents. Atoms are plotted in the same orientation as used in the file. Bonds may, or may not be generated at file import, depending on whether or not the "**Generate Bonds at File Import**" preference has been enabled.

Part of a fixed format (DL_POLY 3) HISTORY file.

```
This is a header line
         2         3        72
timestep     49600        72         2         3    0.001000
   8.165     -0.2000E-09 -0.2000E-09
   0.000       9.200     -0.3000E-09
   0.000       0.000       17.29
O                1   16.000000   -1.200000
 -1.3638E+00  1.6436E+00 -4.4072E-02
 -7.5976E+00 -3.7869E+00 -5.6866E+00
  8.5449E+03  2.0429E+03 -1.0240E+04
O                2   16.000000   -1.200000
  1.6474E+00 -2.9966E+00 -8.6097E+00
  3.2722E+00  1.4009E+00 -4.7746E+00
 -6.9849E+03 -4.6422E+03  2.0552E+03
O                3   16.000000   -1.200000
 -2.6974E+00 -1.8299E+00 -8.5521E+00
  9.0081E+00  6.1361E-01 -4.3083E+00
  9.4882E+02  2.2951E+04 -1.5382E+04
  ...
```

## DMol3

These files are generated by the "DMol3" simulation program which uses density functional theory to calculate molecular structures, transition states, and molecular reaction trajectories.

CrystalMaker supports two types of DMol3 file:

- ".car" - describes a single molecule.
- ".arc" - describes a molecular trajectory of geometry/energy.

The two formats share the same basic structure, with a header, followed by one or more structures.

Part of a DMol3 ".car" file.

```
!BIOSYM archive 3
PBC=OFF
!DATE     May 07 21:52:50 2015
C1       2.349829781   -2.274336230    8.135554924 dmol    1     C   0.000
C2      -2.162304958   15.810512076   -1.345103624 dmol    1     C   0.000
C3       1.839355070   -2.495031830    6.727545843 dmol    1     C   0.000
C4       0.013630104   -1.526278557    4.189209502 dmol    1     C   0.000
C5      -2.509885181   14.382229214   -0.906994596 dmol    1     C   0.000
...
S269    -1.405180020    7.781206012    0.215391076 dmol    1     S   0.000
end
end
```

**Visualizing the Trajectory** When importing a ".arc" file, the individual structures are loaded in the same window, as separate View thumbnails. These can then be synchronized, animated, and exported as a movie. This is an ideal way for visualizing the progress of a refinement. The energies of each structure are presented in the Notebook pane.

**Orientation & Bonding** When presented with a crystal structure, CrystalMaker derives an orientation matrix to relate the given orthogonal coordinates of atoms, to their fractional (crystallographic) equivalents. Atoms are plotted in the same orientation as used in the file. Bonds may, or may not be generated at file import, depending on whether or not the "**Generate Bonds at File Import**" menu option is selected.

# Cambridge FDAT

The "FDAT" file format is used by the Cambridge Crystallographic Data Centre, for their widely-used Cambridge Structural Database of organic structures. FDAT files are also generated by the Daresbury Crystallographic Database Service. An example FDAT file is listed below.

CrystalMaker extracts most information contained in an FDAT file. Many of the header flags (e.g., errors, refinement, data collection) are interpreted, and diagnostic messages printed in the Notebook pane. Errors in unit cell parameters are also extracted and used for bond-distance error propagation.

### Symmetry

Although the spacegroup symbol and number is given, CrystalMaker prefers to use the symmetry operators instead—this avoids problems with non-standard settings!

On a technical note, CrystalMaker does a lot of behind-the-scenes work converting the CSD symmetry operators to conventional general equivalent positions: if there's a centre of symmetry at the origin we add the extra operators, and we also use the lattice type to "prune" the (redundant) symmetry operators corresponding to lattice translations. Thus, if one examines the imported general equivalent positions (GEPs) using the Symmetry Options dialog, they should correspond to equivalent positions listed in the International Tables for Crystallography.

### Atoms

CrystalMaker only imports atoms in the asymmetric unit; symmetry-generated atoms, if listed in the file, are ignored. The atom colours correspond to CrystalMaker's default atom colours: these can be edited or imported from a text file using the Elements pane in the Preferences panel. If you import a large number of organic structures, we recommend importing the CSD Default Radii element table, and then saving these data in your preferences file.

### Automatic Bond Generation

CrystalMaker uses a very concise way of representing bonding information—the bond specification cards. The individual bonds listed at the end of the FDAT file are therefore largely irrelevant. However, we search the bonds list to deduce the intended bonding pattern, and use this as a basis for CrystalMaker's own bond search. Thus, if the FDAT bond list contains C–C, C–H and C–O bonds, we create three separate bond specifications for these bonds. To determine the maximum bond lengths for each bond specification, we use the bond length tolerance in the CSD file (usually 0.40 Å) plus the sum of the atomic radii involved. Usually these radii are listed in the FDAT file. If the radii can't be found in the FDAT file, CrystalMaker searches its own default radii—these are the radii that appear in the Elements Editor window. If a radius value still can't be found, a default value of 1.0 Å is used.

Because of the way CrystalMaker defines bonds, you may find that not all "requested" bonds can be found, and an alertbox will be displayed after the crystal has been imported. For example, if a molecule contains H-C and H-O bonds so that some H's are bonded to carbon but not oxygen, and vice versa, error messages will be printed in the Output Log. (Obviously, the carbon H will not have any bonds to O, and the oxygen H won't have any bonds to carbon). In these cases, you can disregard the messages.

If you still don't get the bonds you want, you can easily change the bonding specifications using the Bonding Inspector.

An FDAT file for an organometallic molecule.

```
#AABHTZ  13770506       18  9  0  0  0  1  5 35  0  0 371321000000000000000000076
 11372 10272  7359 10875  7107  9616333222 9 5 9 6 4 8  0  0  2P-1       240
R=0.0410
211 0121 0112 0
C  68H  23O  68N  68CL 99
CL1   -33550   9980  10610 CL2   -64070 -30840  32700  C1   -47750   3880  23070
C2    -57270  13370  34240 C3    -68450   9160  44830  C4   -70210  -4450  44470
C5    -60690 -13870  32950 C6    -49040 -10070  21810  C7   -38440 -19380   8860
N8    -36680 -29770  13510 N9    -26290 -38000    990  C10  -18570 -36530 -17520
N11   -21960 -38590 -33470 N12   -11480 -36040 -48430  C13   -2540 -32560 -40600
N14    -6420 -32680 -21040 N15      230 -28370  -7410  C16   -3050 -16060   7440
C17     4050 -12440  22150 O18   -11020  -8830   7930  C19  -23940 -48600   7180
C20   -33070 -50930  25480 O21   -14540 -55420  -2960  H2   -55800  23200  34700
H3    -75200  15700  53100 H4    -78400  -7800  53000  H7   -32600 -17500  -3200
H13     5700 -29600 -46900 H15     4600 -34000  -5700  H171   8100  -3600  21700
H172   10500 -19800  18900 H173    -600 -10700  33300  H201 -31300 -59800  27500
H202  -32900 -45100  37400 H203  -41300 -52500  24300
3 7 4 5 6 7 8 3 8 910111213141216171818112121 4 5 6 915171919192222221516
```

# GRD

CrystalMaker can import 3D volumetric data from the "GRD" file format (which is virtually identical to CrystalMaker's Voxel format, with just one additional header line).

GRD files contain no atoms, so when *opening* a file, CrystalMaker will generate a dummy structure for you: a primitive lattice with (hidden) atoms at the corners of the unit cell. Alternatively, you can load the volumetric data values directly into an existing structure's **Volumetric Data** list (e.g., by dragging-and-dropping the file into the list).

The "GRD" format is very simple. It consists of:

- Title line.
- Unit cell parameters: $a$, $b$, $c$, $\alpha$, $\beta$, $\gamma$ (distances in Å; angles in degrees).
- Header line with three integers: $Nx$, $Ny$ and $Nz$. These are the numbers of data points along the unit cell's $x$, $y$ and $z$-edges, respectively.
- A series of floating-point numbers corresponding to the $Nx \,.\, Ny \,.\, Nz$ points.

The data points can be arranged on multiple lines if required, as long as they are arranged in the correct order: scanned along $z$, then along $y$, and finally along $x$ (i.e., $\Delta z > \Delta y > \Delta x$).

Part of a GRD file (long lines have been truncated).

```
Voxel data for "Electron Density" exported from CrystalMaker X for macOS
10.0 10.0 10.0 90.0 90.0 90.0
104    104    233
 8.798907e+01     8.725596e+01     0.000000e+00     8.508385e+01   ...
 3.303827e+01     3.775127e+01     0.000000e+00     4.216966e+01   ...
...
```

## GROMACS

GROMACS is another energy-modelling program, designed for biological systems. An example file is listed below:-

An example GROMACS file.

```
MD of 2 waters, t= 0.0
    6
    1WATER  OW1    1   0.126   1.624   1.679  0.1227 -0.0580  0.0434
    1WATER  HW2    2   0.190   1.661   1.747  0.8085  0.3191 -0.7791
    1WATER  HW3    3   0.177   1.568   1.613 -0.9045 -2.6469  1.3180
    2WATER  OW1    4   1.275   0.053   0.622  0.2519  0.3140 -0.1734
    2WATER  HW2    5   1.337   0.002   0.680 -1.0641 -1.1349  0.0257
    2WATER  HW3    6   1.326   0.120   0.568  1.9427 -0.8216 -0.0244
   1.82060   1.82060   1.82060
```

Please note that GROMACS does not uniquely define element symbols, relying on atom labels instead. CrystalMaker will assume that the structure is organic, and use the first letter of the atom label to assign the element symbol (e.g., an atom with label "`HE1`" would be interpreted as "`H`", not "`He`").

# GSAS Experiment

GSAS ("General Structure Analysis System") is a computer program for crystal structure refinement from both single-crystal and powder diffraction data, using x-rays or neutrons. The software was developed at the Los Alamos National Laboratory by Larson & Von Dreele (2004).

CrystalMaker can input GSAS "experiment" files. These have a precise, fixed format, which is checked on import. Key requirements include the presence of at least one **HSTRY** history statement, a **VERSION** descriptor, the presence of cell parameters and atomic coordinates, and a **ZZZZ**... terminator line.

## File Import

Unit cell data, symmetry and structural data (type "A" and type "B" lines) are recorded:

- **Phase name.** This is used for the window title.
- **Cell parameters and errors.** Error values for the cell parameters are recorded and can be used in error propagation.
- **Site occupancies.** The chemical elements and their occupancies are used for atom colours, radii and automatic bond generation. The occupancies are also used in CrystalDiffract and SingleCrystal.
- **Atomic displacement parameters.** Temperature factors are extracted from the GSAS file; these may be either isotropic or anisotropic, depending on whether the "B" data line contains an "I" or "A" flag, respectively.

```
    VERSION    6
    DESCR   GSAS Calculation from CERIUS2
    HSTRY257 EXPEDT  V-UX 6.0 19-Feb-95 19:55:16             L   O
    HSTRY258 GENLES  V-UX 6.0 19-Feb-95 19:55:26 Sdsq= 0.140E+05 S/E=  1.82
    HSTRY259 EXPEDT  V-UX 6.0 19-Feb-95 19:57:08             LA  O
    HSTRY260 GENLES  V-UX 6.0 19-Feb-95 19:57:18 Sdsq= 0.136E+05 S/E= 0.163E-01
    HSTRY303 POWPREF V-UX 6.0 21-Apr-95 17:14:08
    HSTRY304 EXPEDT  V-UX 6.0 21-Apr-95 17:27:16             L   O
    DSGL CDAT1  DRAD ARAD NOFO
    GNLS  RUN on 21-Apr-95 at 17:28:37   Total cycles run 317       21178.
    GNLS CDAT1  MXCY  3
    AFAC  O     3.048513.2771 2.2868 5.7011 1.5463  .3239  .867032.9089  .2508 RHF
    AFAC  O_    15.999 .5805      .00019
    AFAC  O_SIZ      1.09      0.89 1.40  108
    AFAC  O_XAB  988.0 590.6 293.1 30.48 17.21
    AFAC  O_XAN   .090  .073  .069  .052  .047  .032  .008  .006  .003  .004
    AFAC CA     8.626610.4421 7.3873  .6599 1.589985.7484 1.0211178.437 1.3751 RHF
    AFAC CA_     40.08  .490         .43
    AFAC CA_SIZ      2.17     1.97  2.00  007
    AFAC CA_XAB  33250 21230 11410  1264 637.1
    AFAC CA_XAN  -.221 2.514  .163 1.904  .341 1.286  .203  .306  .137  .193
...
```

Part of a GSAS experiment file.

## GULP

CrystalMaker can read from output files generated by Julian Gale's "General Utility Lattice Program". This is a force-field based program that is primarily designed to relax inorganic structures.

GULP output files generally contain at least one pair of structures: an unrelaxed input structure, and the output structure. CrystalMaker will endeavour to extract all structures from the file, so you can readily ascertain how well the software managed to relax your input.

GULP output files are extremely verbose, so it is not particularly helpful to include an example here.

# ICSD

These files are typically produced as a result of searching structural information from the Inorganic Crystal Structures Database (ICSD). The file format is flexible, and allows the inclusion of structural errors, Wyckoff site symbols, and oxidation states. A typical example is given below.

CrystalMaker ignores error information and temperature factors (e.g., the ITF values listed in the example below). The essential crystallographic data are imported, but CrystalMaker will use the spacegroup number, in preference to any symbol. Any titles, reference & author information are copied to the notebook pane.

An ICSD output file for the SiP2O7 structure.

```
COL  ICSD Collection Code 8096
DATE Recorded Jan 1, 1980
NAME Silicon diphosphate - A IV
FORM Si P2 O7
     = O7 P2 Si
TITL Refinement of the crystal structure of silicon diphosphate,
     Si P2 O7 AIV - a phase with six-coordinated silicon
REF  Acta Crystallographica B (24,1968-38,1982)
     ACBCA 35 (1979) 724-725
AUT  Hesse K F
CELL a=4.713(1) b=11.987(2) c=7.628(2) alpha=90.0 ·=91.2(0) Á=90.0
     V=430.8 Z=4
SGR  P 1 21/n 1    (14) - monoclinic
CLAS 2/m   (Hermann-Mauguin) - C2h (Schoenflies)
PRS  mP40
ANX  AB2X7
PARM Atom__No OxStat  Wyck ——X—— ——Y—— ——Z——  -SOF-
     Si     1  4.000    4e  0.2195(4)   0.8505(2)   0.3474(3)
     P      1  5.000    4e  0.7991(4)   0.5182(2)   0.1962(2)
     P      2  5.000    4e  0.7203(4)   0.697(0)    0.4483(3)
     O      1 -2.000    4e  0.7073(10)  0.5725(4)   0.3743(6)
     O      2 -2.000    4e  0.0805(10)  0.4645(4)   0.2364(6)
     O      3 -2.000    4e  0.5788(10)  0.435(0)    0.1412(6)
     O      4 -2.000    4e  0.8349(10)  0.6109(4)   0.0651(6)
     O      5 -2.000    4e  0.6224(9)   0.6873(4)   0.6315(6)
     O      6 -2.000    4e  0.0215(10)  0.7364(4)   0.4303(6)
     O      7 -2.000    4e  0.5153(9)   0.7624(4)   0.3379(6)
WYCK e10
ITF  Si  1   B= 0.4800
ITF  P   1   B= 0.3500
ITF  P   2   B= 0.3400
ITF  O   1   B= 0.4400
ITF  O   2   B= 0.6000
ITF  O   3   B= 0.4500
ITF  O   4   B= 0.5700
ITF  O   5   B= 0.3400
ITF  O   6   B= 0.5300
RVAL 0.050
```

## LAMMPS

LAMMPS is an energy-modelling program developed at Sandia National Laboratories in the USA. CrystalMaker supports the coordinates "dump" format, an example of which is listed below:-

The start of a LAMMPS dump file. Three atom lines are shown; each has the same atom ID, "1".

```
ITEM: TIMESTEP
11000
ITEM: NUMBER OF ATOMS
8000
ITEM: BOX BOUNDS pp pp pp
0 18.8207
0 18.8207
0 37.6414
ITEM: ATOMS id type xs ys zs
7936 1 0.0515603 0.00797728 0.00467763
6719 1 0.00242674 0.0395856 0.0162416
7837 1 0.1169 0.0539664 0.00190204
...
```

### Warning: Dummy Element Symbols!

Please note that LAMMPS does not embed element symbols in its output file, only numeric atom IDs. CrystalMaker has absolutely no way of "mind reading" what these numerals are supposed to represent. The program therefore assigns dummy element symbols in the form: A*n* where *n* is the atom ID.

You can easily edit these symbols in the Atoms Inspector: simply double-click on the symbol in an element row and enter the correct element symbol. CrystalMaker will then automatically reassign the symbol to all sites and atoms, and replot your structure.

## Molfile

The "Molfile" format is used by Elsevier MDL for representing and communicating chemical information. There are actually two current formats, of which the older—and ubiquitous—V2000 format is supported by CrystalMaker. A more-complex "V3000" format is less-widely used, and is not currently supported by CrystalMaker.

The V2000 Molfile format comprises a 3-line header block, followed by a "Connection Table" with atom data, bonding and properties blocks.

**Fixed Format:** Please note that this is a FORTRAN-derived fixed-format, so great care should be exercised when attempting to edit this format: numbers must appear in the correct columns!

Molfile for glycine

```
  MDL-Draw09130610242D

  4  3  0  0  0  0  0  0  0  0999 V2000
  -11.8231    3.3413    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
  -11.8231    4.2502    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  -11.0216    4.5353    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  -11.0216    5.3853    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
  1  2  1  0  0  0  0
  2  3  1  0  0  0  0
  3  4  2  0  0  0  0
M  END
```

# PDB

The Protein Data Bank, or PDB (formerly the "Brookhaven PDB") contains a wealth of information on macromolecules (**http://www.rcsb.org**). PDB Data files are text files, presented in a fixed format, containing the orthogonal coordinates of atoms in a molecule, together with site occupancies, oxidation states and information on which atom belongs to which sub-molecular group.

**Fixed Format:** As with the Molfile format, please take great care if you need to edit a PDB file: this is a fixed-format data structure in which specific entries need to be in specific text columns.

## File Import

CrystalMaker imports comments and author information from the PDB file, and displays these in the Notes pane. Structural data are processed differently, depending on whether a full crystal has been saved.

**Molecule Import.** Many PDB files contain only orthogonal coordinates for a single molecule - and not the complete crystallographic structure. These files can be loaded only as "molecules": an isolated cluster of atoms with no lattice periodicity. Such structures are not suitable for diffraction calculations.

**Full Crystal Import.** Files that do contain crystallographic data (e.g., a `CRYST1` card), with cell parameters and asymmetric unit information, are loaded as crystals; the original "molecule" view is preserved, but the full crystallographic data are available, letting you extend the range to include multiple unit cells and, of course, take advantage of our diffraction software to simulate single-crystal or powder diffraction patterns.

When attempting to load a PDB file that is presented as a crystal, CrystalMaker checks the data to ensure that this can actually be plotted as a crystal. It is not uncommon to find mutually-incompatible sets of unit cell parameters and atomic coordinates! In these cases, the structure simply cannot be displayed as a crystal and a warning message will be issued; the structure will then be displayed in "molecule mode".

**Automatic Bond Generation.** CrystalMaker will search out, and plot, nearest-neighbour bonds in the molecule. Bonds are detected if two atoms lie within 15% of the sum of their radii It is therefore essential to ensure that you are using the appropriate set of radii before you import a PDB file:

- For organic structures, we recommend that you use the "**CSD CrystalMaker Covalent Radii**" element table, which you can load via the Atoms Inspector's contextual menu, or set as a preference via the **Preferences** panel.

Having found nearest-neighbour radii, CrystalMaker also constructs the corresponding bond specifications (which you can edit via the Bonds Inspector).

### Multi-Structure PDB files

If your PDB file contains more than one structure CrystalMaker will add each structure to the document. This way you can easily animate your results.

A very-basic PDB file, containing just atom lines.

```
ATOM  1  N   GLY  1   0.162  -0.202   0.000  1.00  0.00
ATOM  2  CA  GLY  1   1.612  -0.031   0.000  1.00  0.00
ATOM  3  C   GLY  1   1.985   1.432   0.000  1.00  0.00
ATOM  4  O   GLY  1   1.137   2.319   0.000  1.00  0.00
ATOM  5 1H   GLY  1  -0.299  -1.179   0.000  1.00  0.00
ATOM  6 2H   GLY  1  -0.513   0.641   0.000  1.00  0.00
ATOM  7 1HA  GLY  1   2.055  -0.519   0.888  1.00  0.00
ATOM  8 2HA  GLY  1   2.055  -0.519  -0.888  1.00  0.00
ATOM  9  HC  GLY  1   3.052   1.653   0.000  1.00  0.00
```

### Molecular Export

If your structure is a *crystal* then you have the option of exporting the visible atom son the screen as a self-contained "molecule". When you do this, CrystalMaker generates orthogonal coordinates $\{x_o y_o z_o\}$ using the standard convention:-

- The new $x_o$-axis is parallel to the crystal's $x$-axis.
- The new $y_o$-axis lies in the crystal's $xy$ plane and is perpendicular to $x_o$.
- The new $z_o$-axis is perpendicular to $x_o$ and $y_o$.

### Crystal Structure Export

If your structure is a crystal you also have the option to export it as a PDB crystal, in which case the full contents of one unit cell will be saved in the file.

We should note that the PDB format is **not recommended** as a general crystallographic format (it is, after all, a highly-specialised format for the purpose of depicting protein structures—not zeolites!). There are some fundamental limitations in the format which preclude its wider use:-

- **Complex space groups cannot be represented**. The PDB format requires that space group characters should be in full international notation—but also limits the number of characters to 11, which is too few for some space groups.
- **There is no way to indicate different origin choices**. Whilst one could convert atomic coordinates to the default origin choice, there is no way to shift the origin of the unit cell to the correct position.

As a universal workaround, we export PDB crystal structures using the space group 'P 1'. Note that one complete unit cell is then shown. If you simply want to export the visible atoms on the screen, you may prefer to export your structure as a PDB "molecule".

## RMCProfile

RMCProfile is a program for modelling the local structure of crystalline materials using the Reverse Monte Carlo technique. It is the product of an academic collaboration between scientists at the ISIS neutron source(Rutherford-Appleton Laboratory), Oxford, Cambridge and NIST.

CrystalMaker can read from, and write to, RMCProfile version 6 files. An example of this format is shown below.

Part of an RMCProfile file, generated by CrystalMaker X

```
(Version 6f format configuration file)
(Generated by CrystalMaker X for macOS version 10.0.0b5)
Metadata date:      6-5-2017
Number of types of atoms: 3
Atom types present:         Na O Si
Number of each atom type:   4 32 16
Number of atoms:    52
Supercell dimensions:    1 1 1
Cell (Ang/deg): 8.29700 12.99400 7.14400 90.00000 116.01000 90.00000
Atoms:
1 Na [1]     0.277500     0.000000     0.138500 1 0 0 0
2 Na [1]     0.722500     0.000000     0.861500 2 0 0 0
3 Na [1]     0.777500     0.500000     0.138500 3 0 0 0
4 Na [1]     0.222500     0.500000     0.861500 4 0 0 0
5 O [1]     0.000000     0.141100     0.000000 5 0 0 0
6 O [1]     0.000000     0.858900     0.000000 6 0 0 0
7 O [1]     0.500000     0.641100     0.000000 7 0 0 0
8 O [1]     0.500000     0.358900     0.000000 8 0 0 0
9 O [2]     0.612600     0.000000     0.285200 9 0 0 0
...
```

## SDfile

The "SDfile" format is used by Elsevier MDL for representing and communicating chemical information for multiple structures.

Each SDfile contains one-or-more structures, presented as a Molfile, followed by a series of data headers and data fields. The data headers all begin with a right-angled bracked (">") and include a data title, given in angled brackets. Each structure entry ends with a "$$$$" line.

CrystalMaker will read each structure into the same window, represented by thumbnails in the Views pane of the Overview window. For each structure, the data headers and associated data items are printed in the Notes pane of the sidebar.

Please be aware that some SDfiles may contain thousands of structures; generating all of these may take some time. CrystalMaker will warn you, in advance, if the file contains more than 50 structures.

Part of an SDfile, showing the embedded "Molfile" data.

```
> <MODELREGNO> (MFCD00001351)
1298

> <MODELSTRUCTURE> (MFCD00001351)

  MDL-Draw09130610392D                          1305

 11 12  0  0  0  0  0  0  0  0999 V2000
   -0.0166    1.3730    0.0096 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.0021   -0.0041    0.0020 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.4861    1.4661   -0.0043 C   0  0  1  0  0  0  0  0  0  0  0  0
   -1.2288    2.0490    0.0291 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.5067   -0.0563   -0.0126 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.1914   -0.7128    0.0093 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.0405    2.0837   -1.2621 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.4151    1.3429    0.0408 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.3965   -0.0393    0.0241 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.0311    3.4171   -1.4157 O   0  0  0  0  0  0  0  0  0  0  0  0
    2.4934    1.3785   -2.1325 O   0  0  0  0  0  0  0  0  0  0  0  0
  1  2  2  0  0  0  0
  1  3  1  0  0  0  0
  1  4  1  0  0  0  0
  2  5  1  0  0  0  0
  2  6  1  0  0  0  0
  3  7  1  0  0  0  0
  4  8  2  0  0  0  0
  6  9  2  0  0  0  0
  7 10  1  0  0  0  0
  7 11  2  0  0  0  0
  3  5  1  0  0  0  0
  8  9  1  0  0  0  0
M  END

> <MOLFORMULA> (MFCD00001351)
C9 H8 O2

$$$$
```

# SHELX

SHELX data files are used by the SHELX-76 and SHELXL-93 crystal structure refinement programs (Sheldrick, 1993). CrystalMaker imports SHELX data files as crystals. SHELX datafiles use symmetry operators (**SYMM** cards), but are not required to contain the identity operator (+x, +y, +z). CrystalMaker will add this if it is not included.

**Tip:** SHELX control cards (e.g., "SYMM", "CELL") must be in upper-case for them to be recognized by CrystalMaker. This is important, because the same file extension, ".str", is claimed by at least two other programs, and CrystalMaker needs some additional cues as to which format is which.

CrystalMaker can read atomic displacement parameters from SHELX files, providing these are in the order: $U_{11}$ $U_{22}$ $U_{33}$ $U_{23}$ $U_{13}$ $U_{12}$. Atom lines may contain a single, isotropic temperature factor, instead of the six anisotropic components.

A very-simple example of structural data from a SHELX file.

```
TITL
CELL   0.0000  13.7110  12.7320  18.5710  90.000  90.000  90.000
LATT  7
SYMM -X,+Y,-Z+0.500
AL1   0    0.11000    0.04100    0.16600    1.00000    0.00000
P4    0    0.22700    0.90500    0.05400    1.00000    0.00000
P5    0    0.89100    0.76900    0.93800    1.00000    0.00000
O7    0    0.82200    0.94700    0.12900    1.00000    0.00000
O8    0    0.85800    0.83300    0.00200    1.00000    0.00000
END
```

### Multi-Part Files and Disorder

SHELX allows disordered structures to be modelled in terms of a series of alternative states or "parts".

For example, a carbonate structure might have a $CO_3$ group (shaped like a helicopter rotor, with carbon in the centre and oxygens at the ends of the "rotor blades") in one of three possible orientations. Each orientation would have its own listing in the file, "Part 1", "Part 2" and "Part 3". Other, ordered, atoms would be listed as "Part 0". Plotting the entire structure would show the three rotor orientations superimposed. However, at any instant in time the correct structure would show just a single orientation: atoms from "Part 0" plus one of the three possible orientations of the rotor, "Part 1", "Part 2" or "Part 3". CrystalMaker would therefore show four structures in the Structures List:-

- Composite structure (atoms from Parts 0–3)
- Disordered state 1 (Part 0 + Part 1)
- Disordered state 2 (Part 0 + Part 2)
- Disordered state 3 (Part 0 + Part 3)

By default, the composite structure is shown, but individual states can easily be selected by clicking on their thumbnails.

## STRUPLO

STRUPLO was a polyhedral structures program (Fischer 1985). The data format is similar to CrystalMaker's text format, with various control cards identifying data types.

Files must include cell parameters, and a listing of element types, atom numbers and fractional coordinates for all atoms in the asymmetric unit.

You may, optionally, specify a spacegroup (**SPGR** card), range of fractional coordinates to be plotted (**XYZR**), plus a CrystalMaker-style **BOND** or **BMAX** card to indicate what kind of bonding you require. (See the next section for details about CrystalMaker's text bonding specifications.)

A simple STRUPLO file for a perovskite structure.

```
TITL BaTiO3 Perovskite
CELL 3.9998  3.9998  4.0180  90.00  90.00  90.00
SPGR P 4 m m
XYZR -0.9 2.1  -0.9 2.1  -0.9 2.1
END
Ba  1  0.0000  0.0000  0.0000
Ti  1  0.5000  0.5000  0.4820
O   1  0.5000  0.5000  0.0160
O   2  0.5000  0.0000  0.5150
```

## SYSTRE

SYSTRE is a JAVA program for analysing periodic nets in crystal structures. CrystalMaker can read from its Structure File format (file extension ".cgd") and will show symmetry-related bonds in the structure using colour coding. As connectivity is the raison d'etre of this format, a default "stick" model type is automatically applied.

Because CrystalMaker's bond generation algorithm is based on element-pair/distance combinations, the program has to undertake some additional steps in order to popagate symmetry-related bonds throughout an extended structure. This involves the insertion of "dummy" atoms at the centre of each bond, with unique element symbols.

A simple SYSTRE file for the diamond structure.

```
CRYSTAL
# Structure id (optional; ID and NAME both work)
ID    diamond
# The space group
GROUP Fd-3m
# Cell parameters: a b c alpha beta gamma
CELL 2.3094 2.3094 2.3094 90.00000 90.00000 90.00000
# Atom specification: name coordination x y z
# (decimal numbers or fractions can be used for coordinates)
ATOM 1 4 5/85/85/8
# This ends the structure description
END
```

**Built-In Symmetry-Related Bonding.** As a general note: when working with "regular" structures—without "dummy" atoms—you can readily show symmetry-related bonding by first selecting a bond of interest, and then choosing: **Edit > Select > Symmetry-Related Bonds**. Any bonds related by symmetry to the selection are themselves selected, allowing you to apply a distinctive colour and/or style, via the Selection Inspector.)

# TOPAS

TOPAS is a crystal structure refinement program, designed to offer Rietveld refinement of X-ray powder diffraction data. The program can be controlled via input files that include crystal structure data, an example of which is shown below.

```
str
   space_group fd-3m:2
   ' Space group (HMS): F d -3 m
   phase_name "Spinel"
   ' Formula: Al2 Co O4
   a a_9005212   8.1063
   b =a_9005212;
   c =a_9005212;
   al 90.000
   be 90.000
   ga 90.000
   ' Lattice: Face-centered cubic
   site co_1 x =1/8;                  y =1/8;            z =1/8;            occ co 0.8000 beq 0.331
   site al_1 x =1/8;                  y =1/8;            z =1/8;            occ al 0.2000 beq 0.331
   site co_2 x =1/2;                  y =1/2;            z =1/2;            occ co 0.1000 beq 0.415
   site al_2 x =1/2;                  y =1/2;            z =1/2;            occ al 0.9000 beq 0.415
   site o_1  x !x_o_1_9005212  0.2631 y =!x_o_1_9005212; z =!x_o_1_9005212; occ o  1.0000 beq 0.769
   ' Unit cell volume [A^3]:  532.68
   ' Density (calculated) [g/cm^3]:  4.41000
   CS(cs_9005212, 1000 min 30)
   scale sc_9005212 0.001
   /*
     Reference: O¥Neill H St C, 'Temperature dependence of the cation distribution in CoAl2O4
     spinel Quenched from T = 1000 C', European Journal of Mineralogy 6, 603-609
     (1994).
   */
   ' Orig. COD entry no.: 9005212
   ' Link to original entry: http://sdpd.univ-lemans.fr/cod/cif/9/9005212.cif
```

The format is quite complex and allows the use of named variables. CrystalMaker will extract the full structure, including spacegroup (including origin choice), unit cell parameters (which may have constraints) and the asymmetric unit. The latter includes fractional coordinates, isotropic and/or anistropic displacement parameters and site occupancies (up to a maximum of 3 occupants per site).

In the (rare) case that the TOPAS file contains more than one structure, each structure will be loaded into the same window, and displayed as a thumbnail in the Structures List.

### Reference

Coelho, A. A. (2007) "TOPAS Academic: General Profile and Structure Analysis Software for Powder Diffraction Data." Bruker AXS, Karlsruhe, Germany.

# VASP

The "Vienna Ab Initio Simulation Package", or "VASP", is a program for first-principles calculation of electronic structures and quantum molecular dynamics. The software was developed by researchers at the University of Vienna, but is essentially commercial software in that a licensing fee is charged for its use.

## Structure Files

CrystalMaker provides visualization of structural output from VASP, in terms of the atomic coordinates listed in "`POSCAR`" and "`CONTCAR`" files.

The `POSCAR/CONTCAR` format is essentially a giant listing of atomic coordinates within a single unit cell, whose axial vectors are given relative to an orthogonal basis (see lines 3–5 in the example below).

One major limitation of this format (for VASP versions 4 and earlier) is that only positions are given: with no accompanying atomic species (element types, occupancy), labels, or other useful data. CrystalMaker will assign a default element symbol in these cases—which you should then override using the Crystal Editor, or (more conveniently) by editing element symbols in the Atoms Inspector.

VASP version 5 does now include the option of specifying atom types directly in the structure file, and CrystalMaker will uses these data, where provided.

The start of a VASP POSCAR coordinates file.

```
Ti  O
   1.0
      12.1787000000     0.0000000000     0.0000000000
       0.0000000000     3.7412000000     0.0000000000
      -1.9135761543     0.0000000000     6.2379921699
   8  16
Cartesian
       1.8402291696     0.0000000000     1.8221798928
       8.4248946762     0.0000000000     4.4158122772
       7.9295791696     1.8706000000     1.8221798928
       2.3355446762     1.8706000000     4.4158122772
      -0.1350844279     0.0000000000     4.3985330388
      10.4002082736     0.0000000000     1.8394591311
       5.9542655721     1.8706000000     4.3985330388
       4.3108582736     1.8706000000     1.8394591311
       1.6022482021     0.0000000000     0.0293185632
       8.6628756437     0.0000000000     6.2086736067
       7.6915982021     1.8706000000     0.0293185632
```

## Trajectory Files

CrystalMaker can read from VASP "`XDATCAR`" files, which contain a series of structures corresponding to the "trajectory" of a simulation. Note that these files can be very large! During loading, a progress bar is shown; you can cancel import and simply visualize the structures that have already been loaded.

The resulting "trajectory" comprises a series of structures, represented by thumbnails in the Structures List. We recommend using the **Transform > Synchronize** command to apply the visual settings, scale, range, etc., from the first-loaded structure, to all structures in the list.

**Faster Import:** To speed up the loading of an extended trajectory, you may wish to disable automatic bond generation. This can be done via the program's Preferences panel.

## Volumetric Data

VASP can output volumetric data files to represent the electron localisation function (`ELFCAR`), charge density (`CHG`, `CHGCAR`, `PARCHG`). These files include the crystal structure and can be imported directly into CrystalMaker.

### CHGCAR Files

This file contains a crystal structure and the total charge density (scaled by the unit cell volume). The total charge density is the sum of "spin up" and "spin down" contributions.

For spin-polarised calculations, the `CHGCAR` file contains a second dataset, referred to as "magnetization density", which is "spin up" minus "spin down". CrystalMaker will plot both datasets, if present.

## VESTA

As a service to new users migrating from the Japanese state-subsidised "VESTA" program to CrystalMaker, we provide import for VESTA structures files.

The structures files are very limited in nature, being plain text files with basic details of the crystal structure and its symmetry.

## WIEN2k

"WIEN2k" is a program for electronic structure calculations on solids, developed by researchers at the Technical University of Vienna.

CrystalMaker provides visualization of structural output from WIEN2k "`.struct`" structures files. This is a full crystal format, with unit cell parameters, fractional coordinates of atoms, and symmetry operators. Note that files use a fixed-column format, so care must be taken when editing.

**Tip:** WIEN2k uses an unusual method of specifying rhombohedral structures. Atomic positions are given relative to a rhombohedral cell, but the lattice paramters given are for an hexagonal cell. CrystalMaker automatically converts these to the rhombohedral cell.

The start of a WIEN2k structure file.

```
R   LATTICE,NONEQUIV.ATOMS:  4166_R-3m
MODE OF CALC=RELA unit=ang
   7.581584  7.581584 58.978376 90.000000 90.000000120.000000
ATOM  -1: X=0.38165000 Y=0.38165000 Z=0.38165000
         MULT= 2          ISPLIT= 4
      -1: X=0.51835000 Y=0.51835000 Z=0.51835000
Sr1        NPT=  781  R0=0.00001000 RMT=    2.3600   Z: 38.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.19601000 Y=0.19601000 Z=0.19601000
         MULT= 2          ISPLIT= 4
      -2: X=0.80399000 Y=0.80399000 Z=0.80399000
Zn1        NPT=  781  R0=0.00005000 RMT=    2.3900   Z: 30.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.11440000 Y=0.11440000 Z=0.11440000
         MULT= 2          ISPLIT= 4
      -3: X=0.88560000 Y=0.88560000 Z=0.88560000
P 1        NPT=  781  R0=0.00010000 RMT=    2.1200   Z: 15.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -4: X=0.30509000 Y=0.30509000 Z=0.30509000
         MULT= 2          ISPLIT= 4
      -4: X=0.69491000 Y=0.69491000 Z=0.69491000
O 1        NPT=  781  R0=0.00010000 RMT=    2.0900   Z:  8.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  12      NUMBER OF SYMMETRY OPERATIONS
 1 0 0 0.00000000
 0 1 0 0.00000000
 0 0 1 0.00000000
       1
 0 0 1 0.00000000
 1 0 0 0.00000000
 0 1 0 0.00000000
       2
 0 1 0 0.00000000
 0 0 1 0.00000000
 1 0 0 0.00000000
```

## XCrySDen

CrystalMaker can import the "XSF" and "AXSF" structure format used by various modelling programs. (This format originated with the old, X-Windows-based "XCrySDen" program.)

The XSF format allows for display of either crystal or molecular structures. Crystal structure files relate to a primitive unit cell (although the lattice vectors for a conventional cell are sometimes included as well). Note that there is no provision for specifying symmetry information. Atomic coordinate lines may include an extra set of values corresponding to the force on each atom; these are currently ignored by CrystalMaker.

An XSF file for a crystal structure.

```
# This is a comment line

 CRYSTAL

 # Lattice vectors for the primitive unit cell (in &Aring; units)

 PRIMVEC
    2.7100000000    2.7100000000    0.0000000000
    2.7100000000    0.0000000000    2.7100000000
    0.0000000000    2.7100000000    2.7100000000

 # Lattice vectors for the conventional unit cell (in &Aring; units)

 CONVVEC
    5.4200000000    0.0000000000    0.0000000000
    0.0000000000    5.4200000000    0.0000000000
    0.0000000000    0.0000000000    5.4200000000

 # Coordinates for all atoms in the primitive cell (in &Aring; units)

 PRIMCOORD
 2 1
 16      0.0000000000     0.0000000000     0.0000000000
 30      1.3550000000    -1.3550000000    -1.3550000000
```

### Animated Structure Files

A variant of the XSF format, "AXSF", acts as a container for multiple structures. For crystal structures there are two options, either a fixed-cell format (where the unit cell vectors are given once, at the start of the file), or a variable-cell format (where the unit cell vectors for each structure are listed). CrystalMaker can import both varieties, as well as the simpler animated molecular format.

### Volumetric Data

CrystalMaker can import volumetric data saved in the XSF file. Such data are aperiodic (i.e., cannot be tiled). CrystalMaker requires that the bounding box for the volumetric data be parallel to the (primitive) unit cell axes for the first crystal structure in the file. (CrystalMaker cannot import 2D datasets, or 3D datasets for a molecular structure.)

# XYZ

CrystalMaker can import and export "XYZ" files which comprise lists of atom types (element symbols) and their orthogonal coordinates.

A basic, 12-atom XYZ file.

```
12

C  -9.394        -2.061   -7.164
C  -6.549        -2.402   -5.772
C  -6.549        -2.968   -3.433
C  -9.392        -0.253   -14.627
C  -9.393        -1.494   -9.503
C  -6.548        -0.594   -13.235
C  -6.548        -1.161   -10.896
C  -9.392         0.314   -16.966
C  -6.547        1 .214   -20.698
C  -6.547         0.647   -18.359
C  -9.401        -7.293   -8.431
C  -6.556        -7.634   -7.039
```

The first line of the file is the total number of atoms to be read. The next line is blank. Subsequent lines contain the atom's element symbol, its number, and its orthogonal (structure) coordinates in Ångstrøm units.

You can include more than one structure in an XYZ file, e.g.,

Three structures included in the same XYZ file.

```
4

Si 0.000 0.000 0.000
Si 2.000 0.000 0.000
Si 0.000 2.000 0.000
Si 2.000 2.000 0.000
5

Al 0.000 0.000 0.000
Al 2.500 0.000 0.000
Al 0.000 2.500 0.000
Al 2.500 2.500 0.000
Al 2.500 2.500 2.500
8

Si 0.000 0.000 0.000
Si 2.000 0.000 0.000
Si 0.000 2.000 0.000
Si 2.000 2.000 0.000
Si 0.000 0.000 2.000
Si 2.000 0.000 2.000
Si 0.000 2.000 2.000
Si 2.000 2.000 2.000
```

If you export an existing *crystal* to XYZ format, CrystalMaker generates orthogonal coordinates $\{x_o y_o z_o\}$ using the standard convention:-

- The new $x_o$-axis is parallel to the crystal's $x$-axis.
- The new $y_o$-axis lies in the crystal's $xy$ plane and is perpendicular to $x_o$.
- The new $z_o$-axis is perpendicular to $x_o$ and $y_o$.

## CrystalMaker Text

CrystalMaker has a flexible text format that makes it easy to create your own crystals or molecules. You can create a CrystalMaker text file using a word processor (remember to save in "Text Only" format), or by using CrystalMaker to save a structure as a text file (**File > Export > CrystalMaker Text**).

For crystals, CrystalMaker requires at least:

- Unit cell parameters, *a*, *b*, *c*, α, β, γ
- Optional listing of bond specifications, atom types, etc.
- **ATOM** card, followed by a listing of element symbols, site labels and fractional coordinates for atoms in the asymmetric unit.

You can include other data, for example to specify colour settings, rendering, an orientation matrix, scale factor, and so on. For a detailed description of control cards and data specifications, please see *Appendix B: CrystalMaker Text File Reference*.

### 1. Simple Crystal Input

CrystalMaker text file for the mineral sphene

```
TITL  Sphene P2.1/a
NOTE  Speer & Gibbs 1976
CELL  7.07  8.72  6.57  90  113.9  90
SPGR  P 21/a
BOND  Si  O
BOND  Ti  O
XYZR  -0.5 1.5 -0.5 1.5 -0.5 1.5
ATOM
Ca  Ca     0.2424    0.9184    0.7512
Ti  Ti     0.5134    0.7542    0.2495
Si  Si     0.7486    0.9330    0.7490
O   O(1)   0.7499    0.8202    0.2502
O   O(2)   0.9108    0.8162    0.9347
O   O(3)   0.3827    0.9608    0.1459
O   O(4)   0.9122    0.3165    0.4368
O   O(5)   0.3813    0.4601    0.6468
```

The file begins with a title line (**TITL**) and a reference note (**NOTE**), both of which are optional. These are followed by the unit cell parameters (**CELL**), the spacegroup symbol, (**SPGR**) and two bond specification requests: Si-O and Ti-O bonds. A plot range (**XYZR**) has also been entered, followed by the listing of atoms in the asymmetric unit.

### 2. Defining Symmetry Manually

The next example shows the use of **SYMM** (symmetry) cards to define general equivalent positions, as an alternative to specifying a spacegroup symbol. Note that we have to include the lattice type, using an **LATC** card.

CrystalMaker text file for Cs-Leucite, with general-equivalent positions defined.

```
TITL  Cs-Leucite @ 80 K. Tetragonal
NOTE
Neutron powder diffraction refinement
by Palmer et al. (1997) Amer. Mineral.
CELL  13.54  13.54  13.75  90  90  90
SYMM  X,      Y,      Z
SYMM  1/4-Y,  1/4+X,  1/4-Z
SYMM  1/4+Y,  1/4-X,  1/4+Z
SYMM  1/2+X,  Y,      1/2-Z
SYMM  3/4-Y,  1/4+X,  1/4+Z
SYMM  3/4+Y,  1/4-X,  1/4-Z
SYMM  -X,     1/2-Y,  Z
SYMM  -X,     -Y,     -Z
LATC  I
BOND  Si  O
XYZR  -0.1 1.1 -0.1 1.1 -0.1 1.1
ATOM
Cs  W   0.36382   0.36725   0.12017
Si  T1   0.07041   0.38428   0.15683
Si  T2   0.17107   0.60684   0.12687
Si  T3   0.38649   0.64697   0.08203
O   O1   0.13170   0.29853   0.10767
O   O2   0.11643   0.49137   0.12233
O   O3   0.12912   0.66251   0.22413
O   O4   0.12631   0.66639   0.03492
O   O5   0.28923   0.58912   0.12999
O   O6   0.47933   0.61751   0.15505
```

### 3. Entering Temperature Factors

You can enter isotropic and/or anisotropic temperature factors in CrystalMaker text files, using the new **UISO**, **UANI** or **BANI** control cards, which are described below.

**UISO** This card is used to define isotropic temperature factors (values in Ångstrøms squared). The card should appear on its own line, followed by one or more data lines. Two values are expected per data line: the site label (which must match an entry in the **ATOMS** list), and the Biso value, in Å2.

**UANI** This card is used to define anisotropic temperature factors, Uij (values in $Å^2$). The card should appear on its own line, followed by one or more data lines. Seven values are expected per data line: the site label, followed by the six unique components of the ellipsoid tensor, in the order:

$U_{11}$ $U_{22}$ $U_{33}$ $U_{12}$ $U_{13}$ $U_{23}$

**BANI** Another card for anisotropic temperature factors, this time in the format $B_{ij}$. The card should appear on its own line, followed by one or more data lines. Seven values are expected: the site label, followed by the six unique components of the ellipsoid tensor, in the order:

$B_{11}$ $B_{22}$ $B_{33}$ $B_{12}$ $B_{13}$ $B_{23}$

An example of the use of some of these cards is included below.

CrystalMaker text file with isotropic and anisotropic temperature factors.

```
TITL    Pentanatrium hexahydroxoluminate dihyroxide, Na5[Al(OH)6](OH)2
NOTE
Crystal structure of Pentanatrium hexahydroxoluminate dihyroxide,
Na5 [Al(OH)6] (OH)2. Weinberger et al (1997) Z. Kristal. 212:236

CELL    9.350    9.350    9.610    90    90    90
SPGR    P 4.3 2.1 2
BOND    Al    O
BOND    Na    O
BOND    H     O
ATOM
Al    Al(1)    0.62756    0.62756    0.0
O     O(1)     0.42108    0.63353    0.0039
O     O(2)     0.83410    0.62507    0.0110
O     O(3)     0.62898    0.62763   -0.20193
O     O(4)     0.12094    0.6387    -0.2274
Na    Na(1)    0.87751    0.63244   -0.23217
Na    Na(2)    0.61276    0.86975   -0.27723
Na    Na(3)    0.12479    0.12479    0.0
H     H(1)     0.392      0.573      0.035
H     H(2)     0.856      0.693      0.040
H     H(3)     0.641      0.558     -0.224
H     H(4)     0.122      0.718     -0.213

! Isotropic temperature factors. These must come _after_ the 'ATOM' card.
! Each line must begin with a valid site label, followed by the Uiso value
! in units of A^2.
UISO
H(1)    0.057
H(2)    0.036
H(3)    0.043
H(4)    0.049

! Atomic displacement factors ("Anisotropic temperature factors), expressed
! as Uij values in A^2. (To use Bij values, use the "BANI" control card.)
!
! This card must come _after_ the 'ATOM' card. Each line must begin with a
! valid site label, followed by the six unique components of the Uij tensor
! in the order: U11 U22 U33 U12 U13 U23
!
UANI
Al(1)    0.0960    0.0960    0.0101    0.0005   -0.0002    0.0002
O(1)     0.0110    0.0169    0.0197   -0.0004   -0.0002    0.0031
O(2)     0.0113    0.0156    0.0147   -0.0002   -0.0006   -0.0019
O(3)     0.0146    0.0142    0.0122    0.0006   -0.0004   -0.0010
O(4)     0.0141    0.0163    0.0157   -0.0006    0.0007    0.0000
Na(1)    0.0127    0.0468    0.0161   -0.0004    0.0023    0.0002
Na(2)    0.0158    0.0181    0.0172   -0.0012   -0.0003    0.0025
Na(3)    0.0141    0.0141    0.0199    0.0004   -0.0020    0.0020
```

**Ellipsoids Require Crystals:** Please note that the CrystalMaker text format lets you define atomic displacement parameters ("thermal ellipsoids") for crystal structures only—not for molecules. Without an underlying unit cell, displacement parameters are essentially meaningless.

## Entering Molecular Data

It is also possible to use CrystalMaker's text format for molecules or crystal fragments that do not have translational symmetry. You must tell CrystalMaker that your file contains molecule data by including the **MOLE** card as the first entry.

You should also remember to include orthogonal coordinates for all atoms, in Å.

For molecules, CrystalMaker requires, at least:

- **MOLE** identifier card.
- Optional listing of bond specifications, atom types, etc.
- **ATOM** card, followed by a list of atoms, one per line. Each atom entry should include the element symbol, site label and the *xyz* orthogonal coordinates, in Ångstrøm units.

### Example CrystalMaker Molecule File

This example shows the input for the glycine structure. A title line is followed by a notebook entry (**NOTE**), a detailed list of bond specifications (**BMAX**) and atom type specifications (**TYPE**): giving atomic radii and colours as fractions of red, green, blue components. This file also contains comment lines, each of which must begin with an exclamation mark ("!"), or a C++ style double-slash ("//").

CrystalMaker text file for the glycine molecule.

```
MOLE  CrystalMaker molecule format
TITL  protonated glycine molecule
NOTE
glycine (H+)-B&S: an amino acid.
!
! request a ball-and-stick model
MODL  1
!
! Bond specifications: request C-C, C-O,
! C-H, C-N, H-N and H-O bonds.
BMAX  C   C   0.9638
BMAX  C   O   0.8410
BMAX  C   H   0.6958
BMAX  C   N   0.9360
BMAX  H   N   0.6655
BMAX  H   O   0.6383
!
! Atom types listed here.
TYPE
C     0.95    0.5000  0.5000  0.5000
H     0.57    1.0000  1.0000  1.0000
N     0.95    0.0000  0.0000  1.0000
O     0.89    1.0000  0.0000  0.0000
!
! Atoms listed using orthgonal
! coordinates in Ångstrøm units
ATOM
C   C1     0.4737   -0.1105   -0.2455
C   C11   -0.0787    0.3438    0.3863
H   H1    -0.3590   -0.7214    1.1253
H   H2    -1.0695    0.0747    1.1906
H   H21    1.3546    0.1011   -1.0457
H   H3    -1.0345   -0.5451    0.3448
H   H31   -0.4404    0.8343    0.0651
H   H32    0.3072    0.6438    0.8680
N   N1    -0.6683   -0.2508    0.7834
O   O1     0.4280   -0.8600   -0.3798
O   O2     1.0059    0.4099   -0.6187
```

## CrystalMaker Document

You may save full details of a structure using the **File > Save** or **Save As** commands. The result is a "`.cmdx`" binary data file which can be opened extremely quickly, and which retains full details of your structure, allowing you to replicate your exact screen display.

Note that whilst CrystalMaker X can open binary files created with earlier versions of the software (e.g., CMDF, CMMF), binary files generated by CrystalMaker X cannot be opened by earlier versions of the software. This is because CrystalMaker X uses a 64-bit format, whereas older versions of CrystalMaker are limited to 32-bit.

Please note that simply changing a file extension (e.g., ".cmdf" to ".cmdx") will *not* (miraculously) convert the file! CMDX files are completely different from earlier files and it's important that the program knows which is which—which is why users are advised to leave file extensions alone.

**Batch Export:** If you have a multi-structure document, you can export the individual structures to separate documents using the **File > Export Structures** command.

# CrystalMaker Data Files

## Element Data

CrystalMaker's Preferences panel has an Elements pane which lets you import or export tables of atom radius and colour information. For example, you may find it useful to maintain separate files for different kinds of structures, e.g., organics, organometallics, ionic structures, etc.

CrystalMaker element files are text files with a very simple format:

- An optional **NOTE** with information about the data (this will be displayed in the Element Editor's text field).
- An **ELMT** card, followed by a listing of element symbols, radii in Ångstrøm units, and fractional red/green/blue colour values.

Lines can be any length, but must be terminated by a return character and/or line break.

Part of a CrystalMaker Element data file.

```
NOTE
Default element radii: Using Shannon & Prewitt "Crystal" radii.
ELMT
Al  0.53  0.09751  0.67741  1.00000
As  0.72  0.28579  0.16544  0.31698 // This is a comment
```

The text file can also contain comments—these lines should begin with "**!**" or "//" characters.

### To import an element data file:

1. Open the Preferences panel (Mac users: **CrystalMaker > Preferences**; Windows users: **Edit > Preferences**).
2. Click the **Elements** button in the panel's toolbar.
3. When the Elements pane appears, ensure that its "**List**" tab is selected.
4. Click the **Actions** button (cog icon) at the bottom of the list and choose: **Import Data** from its popup menu. Your newly loaded elements will now be used when generating new structures and bonds.

### To export an element data file:

◆ Choose: **Export Data** from the Element Actions menu.

## Visible Coordination File

Use the **File > Export > Visible Coordination** command to generate a text file that summarizes the connectivity of the displayed structure. This lists each atom that is *visible on screen*. After each atom is a list of the bonded neighbours (if any) and their distances, and the resulting coordination groups are separated by blank lines.

## Crystal Coordination File

The **File > Export > Crystal Coordination** command is designed to provide an accurate summary of the coordination state for an ideal crystal lattice.

The resulting "Crystal Coordination" file lists every atom in a single unit cell—regardless of whether or not this atom is visible on screen. If global bond specifications have been defined, then CrystalMaker will use these to generate a list of nearest neighbours for each atom. The resulting coordination groups are separated by blank lines.

Unlike the **Visible Coordination** command, the Crystal Coordination command uses crystal symmetry to provide a complete bond listing for the unit cell, regardless of the current plot range and/or atom site visibilities.

## Distances & Angles File

CrystalMaker can generate highly-detailed information about the atomic environments in your structure, including bond search output (bond lengths and errors, if provided in an input file) plus bond angle information. These data are exported to a "Distances & Angles File", which is a plain text file, easily read with any text editor or word processor.

The format of the file can be summarised as follows:

**Input Data** The unit cell parameters, spacegroup symmetry, and view direction are listed, and the unit cell volume and density calculated. General equivalent positions are also listed.

**Coordinates** Each atom is assigned a number and all atoms residing within a single unit cell are listed with their fractional and orthogonal coordinates (Å units).

**Bond Distances** For each atom in the asymmetric unit, a list of all atoms closer than the default bond distance is given.

**Bond Angles** For the nearest neighbours listed in the bond length table, a separate listing gives the various bond angles between different combinations of close neighbours.

**Bond Summary** If bonds have been specifically requested then a table of bonded atoms is given. On each line, a centrally-bonded atom is listed, with its atom

number, followed by the atom numbers of its bonded neighbours. This is useful for identifying coordination numbers and polyhedra.

Part of a distances-and-angles file.

```
Bond angles around site T-site (Mg) to the 32 closest neighbours
+-------------------------------------------------------------------------+
| A       B       C        A-B-C [deg]   A-B [A]    B-C [A]    C-A [A] |
+-------------------------------------------------------------------------+
| oxy     T-site  oxy       109.4712     1.9173     1.9173     3.1309  |
| oxy     T-site  oxy       109.4712     1.9173     1.9173     3.1309  |
| oxy     T-site  oxy       109.4713     1.9173     1.9173     3.1310  |
| oxy     T-site  O-site     29.4963     1.9173     3.3498     1.9279  |
| oxy     T-site  O-site    121.4822     1.9173     3.3498     4.6481  |
| oxy     T-site  O-site    121.4822     1.9173     3.3498     4.6481  |
| oxy     T-site  O-site    121.4821     1.9173     3.3498     4.6481  |
| oxy     T-site  O-site    121.4821     1.9173     3.3498     4.6481  |
| oxy     T-site  O-site     29.4962     1.9173     3.3498     1.9279  |
| oxy     T-site  O-site     79.9750     1.9173     3.3498     3.5582  |
```

## Voxel File

CrystalMaker lets you export volumetric data (e.g., density or electron-density maps) as simply "Voxel" text files. These can be loaded back into the program, or shared with your own software.

CrystalMaker's "Voxel" format is very simple. It consists of:

- Title line.
- Header line with three integers: *Nx*, *Ny* and *Nz*. These are the numbers of data points along the unit cell's *x*, *y* and *z*-edges, respectively.
- A series of floating-point numbers corresponding to the *Nx* . *Ny* . *Nz* points.

The data points can be arranged on multiple lines if required, as long as they are arranged in the correct order: scanned along *z*, then along *y*, and finally along *x* (i.e., $\Delta z > \Delta y > \Delta x$). Programmatically, the data points are written out in a triple nested loop, e.g.,

```
for x=1 to Nx
{
    for y=1 to Ny
    {
        for z=1 to Nz
        {
            print value at {x,y,z}
        }
    }
}
```

Part of a Voxel file (long lines have been truncated).

```
Voxel data for "Electron Density" exported from CrystalMaker X for macOS
104    104    233
 8.798907e+01     8.725596e+01     0.000000e+00     8.508385e+01   ...
 3.303827e+01     3.775127e+01     0.000000e+00     4.216966e+01   ...
...
```

Chapter 15

# Gallery

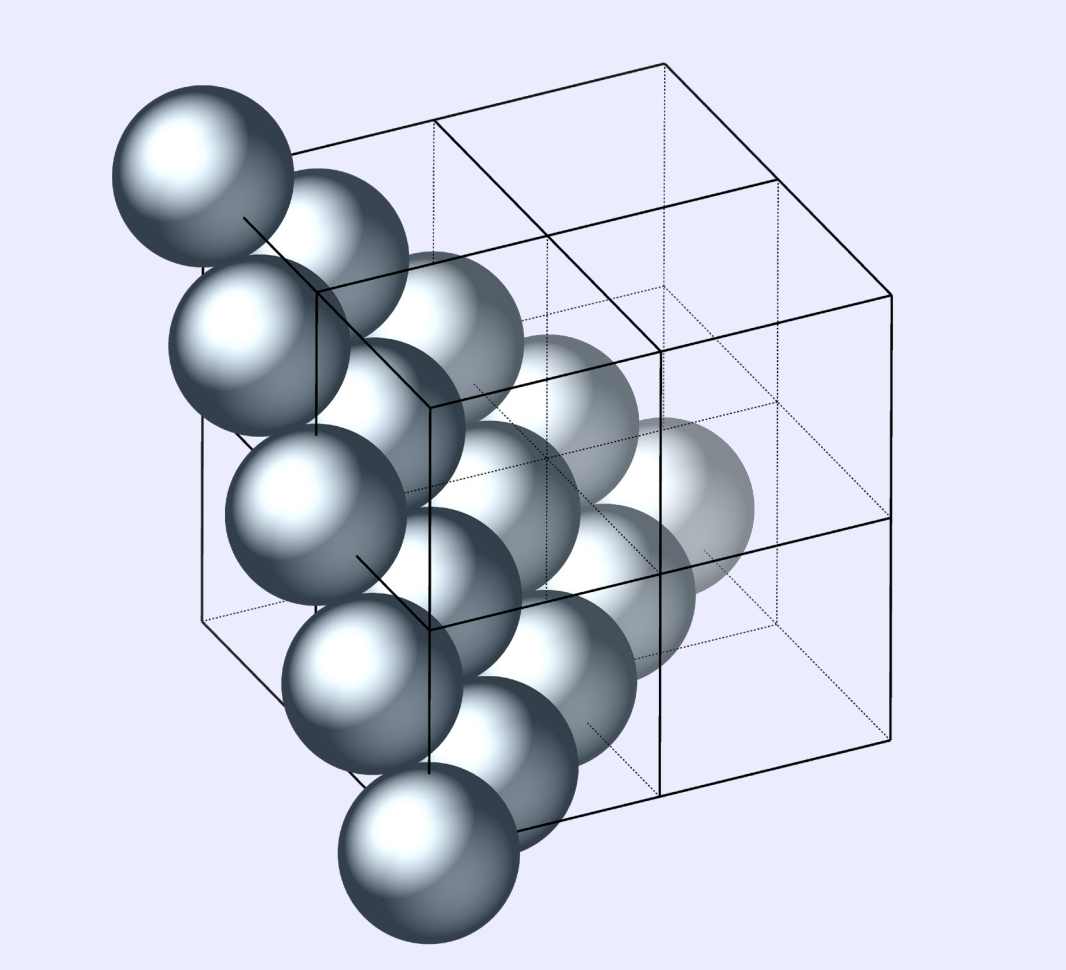
CrystalMaker has powerful graphics capabilities, with the option of photo-realistic rendering and high-=resolution output. This chapter shows some examples of crystal and molecular graphics, created and edited in CrystalMaker, and designed to illustrate potential appliations of the program. Each image is accompanied by a note explaining how it was produced.

To view a gallery of rotatable images, please see the *Examples* collection in the Library window (**View > Library**).

## CrystalMaker Images

You can export images from CrystalMaker using the **File > Export Graphics > 2D Graphics** command. For best results we recommend using a *pixel* format. Note that the PNG or TIFF formats provide *lossless* compression *and* the option of transparent backgrounds.

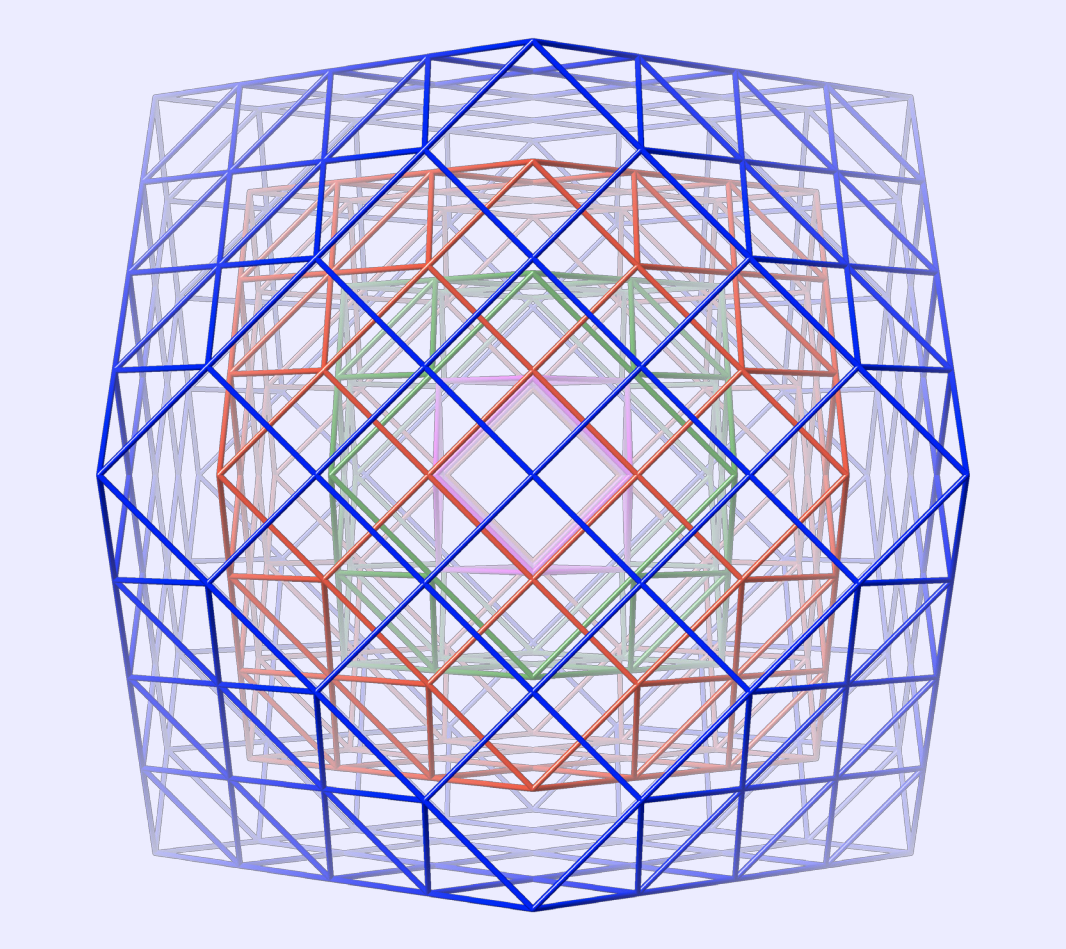
For reference, the images shown in the following page were all exported from CrystalMaker X as PNG images with the "transparent background" option selected.



## Cubic Close-Packed Plane

Isolating a plane of atoms inside a dense structure

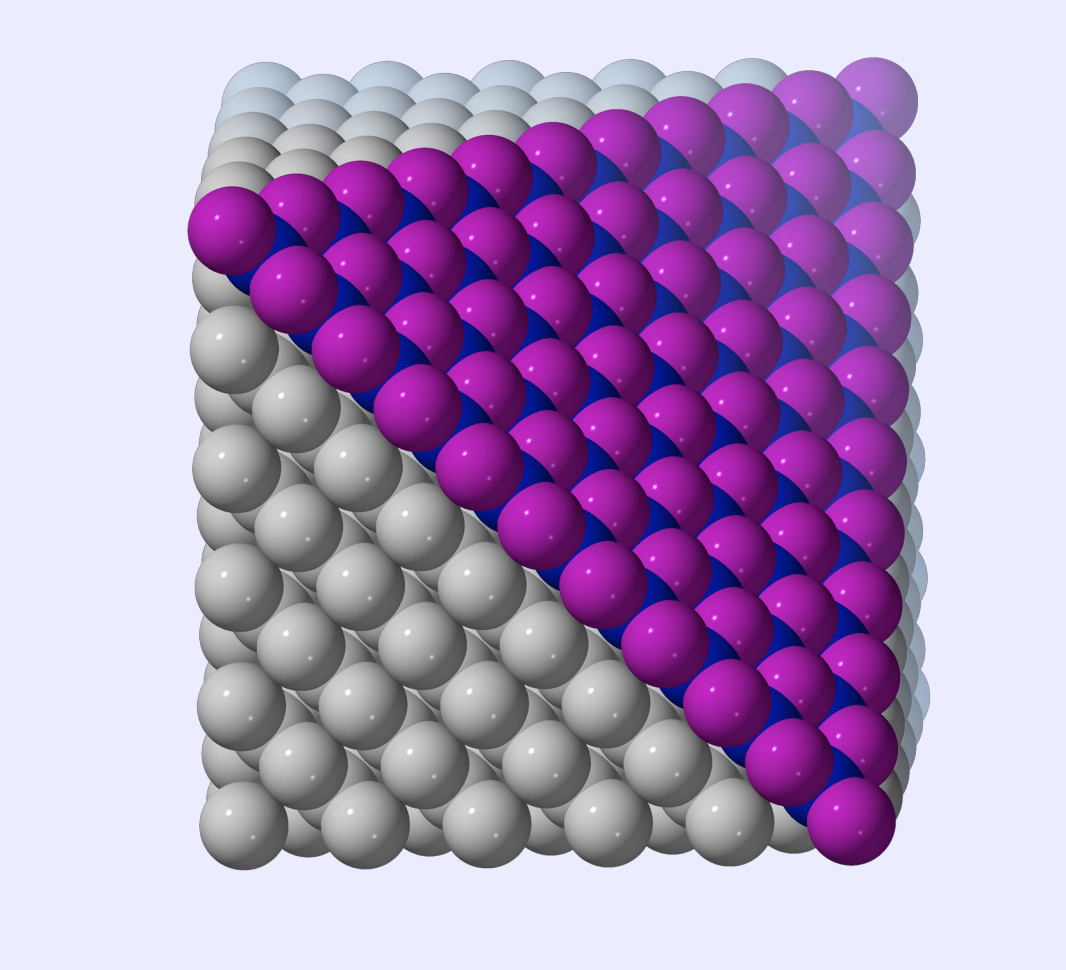
*One cannot use the* **Range** *command to visualise a single {111} plane. Instead, one can either use a pair of lattice planes to define a slab, or simply isolate the layer using the selection tools. I chose the latter method, given that this is such a simple structure. Finally I used the* **Reflectance** *pane of the Rendering Inspector to apply the* **Metal** *preset to the atom spheres.*



## Gold Coordination Cluster

Colour-coded coordination shells in the crystal structure of gold

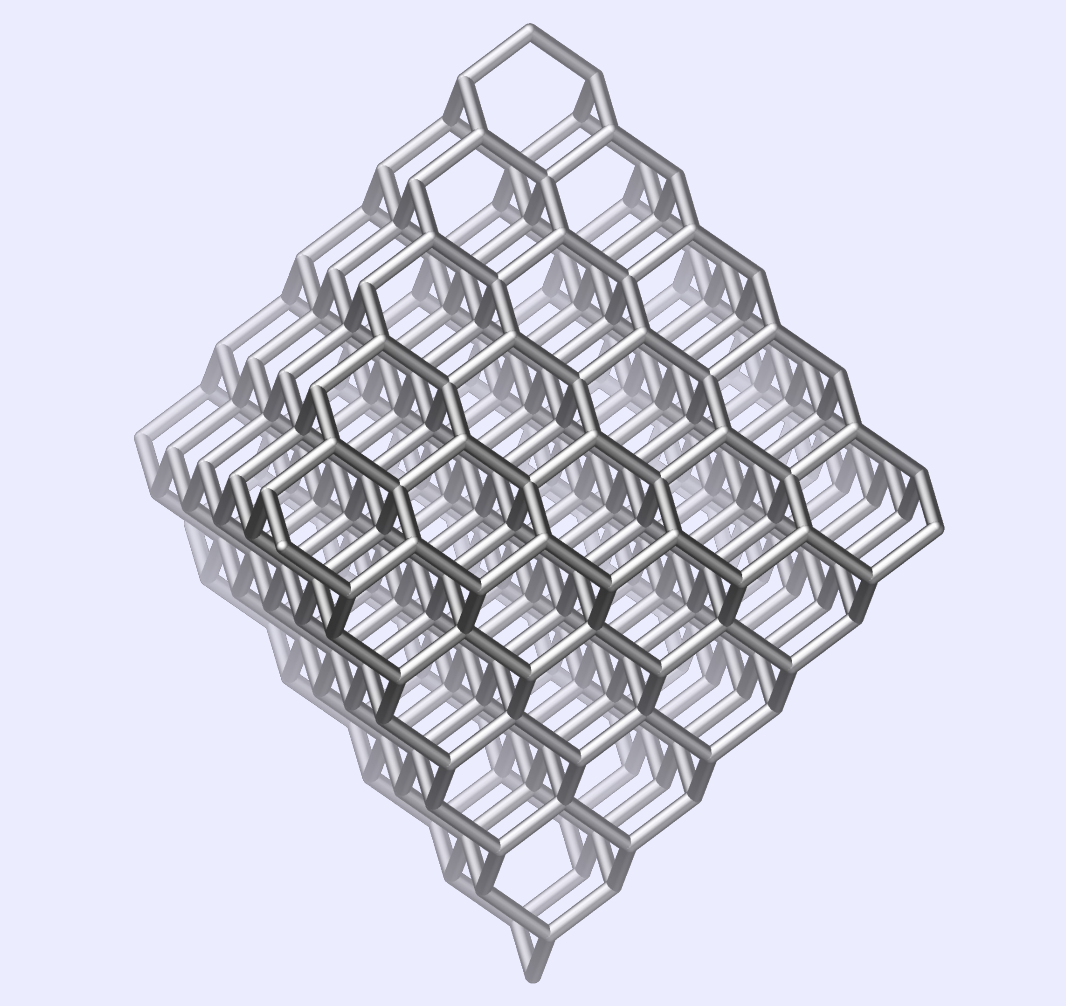
*I started with an extended block of unit cells. I selected one atom towards the centre and used the* **Extend Selection > Nearest Neighbours** *command four times: this resulted in all atoms out to the fourth-nearest-neighbour shell being selected. I then hid all remaining (unselected) atoms using the* **Isolate Selection** *command. I used the Selection Inspector to change the colour of all selected atoms to blue. I then had to work backwards, to colour the inner shells. This I did by repeating the selection process for the inner shells (select the central atom, then use the* **Nearest Neighbours** *command for the appropriate shell) and applying colours as appropriate.*



## Diamond (111) Plane

Colouring atoms with depth to emphasize the 3d structure

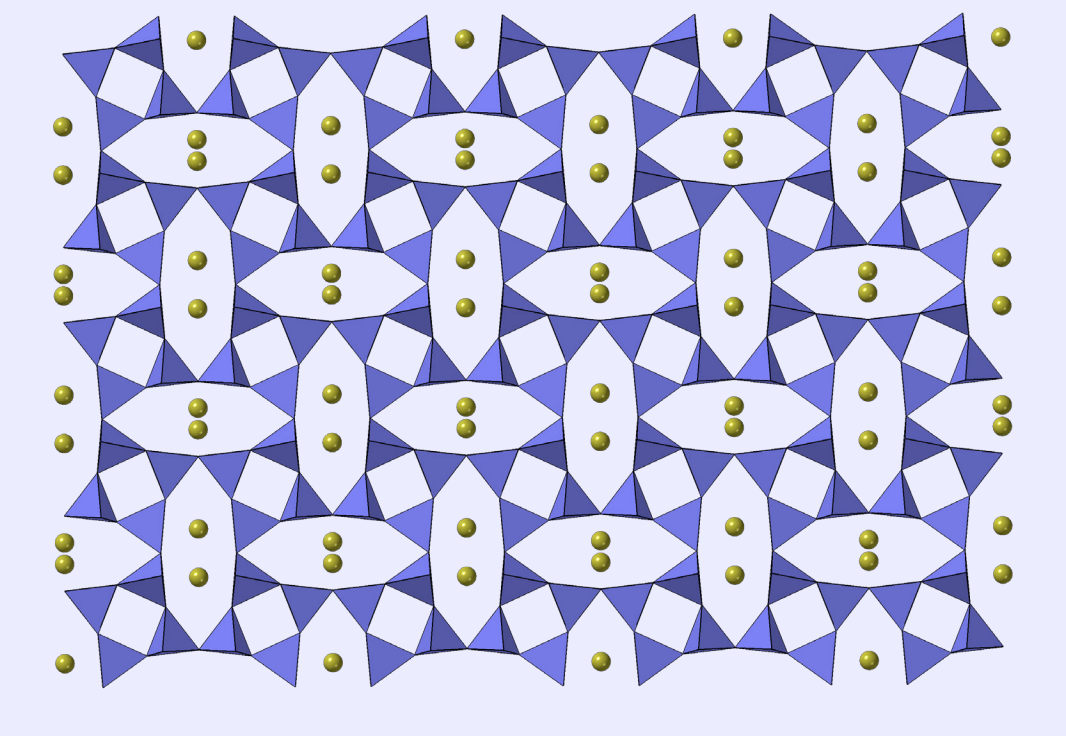
*I started with an extended block of diamond unit cells, shown here as a space-filling model. I added a (111) lattice plane and moved it to one corner of the block before the* **Transform > Slice Crystal** *command to hide the corner atoms. Next I viewed the newly-created surface sideways on. I used the Arrow tool to define rectangular selections around the top atoms (which I coloured purple, using the Selection Inspector) and then the atoms in the next layer down, which I coloured blue. This helps to emphasize the three-dimensional nature of the (111) surfae, with atoms visible at different depths.*



## Diamond Single Crystal

Cleaving a crystal to reveal the crystallographic basis for its habit

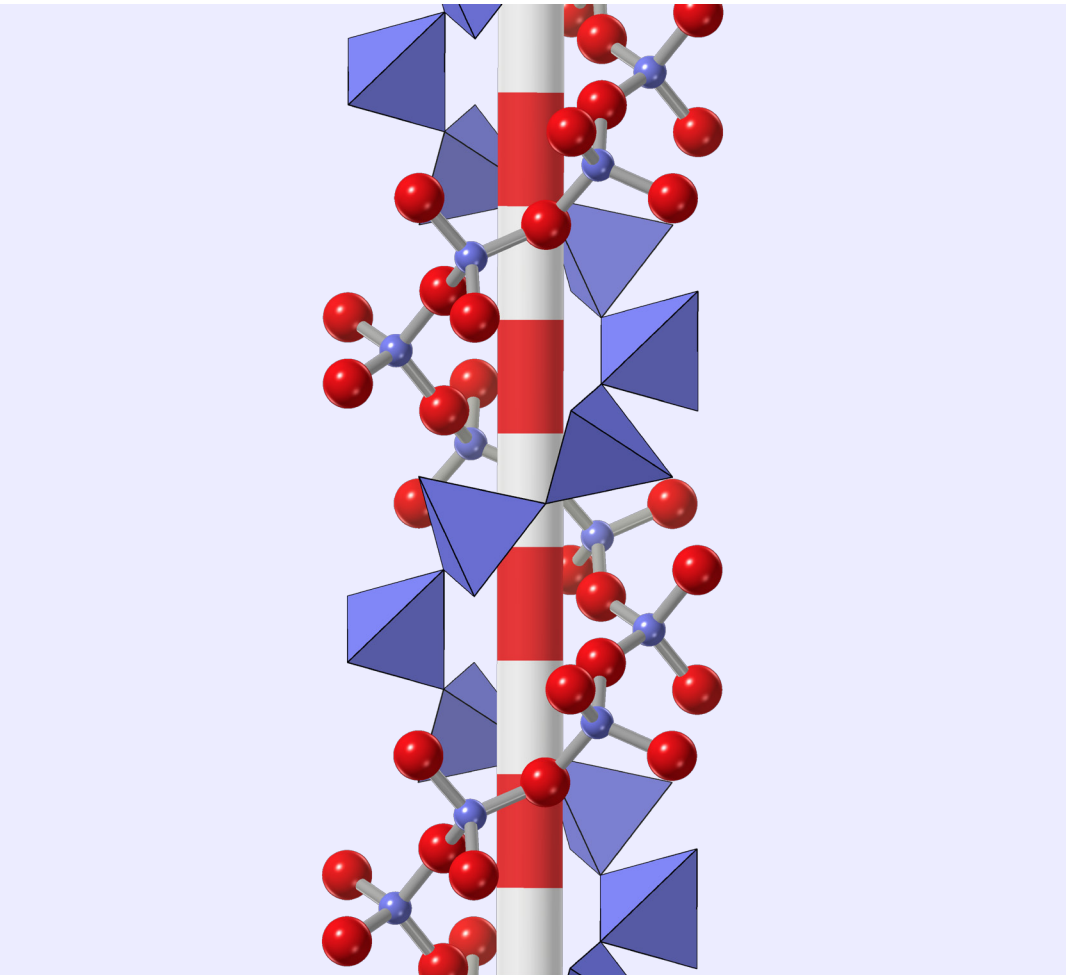
*Natural diamond forms octahedral crystals with {111} faces. This image is an example of how the Lattice Plane tool can be used to define crystal faces. I began with an 8 × 8 × 8 array of diamond unit cells, then progressively "cleaved" octahedral faces: first a pair of opposing (111) faces, next $(11\bar{1})$, then $(\bar{1}\bar{1}1)$ and then $(\bar{1}11)$. Finally I added some depth fading to give a more three-dimensional look.*



## Feldspar Ring Structure

Simplifying a complex structure by focusing on one layer

*Feldspar minerals have complex framework silicate structures, and are notoriously difficult to visualize. A helpful way of understanding the framework topology is to focus on $(20\bar{1})$ planes, as illustrated here. I started with a 4 × 5 × 8 block of unit cells, and added a pair of $(20\bar{1})$ planes which then allowed me to isolate a slab of crystal using the* **Transform > Make Slab** *command.*

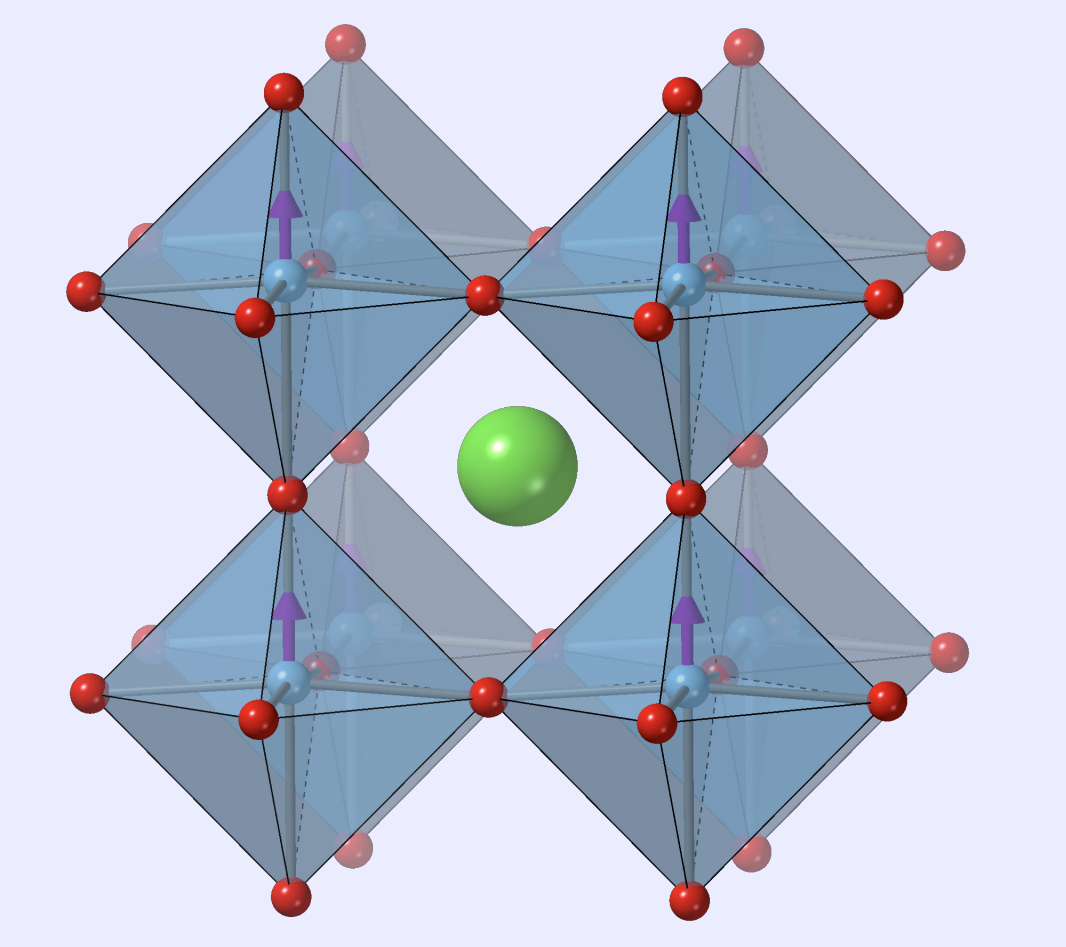


## Quartz Pole

Combining different representations in the same model using the Selection Inspector

*I viewed several unit cells of quartz down [001] and used the lasso tool to outline a double helix. I then rotated this through 90° to see two strands sideways on. I clicked on one polyhedron and used the* **Extend Selection > Fragment** *command to select the entire strand; this then allowed me to specify a ball-and-stick style for the strand atoms (using the Selection Inspector) to distinguish them from the polyhedra in the other strand.*

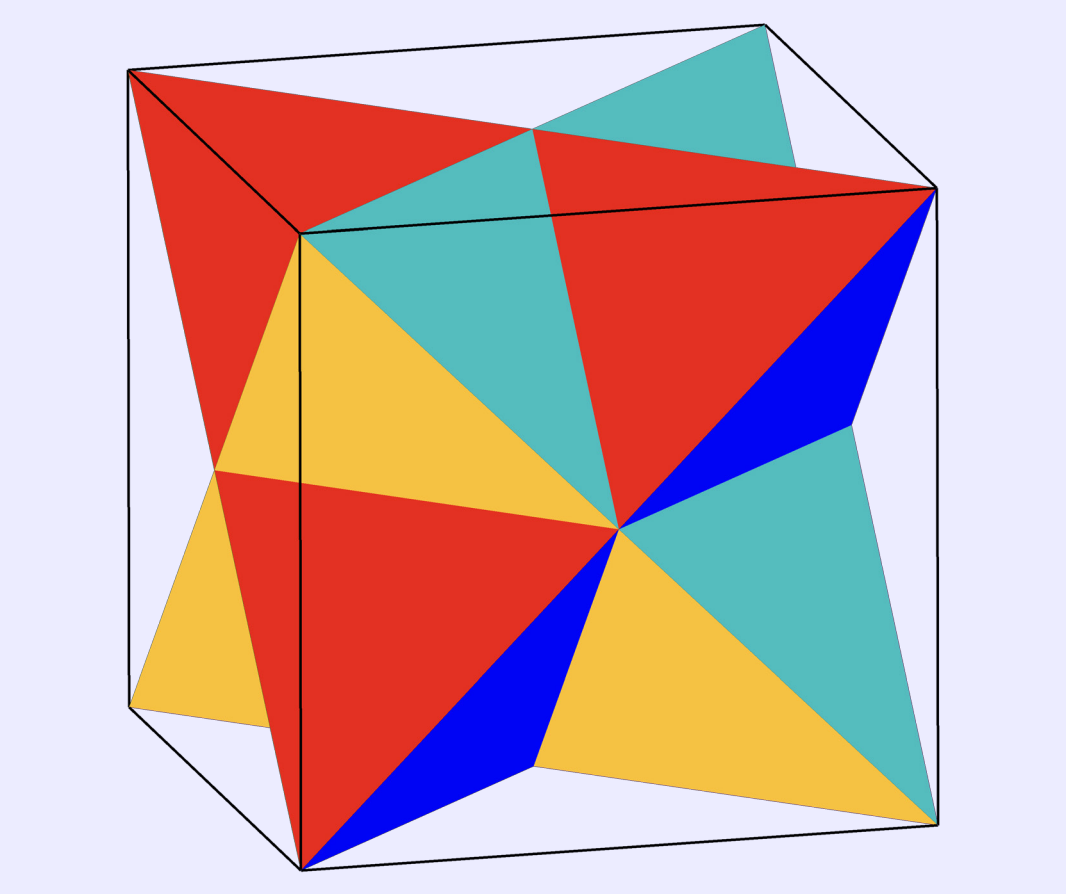
*To emphasize the structural channel, I added a dummy atom with bonds inside the channel. I used the Atoms Inspector to show these as "sticks" in polyhedral mode. Finally, I used the Model Inspector to set a "fat" stick radius.*



## Ferroelectric Distortion in $BaTiO_3$

Combining different representations to highlight physical properties

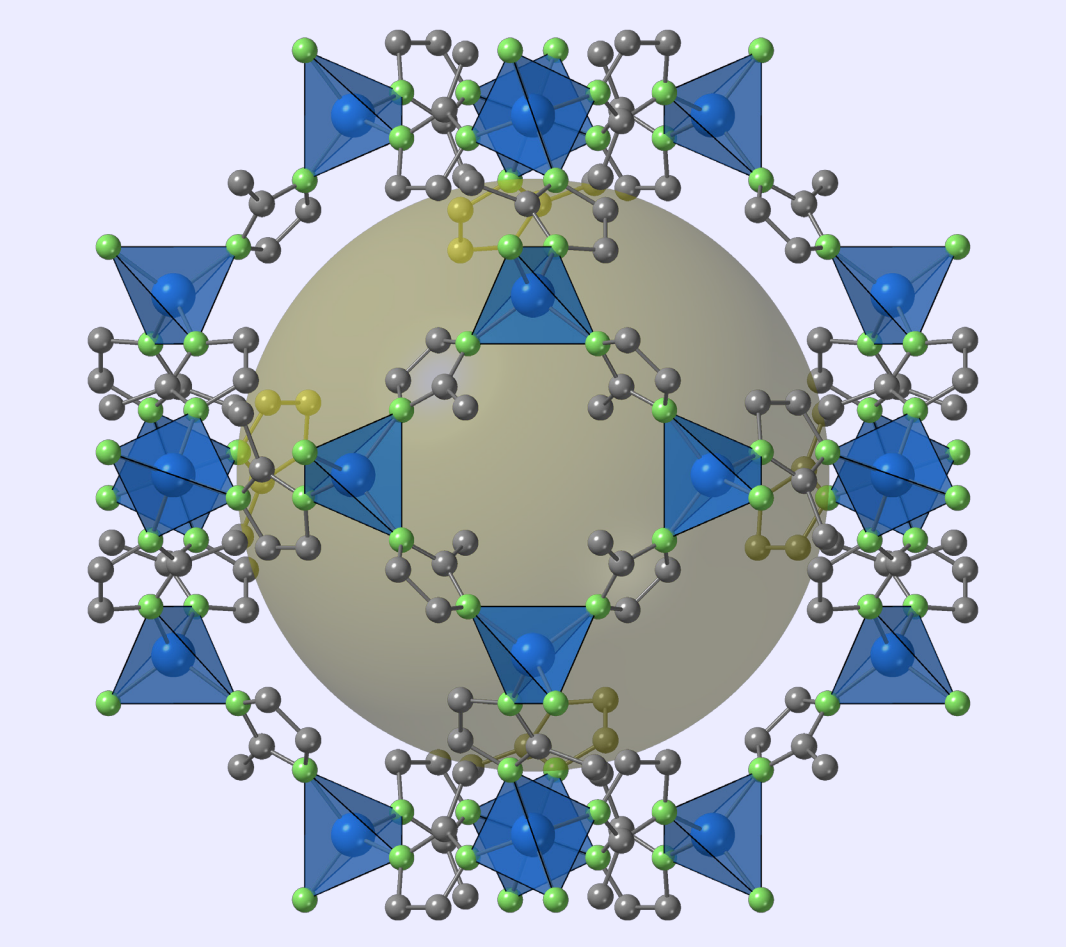
*Barium titanate is an important ferroelectric material. Dipoles are created by the off-centring of Ti cations in $TiO_6$ octahedra (associated with a cubic → tetragonal phase transition). The Ba ion resides in a large, 12-fold coordinated site. I started with a ball-and-stick model, and used the Arrow tool to select the Ti atoms. I then added vectors to the atoms using the Selection Inspector. I then switched to a polyhedral model, specifying translucent polyhedra with ball-and-stick bonds for Ti, and isolated spheres for the Ba and O sites. Because these spheres are plotted at their ball-and-stick sizes, I decided to make the oxygen atoms smaller by reducing their radius from 1.2 to 0.5Å, using the Atoms Inspector.*



## Stella Octangula

Symmetry-related lattice planes

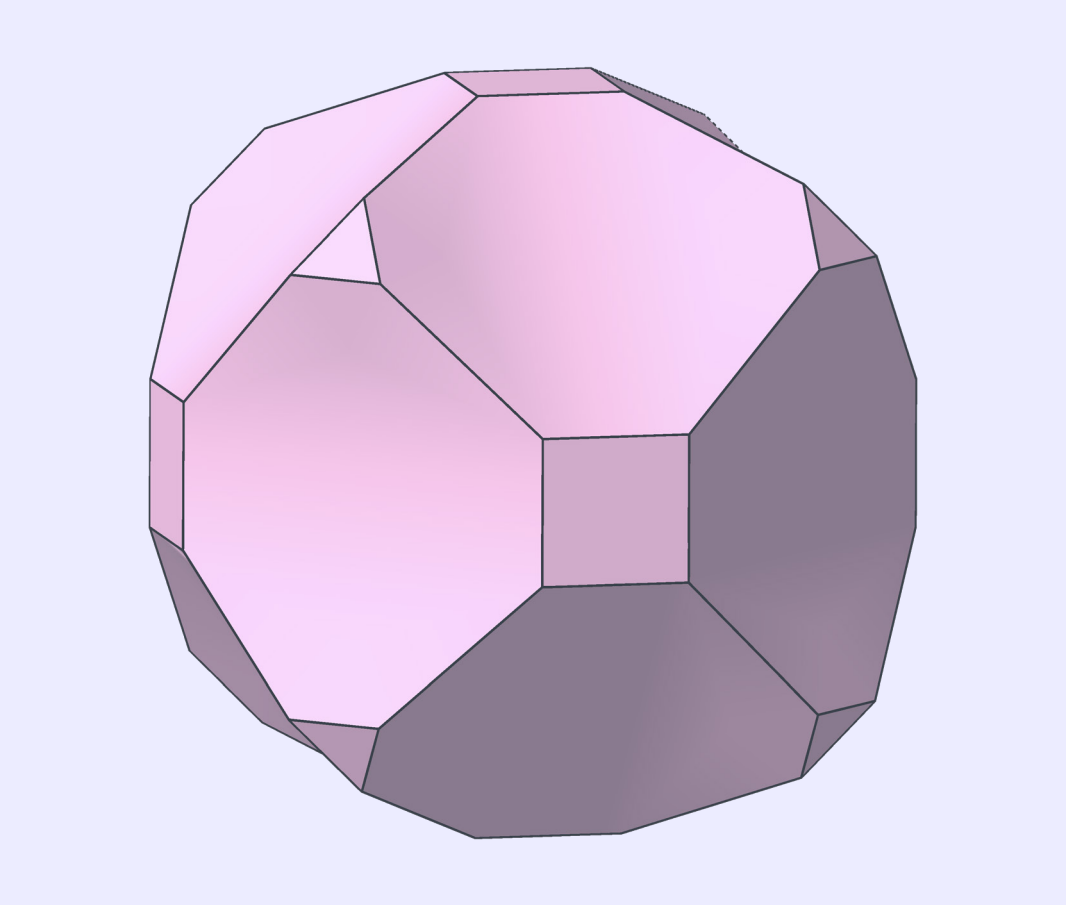
*The full set of {111} lattice planes for a cubic crystal, with each plane shown at its correct intersection with the unit cell axes. To generate this, I used the* **Lattice Planes** *group in the Volume Inspector to add a single (111) plane to a primitive cubic lattice (for which all atoms had been hidden). Next, I used the Actions menu to generate all symmetrically-related planes. These were auto-colorized using the same menu. I then selected all planes in the list and clicked a* **Move** *button to display the position popover; clicking the* **Move to Intercepts** *button ensured that each plane was then moved to its correct position.*



## Metal-Organic Framework

Visualizing a cluster using mixed polyhedra, bonding and a large sphere

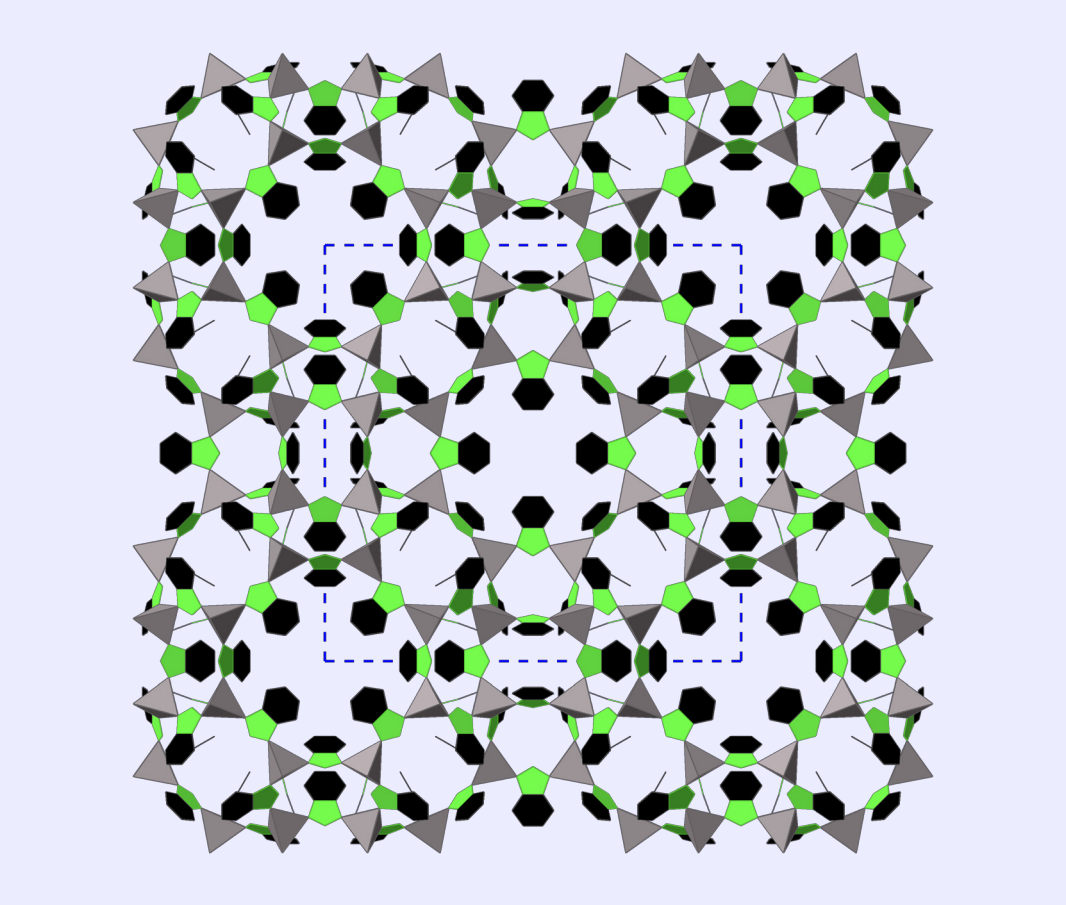
*This structure was built following the import of a crystal structure from a CIF file. I first had to check that I was using the correct, Covalent radii, then I switched to a polyhedral model and used the Atom Inspector to specify ball-and-stick styles for most atoms, apart from Zinc, which had a translucent polyhedral style. Next, I needed to add a translucent sphere in the centre of the unit cell. The symmetry of the crystal would cause problems, so this was discarded. I was then able to click with the Add Atom tool to add a dummy "S" atom, which was assigned a translucent sphere style, and a radius to fit the size of the cavity. To define a radial cluster, I selected the dummy atom and chose:* **Transform > Define Cluster**, *specifying "centre of selection" with a radius of 11.5 Å.*



## Curved Polyhedron

Representing the shape of a cage using a single polyhedron

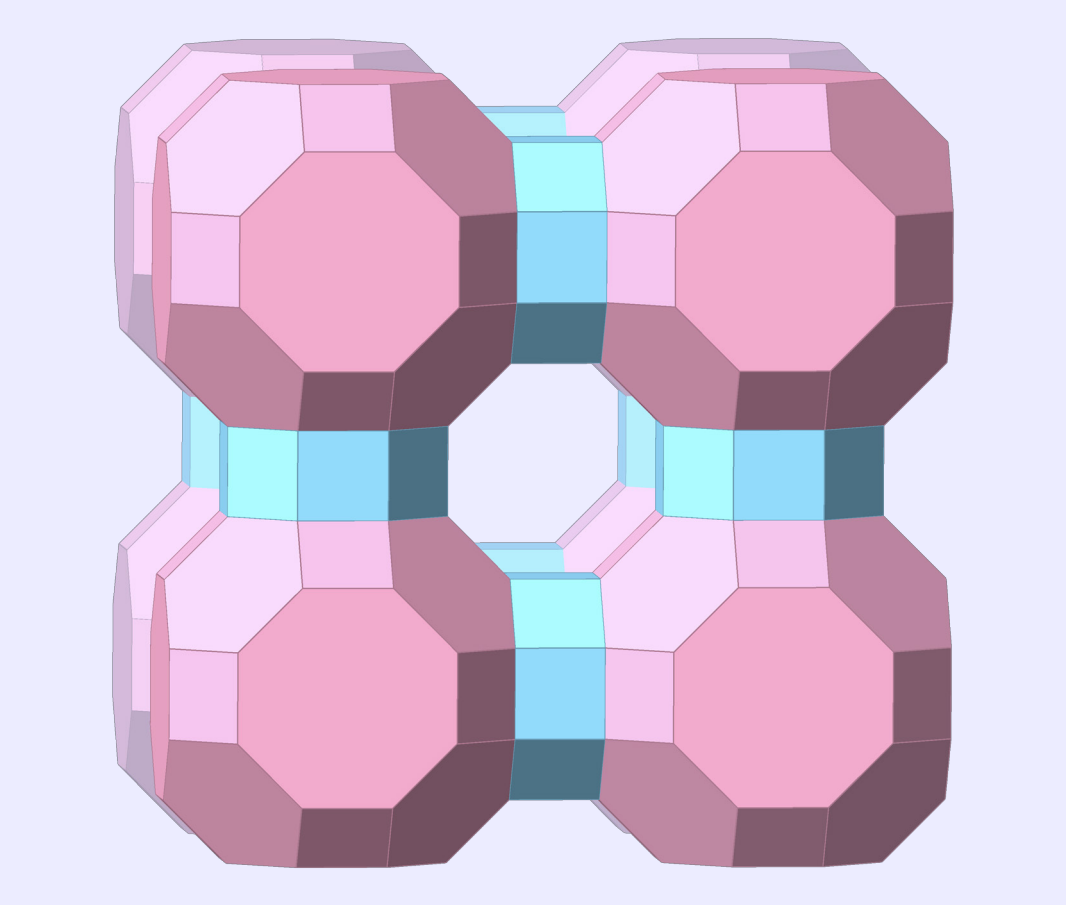
*I started by identifying possible "vertex atoms" to highlight the shape of this Molecular Organic Framework cage. I selected these vertices then used the* **Transform Selection > Add Centroid Atom** *command to insert a dummy atom (with bonds) at the centre of the cage. All other atoms were then hidden. By switching to a polyhedral model I was able to choose a filled polyhedral style for the dummy atom, and blank styles for its vertex atoms. I then used the* **Polyhedra** *group in the Model Inspector to specify concave faces, which gives a better idea of the three-dimensional shape.*



## Simplifying ZIF11

Highlighting the framework with simple polyhedral units

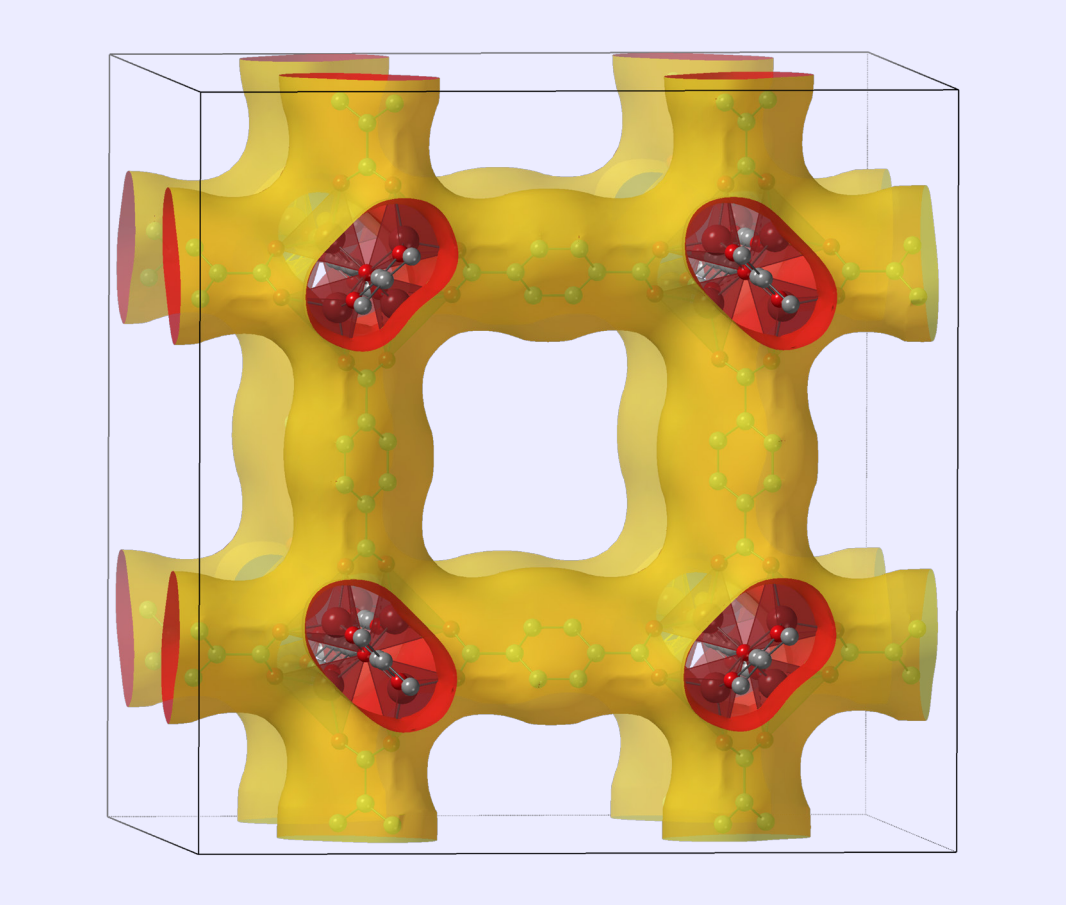
*Zeolitic Imidazolate Frameworks (ZIFs) have immensely complex structures that make it difficult to see the proverbial "wood for the trees". Here I have represented the imidazolate rings by green pentagons, the benzene rings by black hexagons, and the tetrahedral zinc coordination groups by tetrahedra. All apical atoms were then hidden. To show the rings, I used the* **Extend Selection > Ring** *command to select all atoms in a single ring; I then defined a dummy atom at the ring centroid using the* **Add Centroid Atom** *command. The dummy atom was given a "filled" polyhedral style and its vertex atoms given blank styles. Because of symmetry, I only needed to do this for a few rings.*



## Cages in ZIF11

Highlighting the framework with simple polyhedral units

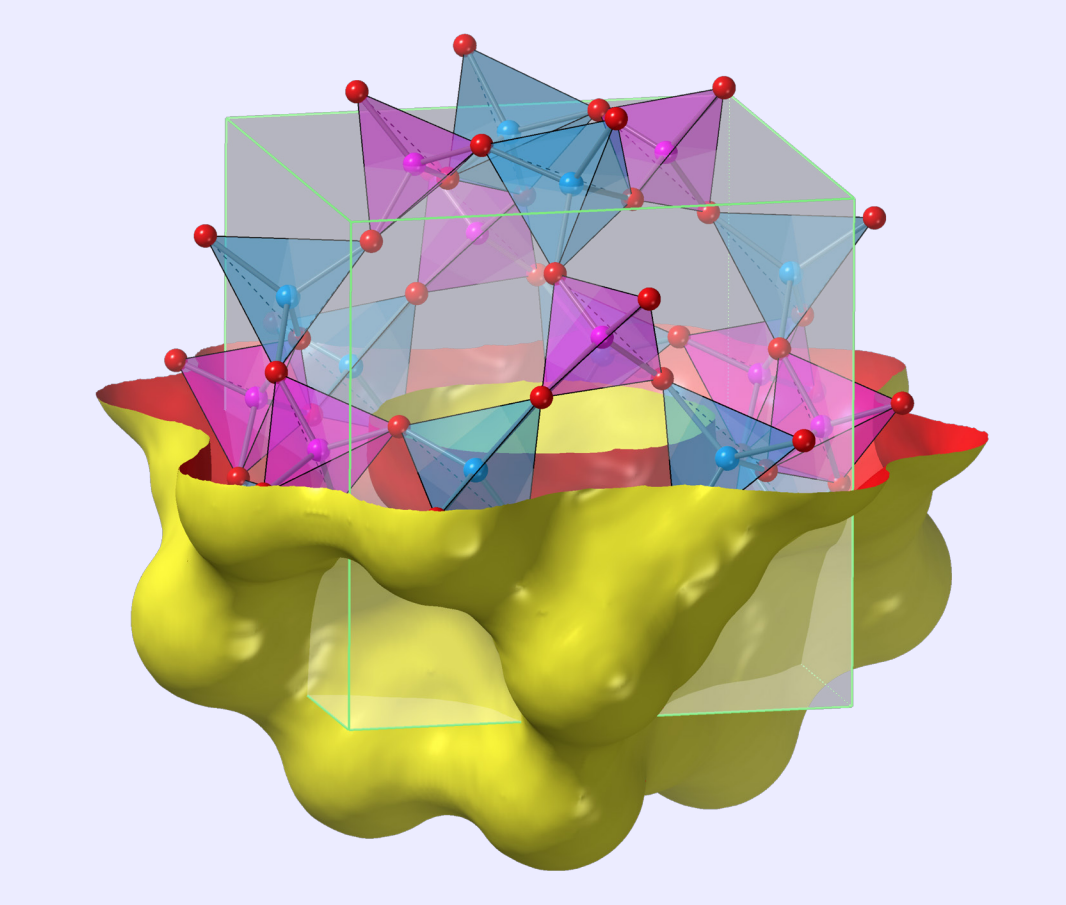
*This is an extreme example of simplifying the ZIF structure! Here I have hidden all atoms apart from Zn: these define the corners of 48-vertex and 16-vertex cages. I again used the* **Transform Selection > Add Centroid Atom** *command to generate dummy atoms at the centres of the cages. I gave each dummy atom a different (dummy) element symbol, and applied different colours to the two symbols. I then switched to a polyhedral model and assigned a blank style to the Zn atoms so that just the cages are visible.*



## MOF Envelope

Emphasizing the overall shape of a channel structure.

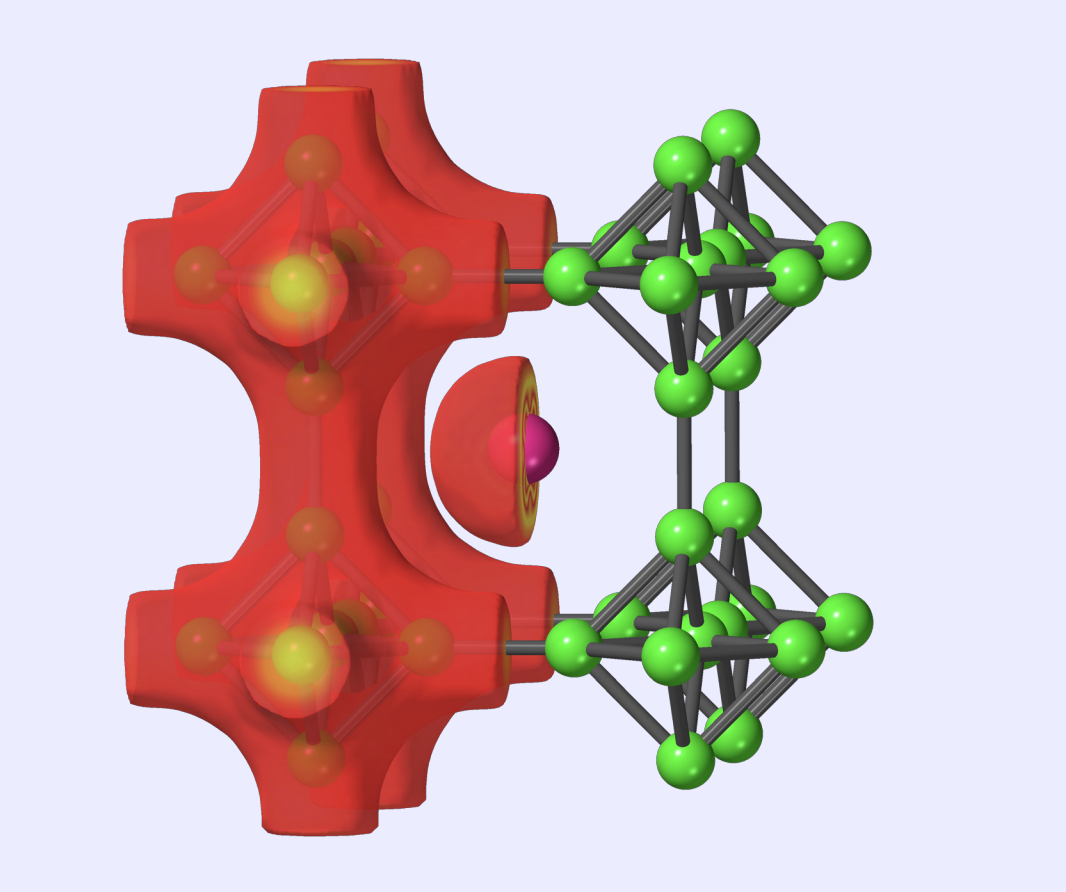
*Metal-Organic Frameworks (MOFs) such as this one ("MOF5") comprise organic "struts" connecting metal/complex "hubs". The overall structure can be difficult to visualize, so here I decided to hide the detail by overlaying a solvent-excluded surface. In this way, one focuses on the overall shape of the network, and can clearly see the free space. The surface was generated using the Volume Inspector; I chose a 1.4 Å radius, so as to show the effective surface available to a water molecule.*



## Sodalite Cage

A stylized representation combined with a surface cutaway.

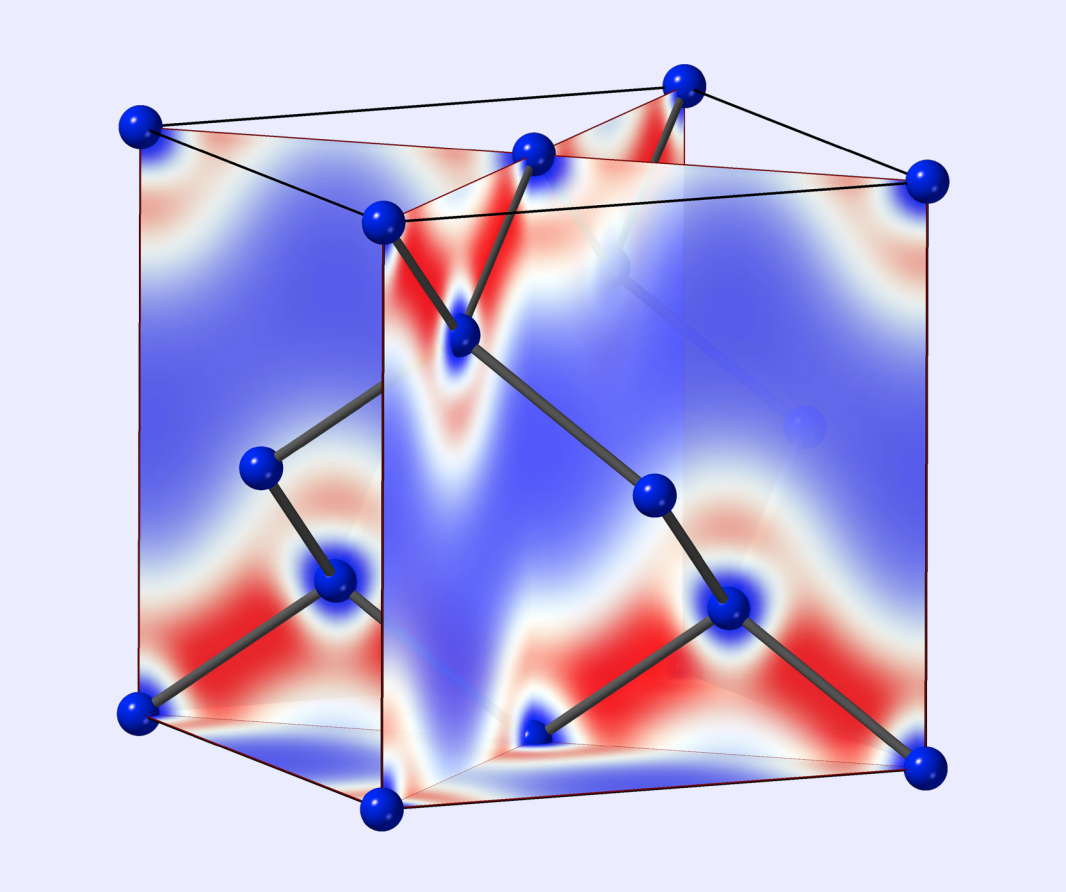
*This picture shows that you can "have your cake and eat it"! I wanted to simplify the quite complex framework structure, using a polyhedral model—but I also wanted to show the effective surface area available to a water molecule (sodalite is a mineral, and water is all-pervasive in nature). I used a translucent polyhedral model, added a unit cell—with translucent faces—and capped this off with a 1.4Å solvent-excluded surface. The problem then was that most of the structure was hidden by the surface… To overcome this, I temporarily hid all the atoms, then used the Arrow/Rectangle tool to select half the surface, hiding the selected voxels. Finally, I brought the hidden atoms back into view.*



## Charge Density in $SmB_6$

Slicing a volumetric dataset to reveal more of the crystal structure.

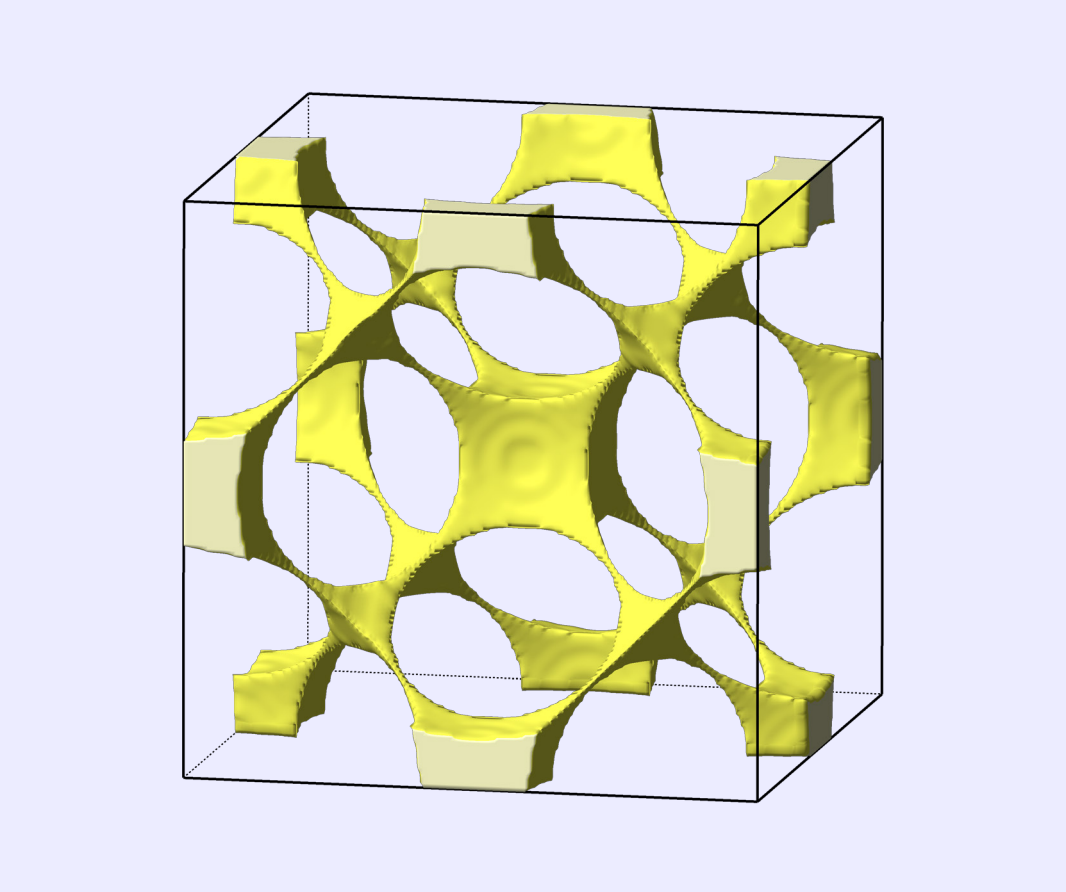
*I started with a CASTEP charge density file (courtesy of Prof Martin Dove, QMUL) which was imported into CrystalMaker. I displayed an iso-volume for the range 1.6–100% and gave this a gradient and a partial opacity. Next I hid all the atoms so that just the volumetric data were visible. Using the Arrow tool to define a selection rectangle, I selected then hid half of the volumetric data. I then made all the atoms visible again. This gave a "split view" of the translucent dataset plus the crystal—and allowed the gradient to be visible on the cut section of the volumetric dataset.*



## Charge Density in Silicon

Lattice plane slices reveal shared electron density and covalent bonding.

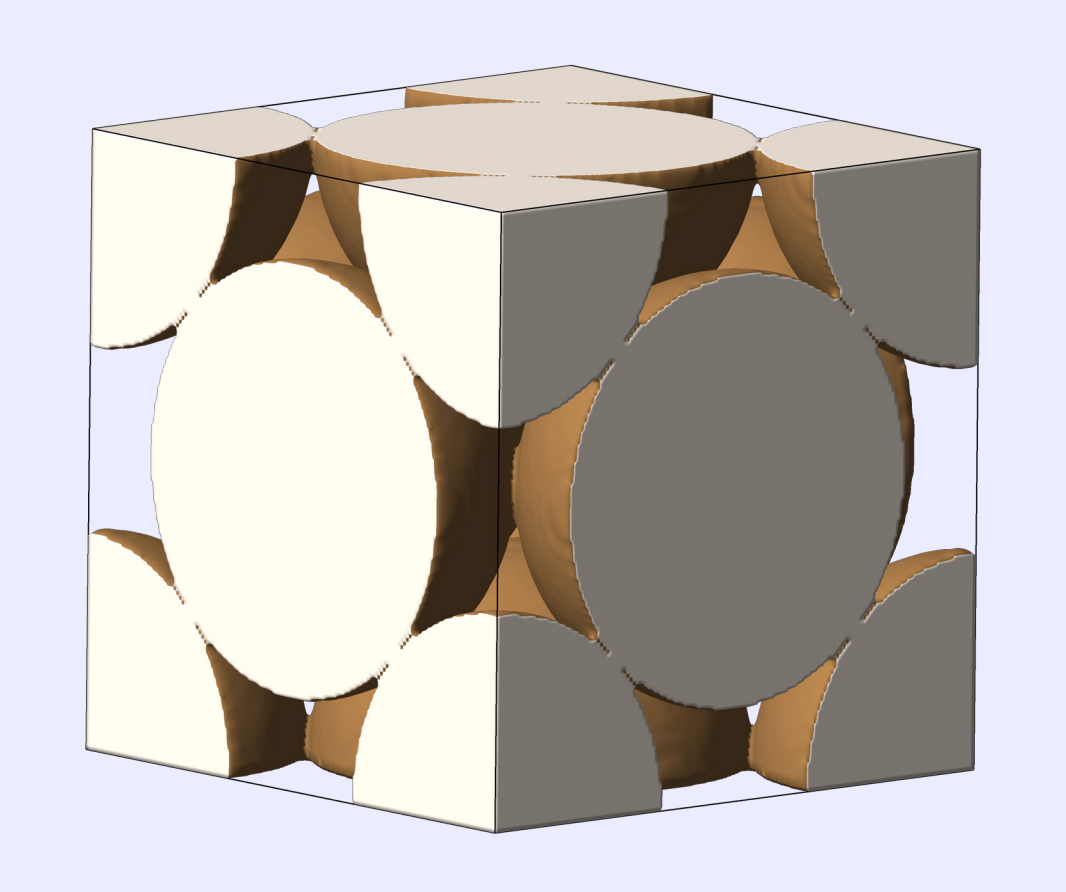
*I started with a VASP file (courtesy of Dr Paul Fons, AIST, Japan) which was imported into CrystalMaker. I chose to display the charge density as lattice plane slices, showing two {110} planes and an (001) plane. I chose a "polar" colour scheme and specified partial translucency (~90% opaque). This view nicely shows the shared electron density between silicon atoms: confirming covalent bonding.*



## Porosity in Copper

Visualizing interstitial space in a cubic close-packed crystal.

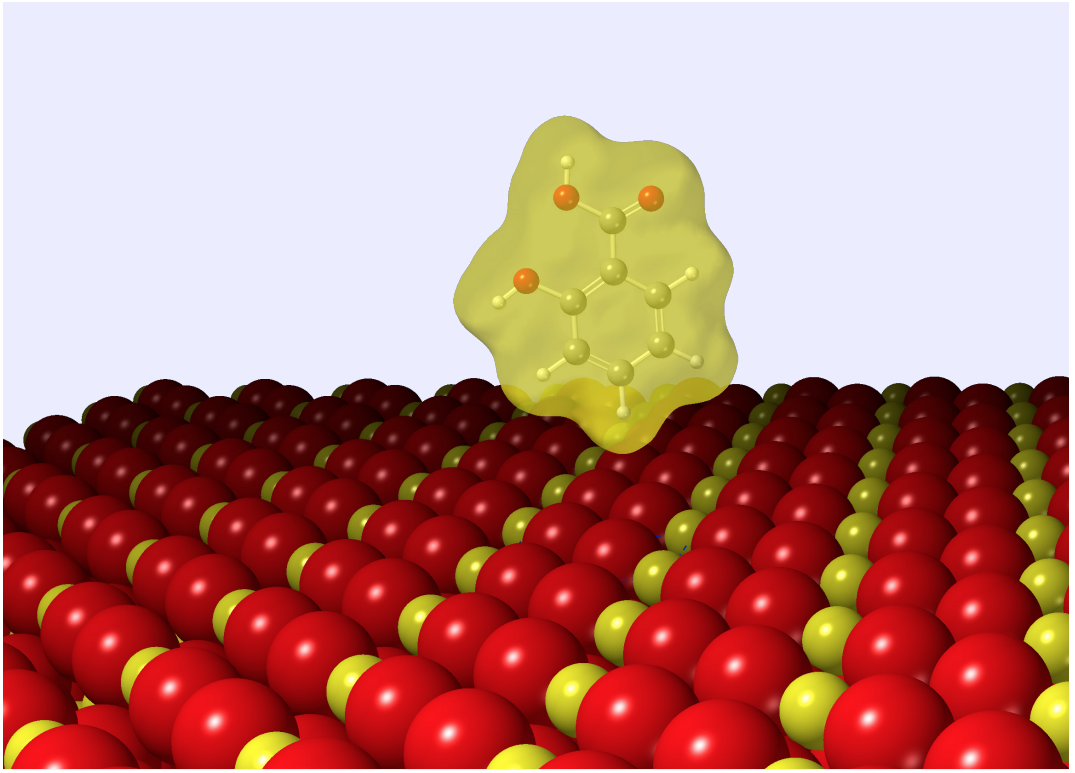
*Porosity visualisation of one unit cell of copper, created using the* **Calculate > Porosity Map** *command. I wanted to emphasize the shapes of the interstices, so I made the copper atoms slightly larger than their atomic radii. This makes it easier to see the tetrahedral interstice shapes. Note the cube-shaped interstice at the centre of the unit cell: this is surrounded by six copper atoms, whose centres define a regular octahedron. The texture you see on the surface of the voids is a sampling artefact, caused when attempting to smooth a finite number of volumetric elements (voxels).*



## Filled Space in Copper

Counting the number of atoms in one unit cell.

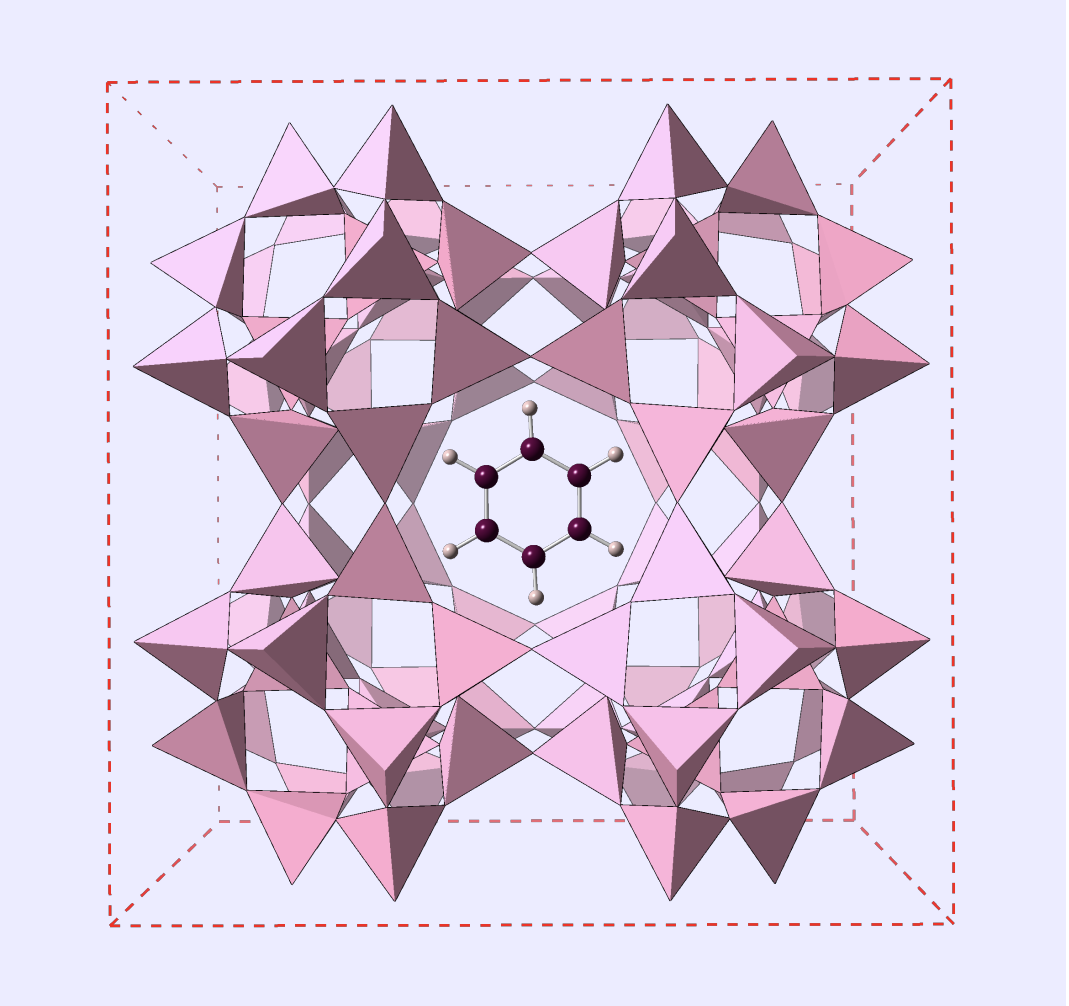
*This is another volumetric visualization, this time showing filled space, rather than empty (void) space. The plot range of one unit cell shows the part of each atom that lies inside this unit cell of copper. To generate this, I hid all copper atoms then specified a high-resolution "porosity map" with the "filled space" option set.*



## Organic Molecule on Rutile (001)

Placing a molecule onto a crystal surface

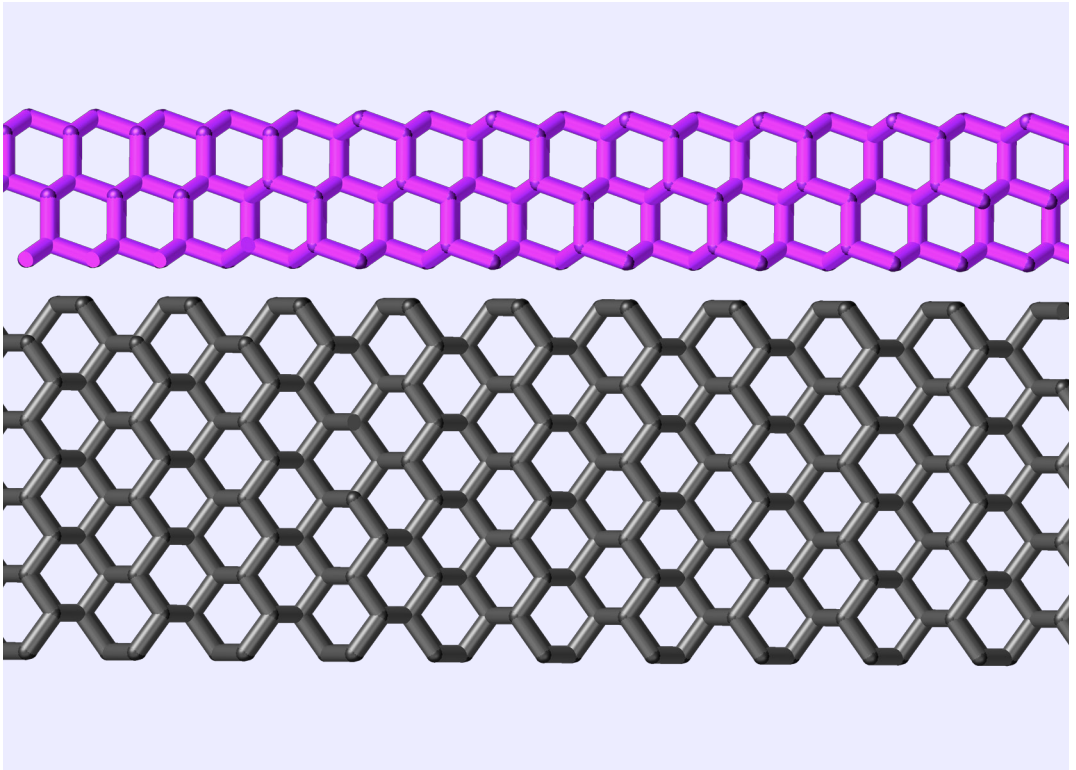
*CrystalMaker X makes it very easy to work with multiple structures in the same window: in this case a crystal surface of rutile and an organic molecule (aspirin). I was able to manipulate the molecule relative to the crystal by locking the crystal then using the Rotate and Move tools to reposition and reorient the molecule. I made the molecule the primary selection and added a Solvent-Excluded surface around it. Returning to the crystal as the primary selection, I set an appropriate scale and added some perspective and depth fading.*



## Benzene Molecule Inside Zeolite Channel

Placing a molecule inside a 'polyhedral' structure

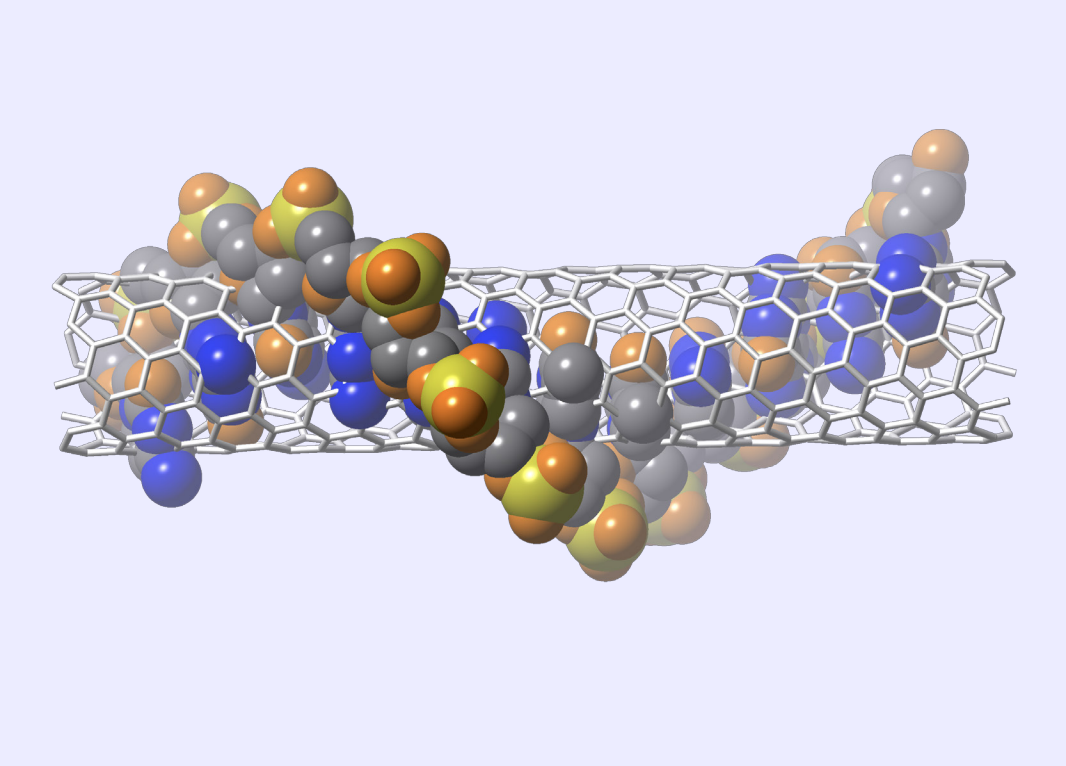
*This is another easy example showing how one can combine multiple structures in the same window. I took the crystal structure of a zeolite, loaded a benzene molecule in the same window, and made both structures visible: the molecule was centred inside the crystal. Note that, if one wished, one could merge the two structures into a single structure (thereby replicating previous versions' "Place Molecule" commands).*



## Silicon Interface

Combining multiple orientations in the same window

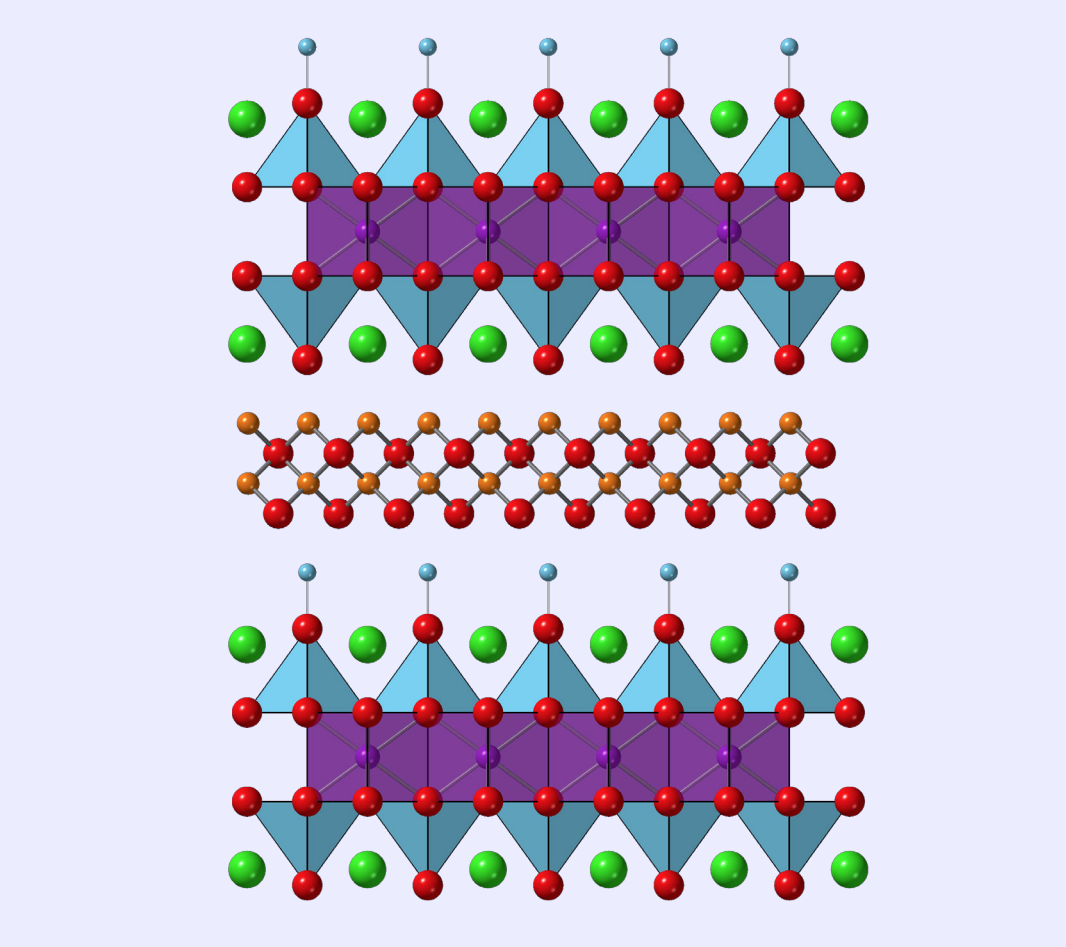
*This interface shows two orientations of the same material: a (111) slab of silicon sitting directly above a (110) slab. I started by loading the silicon structure and generating an extended range of atoms. I then duplicated this structure—giving me two thumbnails in the Structures List. I used a pair of (111) planes to define a slab for the first structure, then repeated the operation for the second structure—using (110) planes. Next, I assigned different colours to each structure. Finally, I made both structures visible by shift-clicking on their thumbnails. Some slight adjustment of positions was necessary, and was achieved by locking one structure and then using the Move tool to reposition the other.*



## Nanotube with DNA Strand

Combining multiple structures & representations in the same model

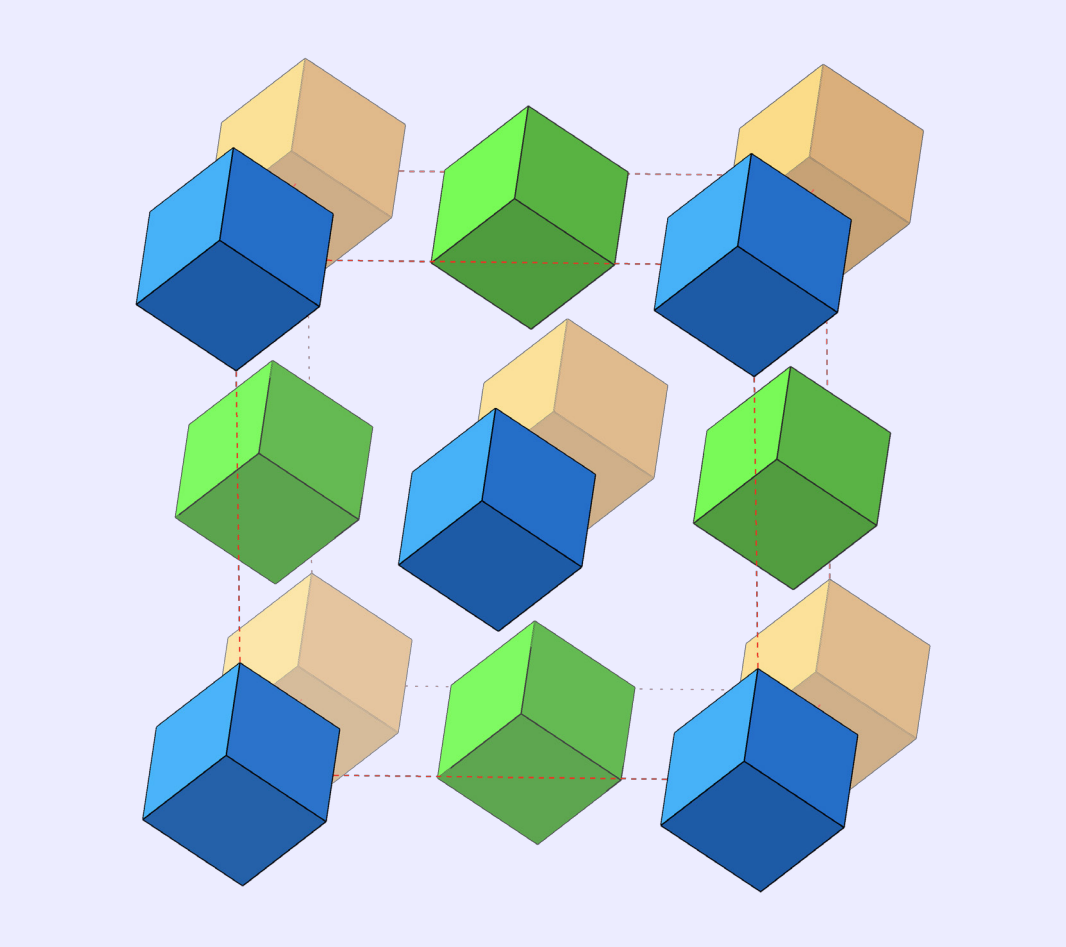
*This is a fanciful construction, designed to show the relative scale of DNA and a carbon nanotube. It was easy to combine the two structures in CrystalMaker X: I just had to hide one of the two DNA strands and set the model types for each structure (stick for the nanotube; space filling for the DNA strand).*



## Intercalated Structure

Merging one lattice into another

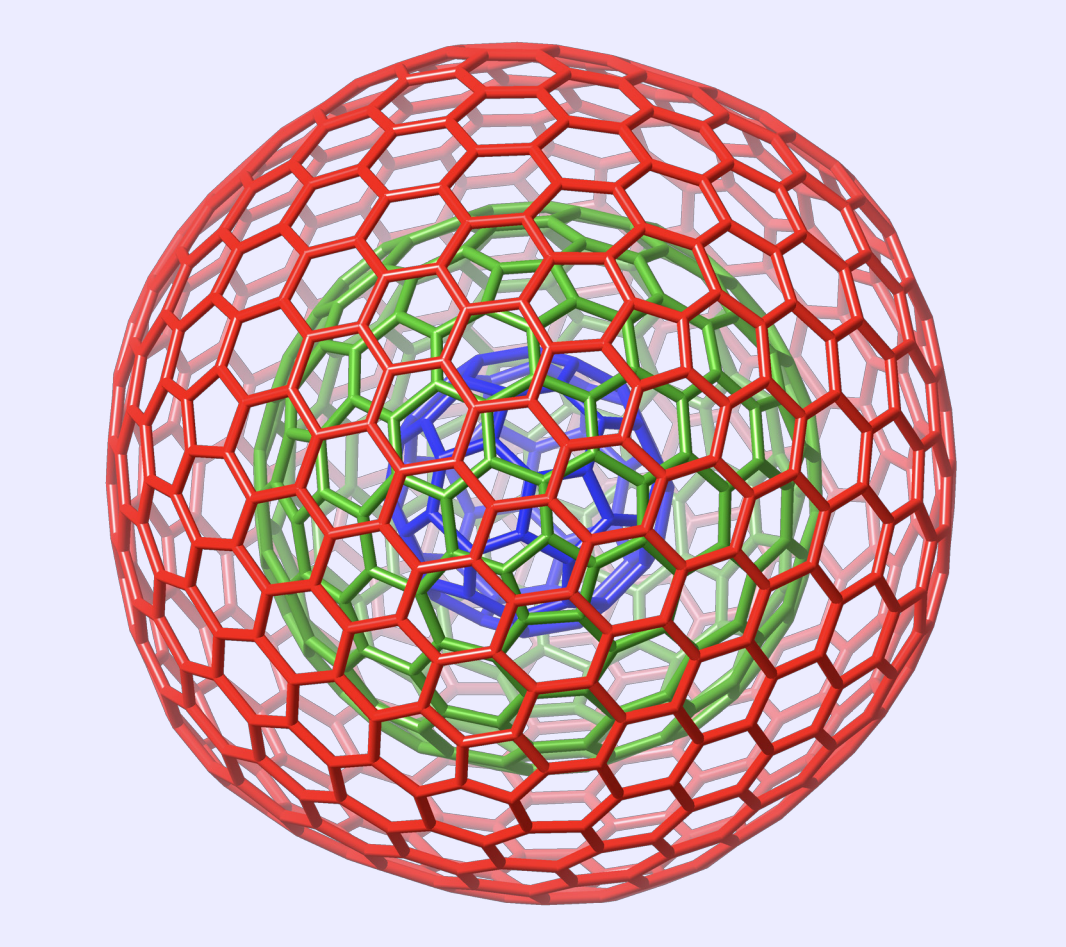
*I started with two separate structures: an YBCO superconductor material and $Li_2O$. I started by inserting space in the YBCO lattice, using an (001) lattice plane to open up 5 Å between the Cu(1) sites and the oxygen layer above. Next, I edited the cell parameter for $Li_2O$ so that it matched the 'a' and 'b' parameters of YBCO. I then made both structures visible and repositioned the $Li_2O$ between the YBCO layers (the latter was locked). Finally, I used the* **Edit > Merge Structures** *command to merge the $Li_2O$ into the host YBCO.*



## Cube Lattice

Using "Molecule Mode" to help tile a rotated cube

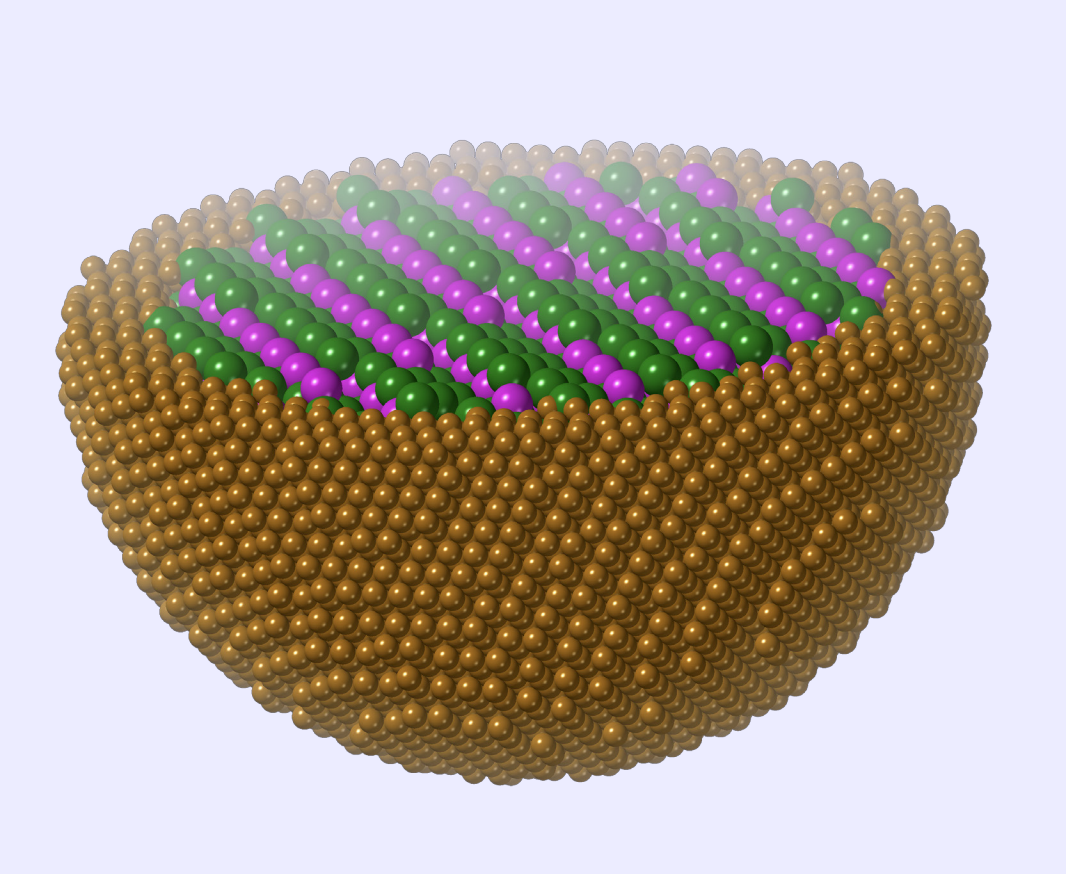
*I built this model starting with a simple cubic primitive lattice. I isolated a single unit cell, comprising eight atoms, and converted this to a "molecule". I rotated my molecule so I was looking along the body diagonal of the cube. Next, I used the* **Molecule to Crystal** *command, in order to tile the rotated cube. This gave me a primitive lattice, with a cube at the centre. I moved the origin to the centre of the cube then edited the structure to give a Face Centred (F) lattice. I also added an atom at the centre of each cube, which then allowed me to define polyhedra. Finally, I selected groups of cubes and edited their colours: according to the relative height, with orange at the "bottom" , green at the centre, and blue at the "top".*



## Matrioshka Balls

Using the Merge Structures command to create concentric molecules

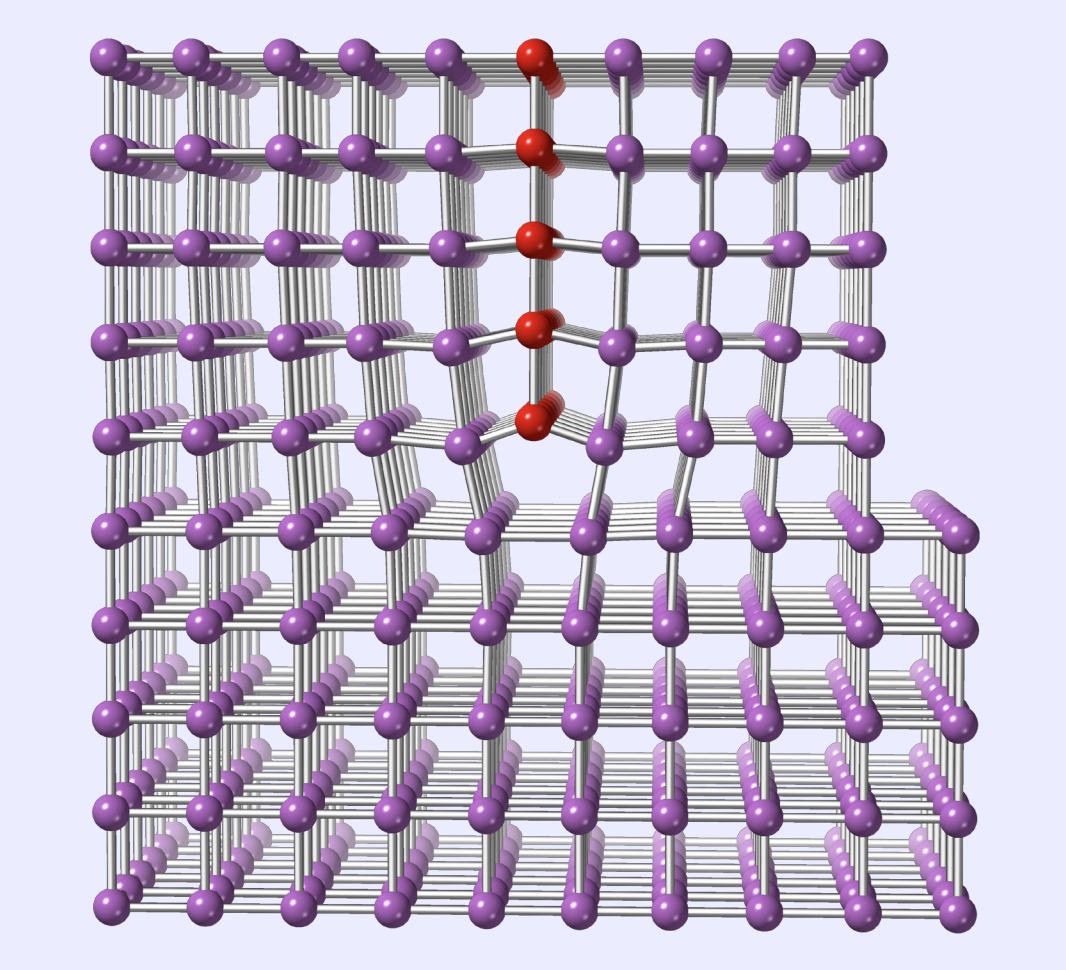
*This was a very easy model to make. I simply started with three separate molecules, each containing a "bucky ball" of a different size and added them to the same window, shift-clicking their thumbnails in the Structures List to make all structures visible (and centred). To merge the separate structures into a single "molecule", one can use the* **Edit > Merge Structures** *command.*



## Sliced Nanoparticle With Surface

Representing a possible structure via clusters and slicing

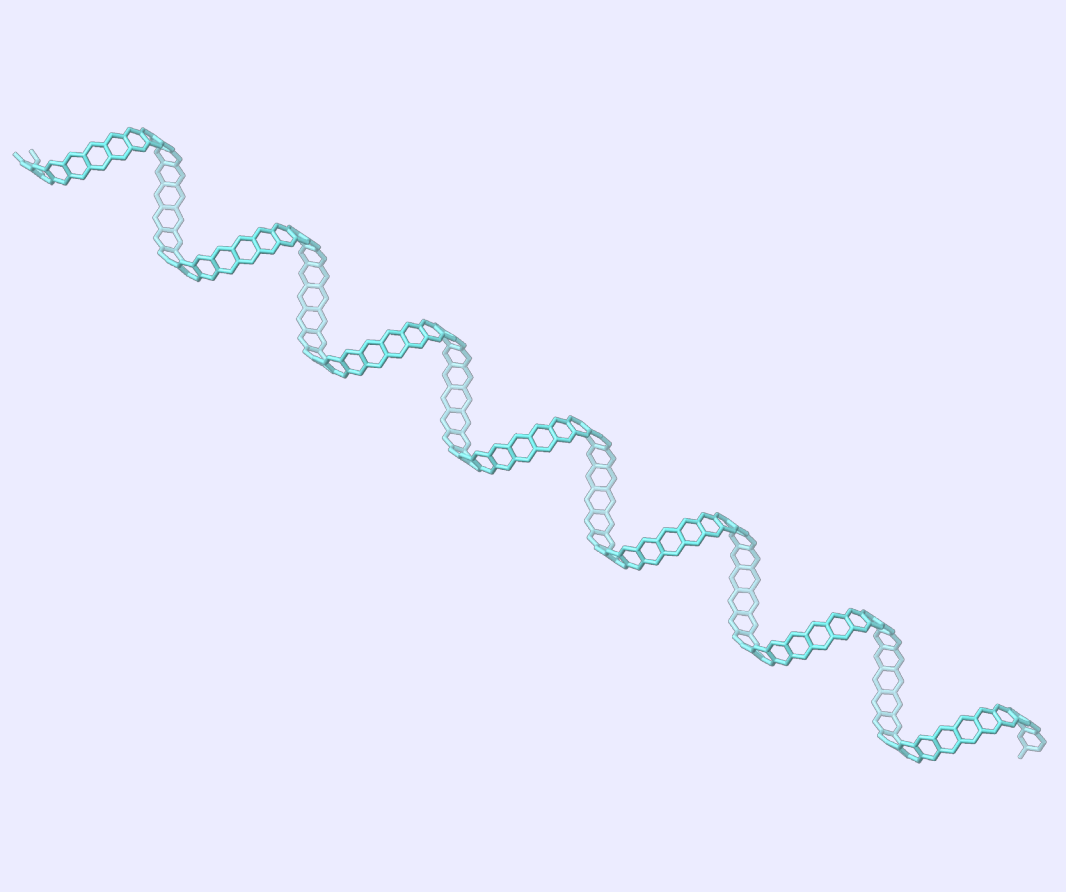
*I used the* **Define Cluster** *command to create a solid sphere of fluorite (green and magenta spheres). This was then converted to a "molecule". I created a hollow sphere of iron (brown), again using the* **Define Cluster** *command, but specifying an inner radius equal to the outer radius of the fluorite sphere. I converted the resulting hollow shell to a "Molecule". The two structures were combined in the same window. Finally, I used the Arrow tool, clicking-and-dragging to define a selection rectangle, and so to hide one hemisphere, thus revealing the contents of this hybrid nanoparticle.*



## Edge Dislocation in a Cubic Crystal

Moving atoms & bonds to display a stylized defect structure

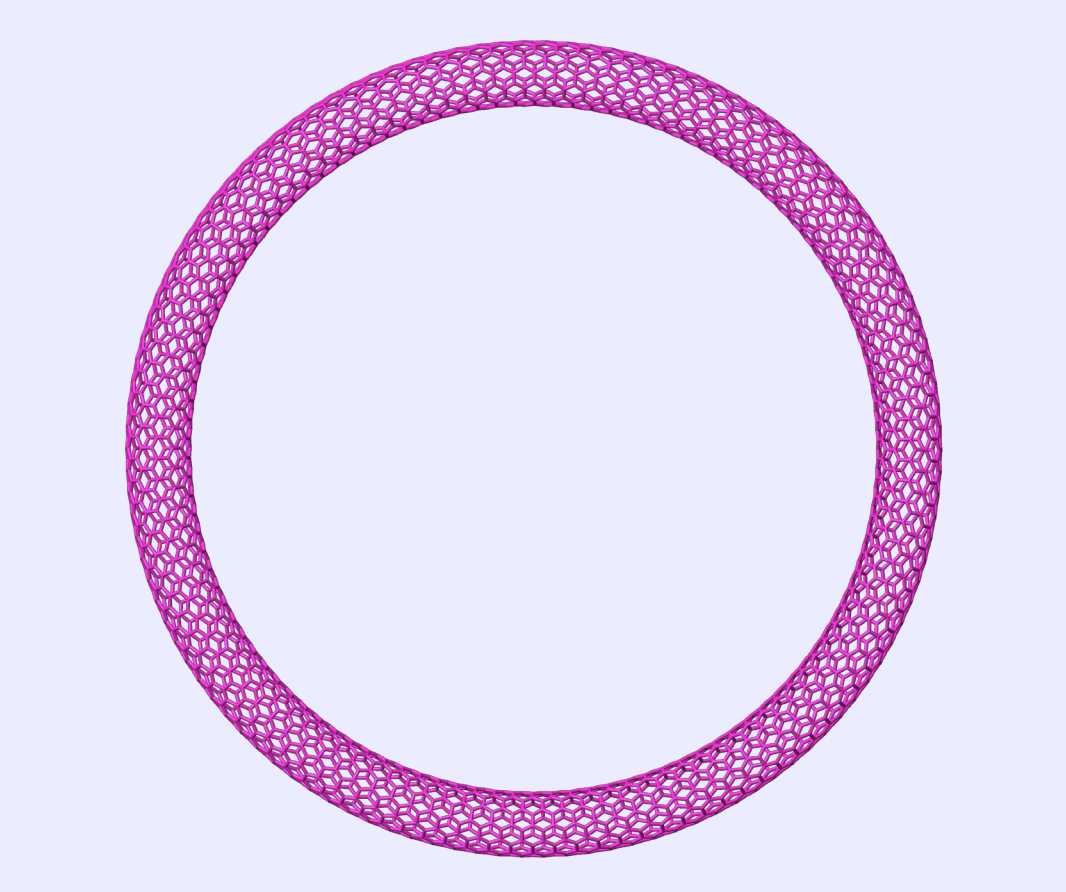
*I created this image using CrystalMaker's atom manipulation tools. I started with a primitive cubic crystal and increased the plot range to create a large block of atoms which was then converted to a molecule. I deleted a half-plane of atoms below the intended slip plane and created a step above the slip plane by deleting another half-plane of atoms on the top right-hand side. A certain amount of atom-level movement was then required to move the atoms around the dislocation core and repair bonding. Finally, I selected the "extra" half plane of atoms at the disclocation core and used the Selection Inspector to change the atom colour to red.*



## Nano Helix

Using the Bend command on an oblique atom strip

*This is an alternative take on the* **Bend** *command, creating a helix rather than the more conventional "nanotube". I started with a Graphite crystal and used the* **Range** *command to create a very-long two-atom strip. The resulting strip was arranged vertically down the screen. I used the* **Rotate** *popover to rotate the strip through 60° about the screen Z-axis. I then rotated the strip through 90° about the screen X-axis, so it was seen "edge on". I selected all atoms and chose the* **Transform > Selection > Bend** *command. Instead of choosing the default radius of 34 Å (which would have given me a one-wavelength helix), I chose a much-smaller radius of just 5 Å, which gave me nearly 7 wavelengths. Finally, I converted my "crystal" to a "molecule" and adjusted the degree of depth fading to accentuate the bends of the helix.*



## Nano Torus

Bending a carbon sheet to create a nanotube and then a nano-torus

*I started with a Graphite crystal and used the Range command to generate a wide strip of atoms. I used the Arrow tool to trim the xy plane to give me a rectangular string and used the Bend command to generate a nanotube. I rotated the new nanotube through 90° about the screen Y-axis, so the tube axis was arranged horizontally, from left-to-right, across the screen. I selected all atoms again, and repeated the* **Bend** *command, accepting the default radius. This yielded a torus shape, which I was able to rotate and apply depth fading to. Finally, I converted my "crystal" to a "molecule".*

# Appendix A

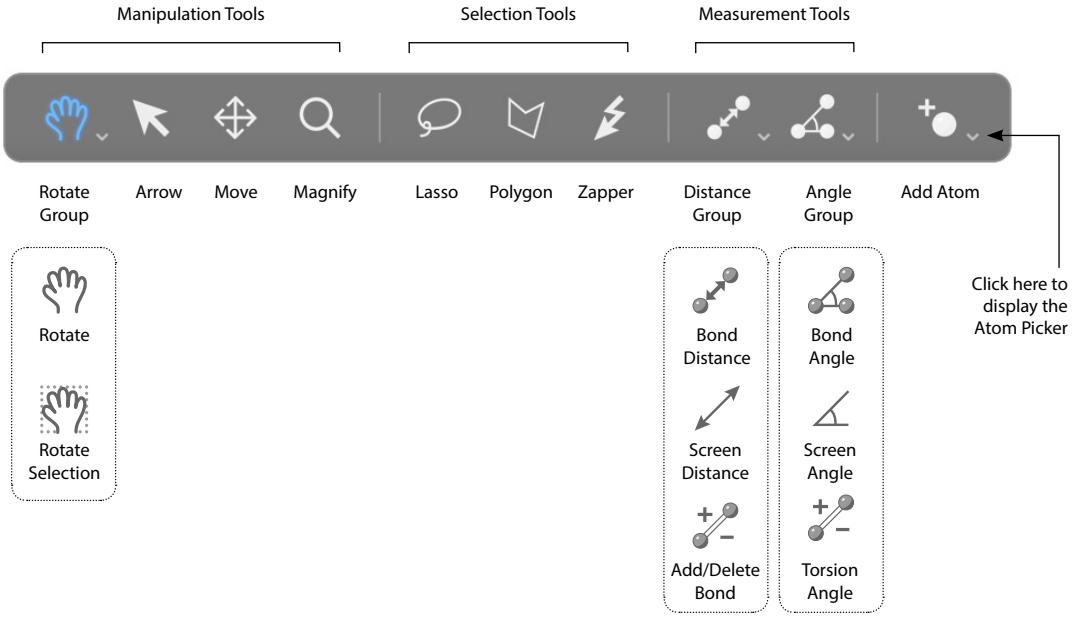
# Toolstrip Reference

This appendix contains a summary of the buttons on CrystalMaker's toolstrip, with some short descriptions of their functions.

## Toolstrip Layout

The toolstrip is divided into different sections, for different functions: Manipulation, Selection, and Measurement tools.

Some tools can be swapped for other related tools, e.g., the Bond Distance tool can be changed to a Screen Distance tool. Swappable tools are indicated by their popup menu symbols (the inverted caret, "v"); clicking this will reveal a popup menu of alternative tools, as summarized in the diagram below:



The toolstrip can be dragged to one of eight different locations: at the four corners or centres of the four edges of the screen. Note that at some positions the toolstrip will have a vertical orientation.

For greater clarity, the toolstrip is automatically hidden when the mouse is moved out of the Graphics pane, or the window is in the background.

#### To keep the toolstrip hidden, do one of the following:

- Choose: **View > Hide Tools**. (Repeat the command to bring the toolstrip back.)
- Right-click in the toolstrip and choose: **Hide**.

#### To move the toolstrip do one of the following:

- Click the edge of the toolstrip and drag it to a new location.
- Right-click in the toolstrip to display a contextual menu, then choose a new location from the **Reposition** submenu.

## Keyboard Shortcuts

You can quickly switch from one tool to another without having to reach for the mouse; just type the keyboard shortcut for the appropriate tool (we've used many of the common Adobe Photoshop shortcuts here). For example, you can switch to the Arrow tool by pressing the letter **A** on your keyboard; you can go back to the Rotate (or "hand") tool by pressing **H**.

The keyboard shortcuts work when the Graphics pane is focused (i.e., you have recently clicked in this pane). At other times, other windows or panes may have keyboard focus, and your typing will appear there.

## Temporary Rotation Mode

Another great time saver is the "temporary rotation mode", which lets you rotate the structure with the mouse—with any tool active—simply by holding down the space key, then clicking and dragging with the mouse.

#### To use "temporary rotation mode":

1. Press and hold the **space** bar on your keyboard; the cursor should change to a "hand" icon.
2. Click-and-drag with the mouse to rotate the structure.
3. Release the **space** bar. Your original tool is active once more.

For example, suppose that you are making an extended selection by clicking on atoms with the Arrow tool. In order to select other atoms you need to rotate the structure. By holding down the spacebar you can do this—and your mouse doesn't need to go anywhere near the Tools palette!

# Manipulation & Information Tools

## Rotate Tool

This lets you rotate an entire structure by clicking-and-dragging with the mouse. If the Rotate-Selection mode is enabled, then only selected atoms will be rotated.

### To change the scale with this tool:

- Hold down the **command** key (Mac) or **control** key (Windows), then click and drag the mouse (e.g., from left-to-right to increase the scale).

## Rotate-Selection Tool

Changes the rotation mode so that any rotations you apply (e.g., with the Rotate Tool, Rotator or the Auto Rotate command) apply only to selected atoms.

This is particularly useful when working in "Molecule Mode", with a placed molecule that you wish to manipulate independently of the host structure.

## Arrow Tool

Lets you identify an atom or polyhedron by hovering over it so that an Atom Info Tip appears. If you click on the atom, information about it is displayed in the Selection Inspector.

You can also use the Arrow tool for selection, and for moving selected parts of a structure:

- Select or deselect atoms by clicking on them (shift-click for multiple atoms).
- Select groups of atoms by clicking on a blank area of the graphics window and dragging a selection rectangle.
- Move selected atoms, by clicking on one of them and dragging. Hold down the **option** key as you drag to duplicate the selection. To constrain movement horizontally or vertically, hold down the **shift** key as you drag.

## Move Tool

Drag the structure across the screen—useful when trying to reposition one structure relative to another (use the Structures List to lock any structures you don't want to move). Click-and-drag to move the (unlocked) structures; hold the **shift** key down to constrain movements to horizontal or vertical.

With the Move Tool active, you can also use the arrow keys on your keyboard to move the structure.

### Magnify Tool

Zoom in or zoom out on a specific point in the structure. (Hold down the **option** or **shift** keys to zoom out).

## Other Selection Tools

### Zapper Tool

A fun shortcut for hiding individual atoms or polyhedra.

Click on an atom or polyhedron you wish to hide. If you hold the mouse button down, a crosshairs appears; releasing the mouse over the atom causes it to vanish in a "puff of smoke"; to spare the atom, simply drag the mouse outside the atom so that the crosshairs disappear.

(Choose **Selection > Show All** to recover hidden atoms.)

### Polygon Tool

Lets you define an irregularly-shaped selection.

To use this tool, click at successive points to define a closed path. To end the selection, click on your starting point again (which should appear highlighted as you move the mouse over it).

### Lasso Tool

Lets you define a freehand selection region.

To use this tool, simply click and drag around the atoms you wish to select. Release the mouse to close your selection region.

## Distance Group

### Bond Distance Tool

This tool lets you measure the three-dimensional distance between a pair of atoms, or the centres of polyhedra, create a new primary bond between the clicked atoms, or display a labelled *secondary* bond.

#### Basic Measurement

To measure bond distances, simply move the mouse over any bond to have its distance displayed.

Alternatively, you can anchor the first measured atom by clicking on it, then as you move the mouse over other atoms, the distance between the two atom centres (as measured in 3D—not the plane of the screen) is updated as you move. Click on the second atom to freeze the measurement and print bond data in the Output Log including:

- Bond distance
- Bond vector
- Projected distance in the plane of the screen

### Bond Generation

When you click on the second atom, an overlay appears with two buttons, prompting you to:

- Create Bond
- Create Distance

If you hold the **shift** key down, the first button changes to **Create Similar Bonds**, allowing you to generate a *bond specification* for the clicked bond which will allow other bonds in the structure to be generated as well.

The **Create Distance** option will generate a *secondary* bond between the two clicked atoms, showing a dashed thin bond cylinder with the bond distance displayed alongside. As you rotate or scale your structure, this measurement will be preserved.

*Note that you also have the option of labelling regular, primary bonds: simply select the bond and select the "Label" checkbox in the Selection Inspector.*

## Screen Distance Tool

Displays a real-time distance measurement in the plane of the plot.

Click once to anchor one end of the tool; the distance, in Ångstrøm units from the anchor to the mouse tip is displayed and updated as you move the mouse. Click a second time to freeze measurement and print the distance in the Output Log.

## Add/Delete Bond Tool

This tool lets you create a new bond, or destroy an existing bond.

To add a new bond, click on a pair of atoms. To generate similar bonds throughout the structure, hold down the **shift** key as you click the second atom.

To delete an existing bond, click on the two atoms at either end of the bond to be removed.

## Angle Group

### Bond Angle Tool

Measures the included angle between three atoms.

With this tool selected, you can move the move and see any included bond angle displayed below.

You can also click on the first two atoms or polyhedra to anchor one side of the angle measurement. As you move the mouse over a third atom (without clicking), the included angle A-B-C is displayed. You can continue to move the mouse, measuring other included angles. To finalize your measurement (and print data in the Output Log), simply click the third atom.

### Screen Angle Tool

Measure angles in the plane of the plot. Click at two points with this tool to anchor one line, then move the mouse to another point and click a third time. The included angle between two line segments is displayed alongside.

### Torsion Angle Tool

Measures the torsion angle between four atoms.

With this tool selected, click on the first three atoms or polyhedra; as you continue to move the mouse, the A–B ^ C–D torsion angle is displayed and updated as the mouse moves over different atoms. To finalize your measurement (and print data in the Output Log), click on the fourth atom.

*The torsion angle is the angle by which the vector AB must be rotated in order to eclipse the vector CD, when viewed along the vector BC. Torsion angles are usually expressed in the range –180° to +180°. According to convention, a clockwise rotation is positive and an anticlockwise rotation is negative.*

# Interactive Structure Building

## Add Atom Tool

This tool lets you add new atoms and, optionally, bonds. Use the Atom Picker to choose which atom to add (see below; the default atom is carbon).

With this tool selected, click anywhere in your structure to add a new atom. If you hold the shift key down as you click, a bond will be created between the last-clicked atom and your newly-created atom.

Click on an existing atom to highlight it; you can then shift-click on another atom (or an empty space to create a new atom) and have a new bond generated.

### To display the Atom Picker:

- Click the popup menu button to the right of the Add Atom tool.

### To choose an element from the Atom Picker:

- Click the element button

### To add different elements to the Atom Picker do one of the following:

- Click the **Sets** button and choose a default set from the popup menu (e.g., Organics, Silicates, etc.)
- Click and hold down the mouse over an element button. A popup menu will appear, letting you choose a new element for that button.

Appendix B

# CrystalMaker Text Format

CrystalMaker lets you define your own structures using a simple, but powerful text format.

A CrystalMaker text file consists of a series of control cards, defining the unit cell parameters, spacegroup symbol and atoms in the asymmetric unit, plus other options such as colours, orientation matrix and rendering settings. This appendix lists all possible control cards. Most of these are optional; the essential cards are marked with asterisks.

Example CrystalMaker text file.

```
TITL  Leucite
CELL  13.055 13.055 13.752 90 90 90
ERRC   0.001  0.001  0.001  0  0  0
SPGR  I 41/a
XYZR  0.9 2.1  0.9 2.1  0.9 2.1
BMAX  Si  O  1.8515
BMAX  K   O  4.0000
```

Main control cards

```
TYPE
K   1.52  0.0955  0.9503  0.0497
O   1.21  1.0000  0.0000  0.0000
Si  0.40  0.6043  0.6043  1.0000
```

Element definitions: radii and RGB colour components

```
ATOM
K  W   0.3659  0.3637  0.1169
O  O1  0.1325  0.3141  0.1099
O  O2  0.0908  0.5112  0.1308
…
Si T1  0.0574  0.3969  0.1665
Si T2  0.1675  0.6116  0.1287
Si T3  0.3930  0.6420  0.0862
```

Asymmetric unit: element type, site label, fractional coordinates

```
ERRS
W   0.0009  0.0007  0.0010
T1  0.0006  0.0006  0.0005
T2  0.0006  0.0005  0.0006
T3  0.0006  0.0006  0.0006
O1  0.0005  0.0004  0.0004
O2  0.0004  0.0004  0.0005
…
```

Errors in fractional coordinates

**Tip:** See *Chapter 14: Data Import/Export* for other examples of CrystalMaker text files.

## Alphabetical Listing of Control Cards

### AREN (see Rendering Settings)

### ATOM (*) - Structural Data

CrystalMaker expects 5 statements per atom:-

- **Element Symbol**, comprising one or two alphanumeric symbols.
- **Site Label** (maximum of 6 characters; *must not contain spaces*). This should uniquely identify a site.
- **Coordinates *x, y* and *z*.** For a crystal, use fractional coordinates for atoms in the asymmetric unit; for a molecule, use orthogonal coordinates for *all atoms to be plotted*.

Format: ATOM
<symbol> <label 1> $x_1$ $y_1$ $z_1$
<symbol> <label 2> $x_2$ $y_2$ $z_2$
etc.

### AVEC - Atom Vector

You can specify a vector that will be displayed from a host atom in the structure. CrystalMaker expects 12 parameters per vector, grouped into the following categories:

- Site label for the host atom.
- Fractional coordinates, *x*, *y* and *z* for the host atom. (You should ensure that this atom can be plotted, with respect to the specified plot range—as given by the XYZR card).
- Vector indices, expressed as a lattice vector, [UVW]. The absolute length of the vector is ignored if the next entry is non-zero.
- The vector length, in Ångstrøms (or enter 0 to have CrystalMaker calculate the length from the [UVW] values). For optimum visibility, recommend lengths of at least 2 Å.
- The fractional red, green and blue colour components for the vector.
- The vector style (1 = "from atom"; 2 = "through atom").

Format: AVEC
<label 1> *x y z* *U V W* <length> <red> <green> <blue> <style>
etc.

### BANI - Anisotropic Temp. Factor

This card is for anisotropic temperature factors, in the format: $B_{ij}$ (please see the UANI card for the more usual case of temperature factors in the Uij format).

The card should appear on its own line, followed by one or more data lines. Seven values are expected per input line: the site label, followed by the six unique components of the thermal ellipsoid tensor, in the order:

$B_{11}$ $B_{22}$ $B_{33}$ $B_{12}$ $B_{13}$ $B_{23}$

### BKCL - Background Colour

The default background colour is black. You may enter your preferred colour by specifying the red/green/blue components as fractions from 0 to 1 (white corresponds to 1, 1, 1)

Format: BKCL <red> <green> <blue>

### BMAX - Bond Distance Specification

Instructs CrystalMaker to search for bonds between atom types which are closer than the maximum distance $B_{max}$ (in Å).

Format: BMAX <element 1> <element 2> $B_{max}$

### BNCL - Bond Colour

You may enter your preferred bond colour by specifying the red/green/blue components.

Format: BNCL <red> <green> <blue>

### BOND - Automatic Bond Specification

Requests that bonds be generated between the specified atom types, provided that the separation of the atoms lies within 15% of the sum of the atomic radii. (Uses radius values supplied in a TYPE card, if present.)

Format: BOND <element 1> <element 2>

### BRAD - Bond Radii

Specifies the radius of bond and stick cylinders, as fractions of the smallest atom radius in a plot.

Format: BRAD <B&S radius> <stick radius>

**BREN** (see Rendering Settings)

### CELL (*) - Unit Cell Constants

(Crystals only). The unit cell lengths must be given in Å, with angles in degrees.

Format: CELL *a b c* α β γ

### COLS - Colour Rendering Scheme

Lets you specify a (colour) rendering mode: 1=Photo Colour; 2=Photo Grey; 3=Black & White mode.

Format: COLS <index>

### Comment Line

You can embed comments within your text file, provided that the comment characters are at the very beginning of the comment line. You must not embed comments inside multi-line data blocks—such as those used by the ATOM, TYPE, NOTE, ERRS cards.

Format: !<comment text>
*or* // <comment text>

### DCUE - Depth Cueing (Fading)

Specifies depth fading and the degree of attenuation with depth. Closest atoms to the viewer are plotted at 100% of their normal reflectance. The furthest atoms are plotted at a fraction of their normal reflectance; this fraction is defined by the "minimum" setting.

The distance interval over which progressive depth fading occurs is controlled by the two fractions: upper and lower. A value of 0 corresponds to the lowest atom plotted (i.e, furthest from the viewer); a value of 1 corresponds to the topmost atom (closest to the viewer).

Format: DCUE <min.> <upper> <lower>

### ERRC - Errors in Cell Constants

(Crystals only). Allows you to enter standard deviation errors (σ) in the unit cell parameters. These data can then be used, with the errors in the structural data (if entered) to calculate errors in bond lengths.

Format: ERRC σ(*a*) σ(*b*) σ(*c*) σ(α) σ(β) σ(γ)

### ERRS - Errors in Structural Data

(Crystals only). If you wish to calculate errors for bond lengths, you should include the standard deviation (σ) errors in the structural data, using the ERRS card.

Format: ERRS
<site label 1> $\sigma(x)$ $\sigma(y)$ $\sigma(z)$
<site label 2> $\sigma(x)$ $\sigma(y)$ $\sigma(z)$
etc.

### LATC - Lattice Type

(Crystals only). This option is for use with the SYMM cards only. It is not required if the SPGR card is used.

Format: LATC <lattice type>

### LTDN - Light Direction

The illumination direction is defined by a unit vector with components $l_{1-3}$, relative to the orthogonal screen axes.

Format: LTDN $l_1$ $l_2$ $l_3$

### MODL - Model Type

Requests a specific model type (the number you enter relates to the order of model types given on CrystalMaker's model menu, that is: 1=Ball & Stick; 2=Space filling; 3=Polyhedral; 4=Wireframe; 5=Stick.

Format: MODL <model reference number>

### MOLE (*) - Molecule Identifier

CrystalMaker assumes that your text file contains data relating to a *crystal*, unless you tell it otherwise by including the MOLE card as the first entry in the text file.

Format: MOLE

### NOTE - Notes

Allows you to enter as much text as you would like, on multiple lines. Each line must contain no more than 72 characters, and must end with a hard return.

Format: NOTE <text>

or: NOTE
<note line 1>
<note line 2>
etc.

### OCCU - Site Occupancies

You can optionally include site occupancy data for your crystal, using the OCCU card—which must be entered *after* the ATOM data.

To define a site's occupancy you need to enter the site label, followed by up to three sets of element symbol / fractional occupancy values. (If any sites are fully ordered, you do not need to include them in the OCCU list.)

If A, B, C, D, E are element symbols, and $f_A$, $f_B$… are the fractional occupancies of each element on a particular site, one would enter the following:

Format: OCCU

<label 1> $A\ f_A\ \ B\ f_B\ \ C\ f_C$
<label 2> $A\ f_A\ \ D\ f_D$
<label 3> $B\ f_B\ \ E\ f_E$
etc.

### OMAT - Orientation Matrix

(Crystals only). If you wish to specify a precise orientation for your crystal—avoiding the ambiguity of the VIEW card, you can enter all 9 coefficients of the orientation matrix, **M**. This matrix converts fractional coordinates, $x_j$ to orthogonal coordinates, $xo$, where: $xo_i = \mathbf{M}_{ij}\, x_j$

Format:

OMAT $M_{11}$ $M_{12}$ $M_{13}$ $M_{21}$ $M_{22}$ $M_{23}$ $M_{31}$ $M_{32}$ $M_{33}$

### OSHF - Origin Offset

(Crystals only). The origin offset (shift) is specified in fractional coordinates.

Format: OSHF $\Delta x\ \ \Delta y\ \ \Delta z$

### PREN (see Rendering Settings)

### PRSP - Perspective

Specifies that perspective should be used, and gives the view distance (Å).

Format: PRSP <view distance>

### Rendering Settings

You may enter reflectance settings for atoms (**AREN**), bonds (**BREN**) and polyhedra (**PREN**). Four values are expected:

1. $K_a$: ambient reflection coef. ($0 \le K_a \le 1$)
2. $K_d$: diffuse reflection coef. ($0 \le K_d \le 1$)
3. $K_s$: specular reflection coef. ($0 \le K_s \le 1$)
4. N: Phong exponent (an integer in the range 1–1000)

Format: AREN $K_a$ $K_d$ $K_s$ N

### RMAT - Rotation Matrix

(Molecules only). If you wish the final orientation of the molecule to be different from the orientation defined by the coordinates, you can enter a rotation matrix, **R**, to transform the coordinates before they are plotted.

If the initial coordinates of an atom are $xo_i$, then the final, plotted coordinates, $xo'_j$ are given by: $xo'_i = \mathbf{R}_{ij}\, xo_j$

Format: RMAT $R_{11}$ $R_{12}$ $R_{13}$ $R_{21}$ $R_{22}$ $R_{23}$ $R_{31}$ $R_{32}$ $R_{33}$

### SCAL - Scale

Specifies a fixed scale in pixels-per-Ångstrøm.

Format: SCAL <scale>

### SHCL - Show unit Cell outline

(Crystals only). You may request a unit cell frame by entering "1" as the index; enter "0" as the index for no unit cell.

Format: SHCL <index>

### SPGR - Space Group symbol

(Crystals only). Spaces should be used to separate symmetry elements associated with different axes. (See *Chapter 5: Building Crystals*, for examples of spacegroup symbols.)

Format: SPGR <space group symbol>

### SYMM - Symmetry operators

(Crystals only). Lets you define symmetry operators in terms of general equivalent positions (GEPs), as an alternative to entering the spacegroup symbol with a SPGR card. Translations are given as fractions (½, ⅔…). The identity operator x,y,z and lattice-related counterparts are not required.

Format: SYMM <GEP>

### TITL - Title Line

A description of the crystal for reference purposes. (Use the NOTE card to enter text for the notebook window.)

Format: TITL <text>

### TYPE - Atom Types

Lets you enter custom atom types, their radii (Å) and RGB colours (fractions red/green/blue). You should ensure that the element symbols match the symbols in the atoms list.

Format: TYPE
<symbol 1> <radius> <R> <G> <B>
<symbol 2> <radius> <R> <G> <B>
etc.

### UISO - Isotropic Temperature Factor

This card is used to define isotropic temperature factors (values in Ångstrøms squared). The card should appear on its own line, followed by one or more data lines. Two values are expected per data line: the site label (which must match an entry in the ATOMS list), and the $B_{iso}$ value, in $Å^2$.

### UANI - Anisotropic Temp. Factor

This card is used to define anisotropic temperature factors, Uij (values in $Å^2$). The card should appear on its own line, followed by one or more data lines. Seven values are expected per data line: the site label, followed by the six unique components of the thermal ellipsoid tensor, in the order:

$U_{11}$ $U_{22}$ $U_{33}$ $U_{12}$ $U_{13}$ $U_{23}$

### VIEW - View direction

[UVW] is the crystallographic view direction, normal to the plot.

Format: VIEW U V W

### XYZR - x, y, & z Range

(Crystals only). Lets you specify a custom plot range in fractional crystallographic coordinates.

Format: XYZR $x_{min}$ $x_{max}$ $y_{min}$ $y_{max}$ $z_{min}$ $z_{max}$

# Appendix C

# Troubleshooting

CrystalMaker is designed to provide workstation-class performance and graphics. This appendix contains some tips for using CrystalMaker safely, and provides some information to help you solve problems on your own.

If, after following this advice, you still have problems, please let us know! See the *Contacting Us* section at the end of this appendix.

## Avoiding Problems

We want you to have the best-possible experience using our software. Here are some tips to stay out of trouble and to ensure that the software gets better the more you use it.

### Stay Up-to-Date

We provide regular, free incremental updates for the current program version. These include new features, performance optimizations, and bug fixes. If you are encountering problems, your first step should be to ensure that your problem hasn't already been fixed, in a program update. Simply visit:

`crystalmaker.com/support`

and click on the **Updates** link.

**You can upgrade older software!** If you are using a previous, unsupported version of the software (e.g., CrystalMaker versions 1–9) we strongly recommend upgrading to the latest supported version (which, at the time of publication is CrystalMaker X).

### Update your graphics drivers

(Windows Users) Most issues are caused by bugs in graphics drivers which do not fully (or correctly) support the range of *OpenGL* features required by CrystalMaker X. Please note that the standard Windows update mechanism does *not* update third-party graphics drivers; instead, you will need to visit the graphics

card manufacturer's website and download the latest drivers from there…

- do *not* assume that your drivers are up-to-date simply because your control panel and/or IT manager claims they are!

Note that graphics intensive software, such as CrystalMaker, are particularly vulnerable to graphics driver issues (which may not affect standard desktop productivity software).

### Save Your Work

If disaster strikes, you have a backup! Note that, when using the program, you can always duplicate the existing structure in the Structures List, so you have a reference copy to return to.

### Check Memory Availability

Ensure there is sufficient memory—especially when working with large structures, animations or when recording video.

### Check Your Disc Regularly

Corrupted system software or damaged disc blocks and result in generally-weird system behaviour and instability across a range of software.

## Troubleshooting Tips

If you do encounter problem using the software, please first ensure that you are using the latest version of the software: as we have already mentioned, we fix *all* bugs that have been reported to us, so there's a very-high likelihood that if it is a bug, there's an update that fixes this. If, after having updated to the latest version, you still have problems, please follow the steps below *before* you contact us. That saves time at both ends, and ensures that, should you need to contact us, we can provide more effective support.

1. Window users: update your graphics drivers! If you are experiencing display issues (e.g., all atoms plotted in the centre of the screen) please ensure that your graphics drivers are up-to-date.
2. Use compatibility mode. If, after updating your drivers, you still have problems, try disabling CrystalMaker's **Use Latest Graphics** preference (see **Compatibility** in the **Graphics** pane of the Preferences panel). This will switch into "compatibility mode", using OpenGL 3.3 graphics commands, instead of the default (and slightly-faster) OpenGL 4.1 version.
3. Garbage in, garbage out? If the problem is related to file import, try checking the file using a plain-text editor:

- Ensure that the file really is a plain-text, ASCII file—and not, for example, a Microsoft Office document!
- Try to verify that the file is valid, and does not contain spurious characters (it is often the case that, during transmission, text files can acquire HTML or other formatting tags that are alien to the original format).
- If you are trying to read a CIF file, verify this by using the free CIF checker at:

  `http://checkcif.iucr.org`

  Please be aware that some third-party programs have serious bugs with their claimed CIF compatibility, resulting in corrupted CIF files being generated, which cause knock-on problems with other software, such as CrystalMaker.

**We're not telepathic!** If, after thoroughly verifying your file, you still have problems, please send us a copy of the file. Sorry, but unless we see the file that's causing problems, it's unlikely that we'll be able to help.

4. Be wary of file extensions! The correct file extensions *must* be used at all times. This allows CrystalMaker to quickly choose the appropriate importer to read a file. We are aware of some cases where users have mistakenly changed file extensions (e.g., ".cmdf" to ".cmdx"), perhaps thinking that this will make earlier files readable by later versions of the program; instead, the program can become confused, trying to fit a certain pattern of bytes in memory into a completely inappropriate template—which can lead to a crash.
5. Mac users: if the program crashes on startup, it may be because the system is trying to restore the last window state, and forcing the program to try to reopen a corrupted file. You can bypass this automatic-window-state restoration by holding down the **shift** key as you launch CrystalMaker.
6. Ensure you have given CrystalMaker sufficient memory: try quitting other programs and try CrystalMaker again.
7. Reset CrystalMaker's preferences. To do this, first display CrystalMaker's Preferences panel (Mac version: **CrystalMaker > Preferences**; Windows version: **Edit > Preferences**) then click the **Reset** button, which is on the top right-hand side of the panel's toolbar.
8. Isolate the cause of your problem: is it unique to CrystalMaker? Can you reproduce the problem on another machine?
9. Use a disc-checking program (e.g., Apple Disk Utility, or Norton Utilities) to thoroughly check your hard drive.
10. As a last resort, if you are having system-wide issues, then a clean installation of your system software may be the only option. System software can get corrupted over a period of time.

## Contacting Us

Providing your software is up-to-date, we're very happy to work with licensed users to help resolve any issues. Please help us to help you by ensuring that you provide the following information:-

- Your name and (if relevant) institution. *Please don't feel offended if we ask for this information!* It is not uncommon for individuals to use stolen software and still expect us to provide free technical support—so we need to know that you're a legitimate customer.
- Your licence code or serial number. Your licence code would have been sent to you when you purchased the software, but you can check your serial number at any time by choosing the program's **About** command (Mac users: **CrystalMaker > About CrystalMaker**; Windows users: **Help > About CrystalMaker**).
- A clear explanation of what the problem is, and how to reproduce it.
- Any files you were using that triggered the bug. These might be text input files (e.g., CIF, PDB, XYZ) or CrystalMaker documents (CMDX) that we can open and use to understand the problem.

Remember: whilst *you* may be acutely aware of a problem, *we* are not sitting with you looking over your shoulder… so the more information you send us, the easier—and quicker—it will be for us to help you. Otherwise, we're working in the dark.

Appendix D

# Basic Crystallography

This appendix aims to provide a very basic introduction to some key concepts which are required in order to use CrystalMaker effectively.

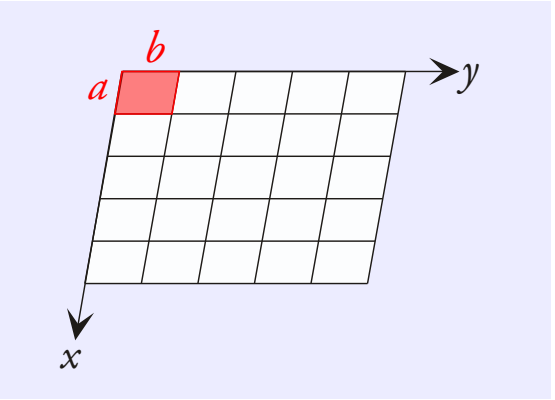
## Lattices and Unit Cells

One of the most important concepts in classical crystallography is that of *repetition* of a basic building unit, to create an extended structure in two or three dimensions.

We could think of a single brick in a wall, or a repeating pattern in a sheet of wallpaper. In any case, it is possible to define a basic, repeating unit, the *unit cell*, which can be *tiled* in two or three dimensions, to yield a periodic structure called a *lattice*.

A simple two-dimensional lattice would consist of a parallel-sided unit cell (a "parallelogram") tiled along *x* and *y* axes, as shown below:

A simple two-dimensional lattice, with one unit cell shaded.




The unit cell is the template for building an extended lattice, and so it is usual to focus on a single unit cell when describing the structure. For this two-dimensional example, the unit cell can be described in terms of just three numbers: the edge lengths parallel to *x* and *y* (*a* and *b* respectively) and the angle between the *x* and *y* axes (which we'll call gamma, γ).

The concept of a unit cell can be applied to three-dimensional lattices. The three-dimensional unit cell is like a building brick which, when stacked with many more bricks, builds an extended structure.

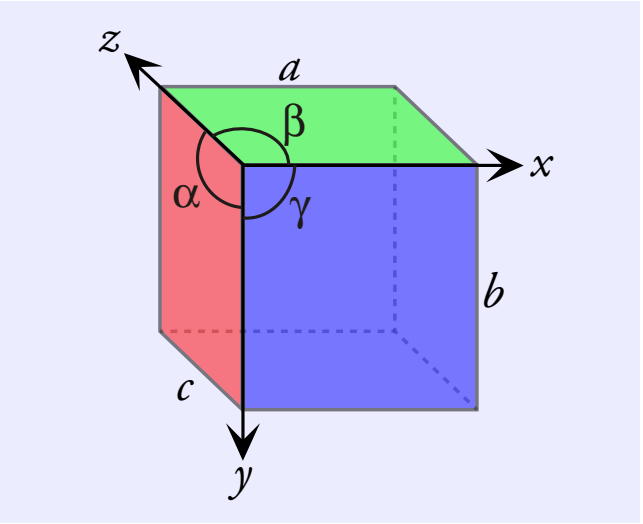
In general terms, a unit cell has a "parallelepiped" shape—e.g., a rectangular block, or in general a slightly-distorted one. The shape of the unit cell is represented by its edge lengths parallel to *x, y,* and *z* axes—and by the angles between these axes. It is conventional to call the edge lengths *a, b,* and *c* (parallel to *x, y* and *z*, respectively), and the interaxial angles α, β and γ where:

$\alpha = y \angle z$

$\beta = x \angle z$

$\gamma = x \angle y.$

It is important to recognize that the inter-axial angles are determined by the atomic arrangement; **they are not necessarily 90°!**




A three-dimensional unit cell showing the inter-axial angles αβγ and cell dimensions abc.

A complete three-dimensional structure is constructed by the repetition of unit cells parallel to the *crystallographic* axes *xyz*.

## Lattice Planes

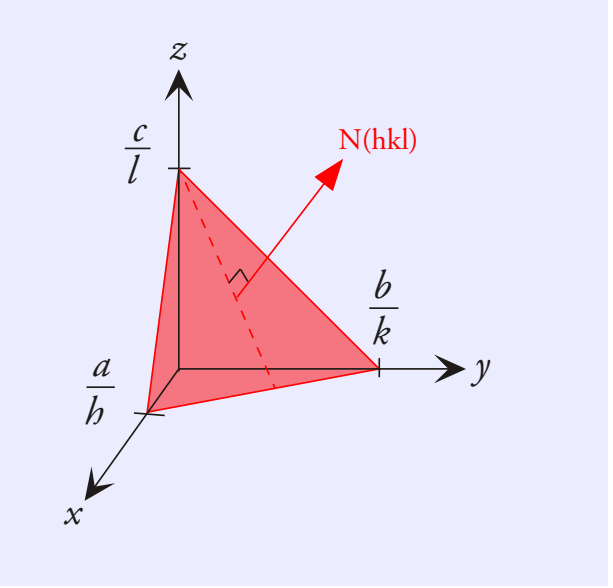
Describing the orientation of planes of atoms is very important—particularly when considering diffraction of radiation, where successive planes of atoms in a crystal act as a diffraction grating.

One way of describing lattice planes is to consider their relationship to the unit cell and its crystallographic axes. Consider a lattice plane passing through a crystal. The plane will eventually cut the *xyz* axes, and its orientation is reflected in the relative values of the *intercepts* along these axes.

Consider a unit cell with edge lengths *a*, *b*, *c*, and a lattice plane cutting through the *xyz* axes. The plane:

- intersects the *x* axis at some fraction of the *a*-repeat distance, *a/h*
- intersects the *y* axis at *b/k*
- intersects the *z*-axis at *c/l*

where *h*, *k* and *l* are integers.



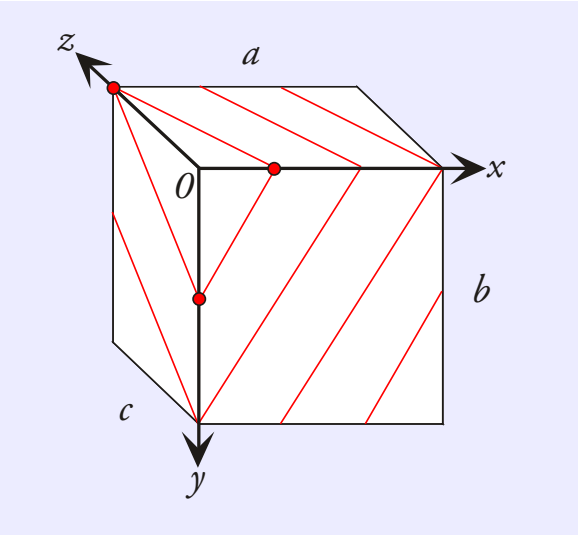

A lattice plane cuts the xyz axes at a/h, b/k and c/l, respectively. The direction of the plane's normal is shown by N(hkl).

The *orientation* of the lattice plane can therefore be reduced to a set of three integers, (hkl), representing the three *intercepts* of the plane with the coordinate axes. These integers are called "**Miller Indices**" (named after W.H. Miller, Professor of Mineralogy at the University of Cambridge in the 18th Century).

It is important to stress that because of the periodic nature of crystal lattices, ***sets of parallel lattice planes occur throughout a crystal lattice***. When determining the Miller Indices of a plane, we use the first plane of a particular orientation from

the origin of the crystal. The block diagram below illustrates such as series of planes; the origin of the crystal is marked "O":

A series of parallel lattice planes, cutting through a single unit cell, with crystallographic axes as shown.




**Quiz**

What are the Miller Indices for this set of planes?

(Answer at the bottom of the next page.)

Please note that in real crystals, the origin of the lattice is *entirely arbitrary*—one is totally free to move the origin to wherever one sees fit. Consequently, there is no fixed *position* for lattice planes in space (one could imagine "sliding" the planes anywhere along their plane normal; their Miller indices would remain the same). The only things fixed are the *orientation* of the plane normal, and the inter-planar spacing (the "d-spacing").

## Lattice Vectors

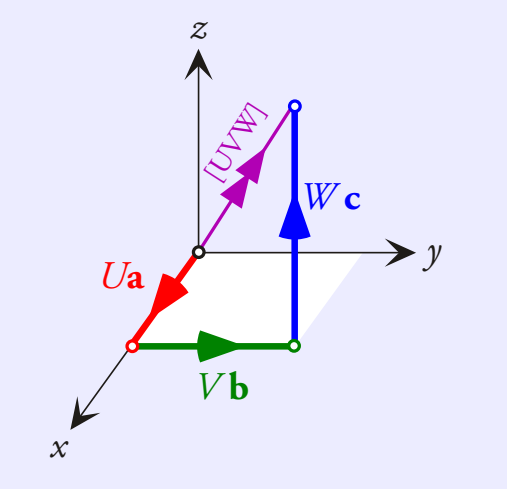
We define vectors parallel to the edges of the unit cell: **a** is a vector of length $a$ that is parallel to the crystallographic $x$ axis; **b** is a vector of length $b$, parallel to the $y$ axis, and **c** is a vector of length $c$ parallel to the $z$ axis.

A general direction in a crystal can be expressed in terms of a sum of the "edge" vectors **abc**:

$$U\mathbf{a} + V\mathbf{b} + W\mathbf{c}$$

Since the vectors **abc** are defined by the unit cell, the vector is usually expressed solely in terms of its components, and abbreviated as [UVW] — the square brackets help to differentiate this *vector* from the Miller Indices referring to a lattice *plane*. It is, however, essential to remember that the vectors **abc** each have specific lengths (they are *not* unit vectors!) and that they are not necessarily at 90° to each other!

A lattice vector [UVW] is expressed in terms of components parallel to the xyz crystallographic axes.




Answer to the previous page's quiz: The Miller Indices are (321). That is, the first plane from the origin cuts the x axis at a/3; the y axis at b/2 and the z axis at c/1.

## Miller-Bravais Indices

When working with hexagonal, trigonal or rhombohedral crystals, you may occasionally encounter lattice planes expressed using a four-index ($h\ k\ i\ l$) notation. Such **Miller-Bravais** indices are designed to preserve symmetry relationships (the "$i$" relates to an imaginary "$u$" axis, parallel to $[\bar{1}\bar{1}0]$, which is related by a three-fold axis to the crystallographic $x$ and $y$ axes). However, this notation can be very confusing to most people who expect standard three-index ($h\ k\ l$) notation.

Fortunately, there's an easy way to convert four-index notation to three-index, using the relationship:

$$h + k + i = 0$$

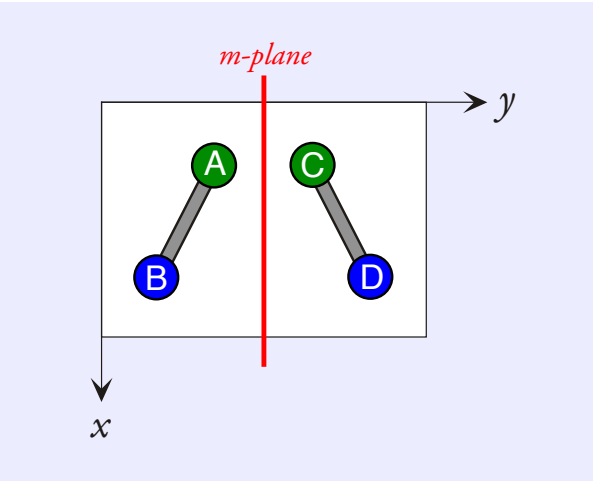
Thus, the lattice plane expressed in four-index notation as $(10\bar{1}0)$ is just (100) in three-index notation. Similarly, the (110) plane in three-index notation becomes $(11\bar{2}0)$ in four-index notation.

## Asymmetric Unit

In a real crystal the unit cell is not a solid "brick", but an area of space containing one or more atoms. Within the unit cell, atoms may have certain symmetry relationships, e.g., one group of atoms related to another by reflection in a mirror plane, or rotation about a symmetry axis. (Ultimately, it is these symmetry relationships that define the symmetry of the crystal as a whole.)

If some atoms in a unit cell are related to others by symmetry, then only a sub-set of the total atoms needs to be considered when describing the structure. This sub-set, or "asymmetric unit" is defined as the minimum group of atoms which, when combined with specified symmetry operators, "generates" the remaining atoms in the unit cell.

As an example, consider the simple two-dimensional unit cell depicted below:




We could specify this structure by listing the fractional coordinates of the four atoms ABCD—but by doing so, we would be missing an important symmetry relationship: the two atoms A & B are related to C & D by a vertical mirror plane. The atoms A & B constitute the asymmetric unit for this structure—and so we need only list their fractional coordinates, and the existence of the mirror plane at $y = 0.5$ (which acts as a "generator" for the atoms C & D).

For real, three-dimensional crystals, we can represent the arrangement of symmetry elements by using a "space group": a self-consistent arrangement of symmetry elements in space. In fact, there's only a finite number of space groups: 230, to be precise, and these are all tabulated in CrystalMaker.

To summarize:

Unit Cell Contents = Asymmetric Unit + Space Group Symmetry

Glossary

# Crystallographic Terms

### Anisotropic Displacement Parameter

A description of the thermal vibration or other state of motion, of an atom in a crystal. The uncertainty in the atomic position is represented by a three-dimensional shape, the surface of which defines a fixed probability of the atom being located within. For harmonic motions of the atom, this is an ellipsoid—a "thermal ellipsoid". This is represented by a symmetric tensor, with six unique components ($U_{ij}$) giving both the magnitude, and the direction of the atom's displacement from its ideal position—hence the term "atomic displacement parameters". This is also referred to as the "anisotropic temperature factor".

### Asymmetric Unit

The smallest group of atoms required to uniquely define a crystal structure.

To define a crystal, one could list all the atoms inside one unit cell. However, if the crystal has some symmetry then some of these atoms will be related to other atoms by the operation of symmetry elements. So, a more concise way of defining a crystal structure is to specify the crystal symmetry (i.e., its spacegroup), and then give the smallest subset of the unit cell (i.e., the asymmetric unit) which, when combined with the symmetry "generates" the remainder of the unit cell.

### Atomic Displacement Parameter

Atomic displacement parameters (sometimes referred to as "thermal ellipsoids", or "temperature factors") are used to describe the relative magnitude, and orientation, of atomic motions (or positional disorder) in a crystal.

In most structures the atoms are not at rest, but vibrate about their mean positions. A statistical analysis of these motions, assuming harmonic vibrations, confines an atom centre to a probability surface whose three-dimensional representation is, in its most general case, an ellipsoid (described by a set of **anisotropic** displacement parameter), sometimes approximated by a sphere (described by a single, **isotropic** displacement parameter).

### Atomic Scattering Factor

X-rays are scattered by the electrons of an atom. Because the diameter of electron clouds is similar to the wavelength of x-rays, the amount of scattering varies with angle. The amplitude of x-ray radiation scattered by a single atom is defined by the atomic scattering factor (ASF). Its angular dependence is summzrized in a 9-coefficient polynomial equation.

Values for the ASF coefficients may be found in the *International Tables for Crystallography*, or in: Doyle & Turner (1968) Acta Crystallographica A24:390-397.

CrystalMaker uses the atomic scattering factors to simulate electron density for a crystal structure.

### Bravais Lattices

The 14 unique three-dimensional lattice types—as derived by the French crystallographer, Auguste Bravais, in the mid-nineteenth century. He showed that, when considering all combinations of lattice types and crystal systems, there was a total of 14 unique lattice, which have become known as the "Bravais Lattices".

### Cell Parameters

*See* Lattice Parameters.

### Crystal

A crystal is a solid material which has a regular internal arrangement of atoms, which sets limits on its range of chemical compositions, and gives it a characteristic crystal shape.

The internal arrangement of atoms can be resolved into an endlessly-repeated unit cell, which contains one or more atoms. The relative arrangment of atoms within the unit cell defines the structure's symmetry, as summarized by the crystallographic spacegroup.

### Crystal System

A crystal system relates to the shape and symmetry of the unit cell, and in particular, to the relative lengths and the angles between the cell edges.

For example, the cubic system is defined by a cube-shaped unit cell, where the cell edges a, b and c are mutually perpendicular, and have the same lengths. On the other hand, the triclinic system is characterized by a "distorted" unit cell, in which the cell edge lengths and their interaxial angles may all be different. The 7 unique crystal systems are summarized below:-

| Crystal System | Unit Cell Dimensions | Essential Symmetry | Bravais Lattices |
|---|---|---|---|
| Triclinic | $a \neq b \neq c$<br>$\alpha \neq \beta \neq \gamma$ | None | P |
| Monoclinic | $a \neq b \neq c$<br>$\alpha = \beta = 90° \neq \gamma$ | One 2-fold (diad) axis | P, C |
| Orthorhombic | $a \neq b \neq c$<br>$\alpha = \beta = \gamma = 90°$ | Three 2-fold (diad) axes | P, C, I, F |
| Tetragonal | $a = b \neq c$<br>$\alpha = \beta = \gamma = 90°$ | One 4-fold (tetrad) axis | P, I |
| Cubic | $a = b = c$<br>$\alpha = \beta = \gamma = 90°$ | Three 3-fold (triad) axes | P, I, F |
| Trigonal (*) | $a = b = c$<br>$\alpha = \beta = \gamma \neq 90°$ | One 3-fold (triad) axis | R |
| Hexagonal | $a = b \neq c$<br>$\alpha = \beta = 90°; \gamma = 120°$ | One 6-fold (hexad) axis | P |

*(*) Note that trigonal crystals can be described in terms of an hexagonal unit cell, although their maximum symmetry is 3-fold, not 6-fold.*

## Diffraction

Diffraction is the process by which waves interact with objects and are disturbed, or bent, from their previous course (e.g., the movement of water ripples around the end of a pier). CrystalMaker is designed to work with two sister programs, SingleCrystal and CrystalDiffract, to simulate diffraction of X-rays, neutrons or electrons from either single crystals, or powdered specimens.

## D-Spacing

The term "d-spacing" refers to the inter-planar separation for a set of lattice planes: that is, the distance between successive planes, measured along the plane normal (at 90° to each lattice plane).

Planes of atoms in a crystal act as miniature diffraction gratings, and their d-spacings control the angles at which radiation is scattered, as summarized in the famous Bragg Equation of 1912.

## Electron Density

The distribution of electrons in a structure. CrystalMaker calculates an "atomistic" electron density by using a Fourier expansion in terms of the **Structure Factors** (which depend on the **Atomic Scattering Factors** for all atoms):

$$\rho = 2 \sum_h \sum_k \sum_l F(hkl) \exp[\, 2\pi i\, (hx + ky + lz)\, ]$$

where $F(hkl)$ is the Structure Factor for the reflexion $hkl$, and $\{x, y, z\}$ are the fractional coordinates of the point in space at which the electron density is to be calculated.

Note that this, calculated, electron density may differ from the true electron density in the crystal, particularly if there is strong directional bonding. The calculation assumes a spherical distribution of electrons around each atom, with the radial electron density determined by the shape of the **Atomic Scattering Factor** for that atom. Nevertheless, this "ideal" atomistic electron density is useful, particularly as it relates to the process of diffraction, and provides an important reference when trying to understand actual electron density (e.g., derived from computational studies) in the crystal.

### Form Factor

*See* Atomic Scattering Factor.

### Fractional Coordinates

For crystal structures it is conventional to define atomic coordinates relative to the unit cell dimensions; these relative coordinates are expressed as fractions of the unit cell dimensions along the crystallographic x, y, and z axes.

For example, if an atom in a cubic crystal has orthogonal coordinates {x = 2 Å, y = 4 Å, z = 6 Å} and the unit cell parameter $a$ (= $b$ = $c$) is 10 Å, then its fractional coordinates are {0.2, 0.4, 0.6}.

### General Equivalent Position

Crystallographic symmetry includes lattice translations (defined by the lattice type), plus additional symmetry operations associated with each lattice point. These symmetry operations, which may include mirror or rotational symmetry, can be summarized by listing the relative coordinates to which a single atom is mapped.

For example, consider a crystal whose unit cell contains just a single symmetry element: a mirror plane parallel to the x and z axes, and passing through the y axis at the origin. The mirror plane will reflect (or map) a point at {+x, +y, +z} to the position at {+x, -y, +z}. In other words, the positions {+x, +y, +z} and {+x, -y, +z} are symmetrically-equivalent - and are referred to as "general equivalent positions" for this crystal.

### Interpolate Structures

CrystalMaker provides an Interpolate Structures command, which places one or more new structures between a pair of end-member structures. The new structures are created by averaging the end-members in the appropriate proportions (e.g., inserting three structures between "A" and "B" would yield three intermediate structures: 0.25A + 0.75B, 0.5A + 0.5B and 0.75A + 0.25B). This process of generating intermediates and then inserting them into a list is called "interpolation". It is useful for making animations smoother.

### Isotropic Displacement Parameter

A representation of the thermal (or other) motion of an atom, assuming equal motions in all directions. The radius of the sphere is the atom's mean-square displacement, $< u^2 >$, written $U_{iso}$ (in units of Å$^2$).

N.B., the isotropic *displacement* factor, $U_{iso}$, is related to the atom's isotropic *temperature* factor, $B_{iso}$, by a factor of $8\pi^2$, i.e.,

$$B_{iso} = 8\ \pi^2\ U_{iso}\ .$$

### Lattice

A lattice is defined as a regular arrangement of points throughout space. This is a mathematical concept, used to describe the regular repetition, throughout 3-d space of individual atoms, or groups of atoms (i.e., the asymmetric unit).

The basic building brick of a crystal, the unit cell, has lattice points at each of its eight corners. It may also have lattice points at the centres of certain faces, or at the centre of the unit cell. This arrangement of lattice points within the unit cell defines the lattice type of a crystal: *P* (Primitive); *I* (Body-centred, from the German Innenzentrierte; "inner-centred"); *A*-, *B*- and *C*-face centred; *F* (all-face-centred) and *R* (Rhombohedral).

### Lattice Parameters

Six numbers which uniquely define the size and shape of the unit cell. These are the lengths of the unit cell edges, *a*, *b*, *c*; and the inter-axial angles α, β, and γ.

### Lattice Plane

A lattice plane is a plane of lattice points in a three-dimensional structure The orientation of a lattice plane can be given in terms of its intercepts along the unit cell axes xyz. These are summarized using Miller Indices, (hkl).

### Lattice Vector

A lattice vector is defined as a vector between two lattice points. The orientation of the vector can be expressed in terms of its coefficients U, V, and W, parallel to the unit cell vectors **a**, **b**, and **c**, respectively, giving the vector equation:

$$U\mathbf{a} + V\mathbf{b} + W\mathbf{c}$$

which is generally written in a shorthand form as:

$$[UVW]$$

Note that the unit cell vectors are not necessarily mutually orthogonal, neither may they be of equal length. So, for example, in an orthorhombic crystal ($a \neq b \neq c$), the lattice vector [100] probably has a different length from the vector [010].

### Miller Indices

Miller Indices are sets of three integers, designated h, k, l, which uniquely define the orientation of a lattice plane, relative to a crystal's unit cell.

A lattice plane's orientation can be defined in terms of its intersections with the three crystallographic axes, x, y, and z. If a unit cell has edge lengths a, b, and c, and the first lattice plane from the origin cuts these axes at $a/h$, $b/k$, and $c/l$, then the Miller Indices of that plane are: ($h\ k\ l$).

### Mineral

A mineral is a naturally-formed crystal. That is, a solid body, formed by natural processes, that has a regular arrangment of atoms which sets limits to its range of chemical composition, and gives it a characteristic crystal shape.

Examples of minerals include diamond, quartz and feldspar, but not glass, which although solid, does not have a regular internal structure.

### Molecular Cell

In CrystalMaker, this refers to the full contents of the unit cell, optimized to show intact molecules. (Some atoms may lie outside the main cell, and some atoms inside that cell may be hidden, so as to depict intact molecules straddling the cell edges.)

### Molecular Crystal

Molecular crystals are crystal structures which contain discrete bonded units ("molecules") with no (strong) bonding between the units. (In reality, weak Van der Waals or hydrogen bonds may exist to hold the molecular units in place—but these weak bonds are rarely displayed in crystal plotting programs.)

Examples of molecular crystals include the structures of organic molecules, and some inorganic compounds such as sulphur hexafluoride. Examples of non-molecular crystals (i.e., with strong, long-range bonding) include most minerals (e.g., quartz, feldspar, garnet), ceramics, oxides, and so on.

### Molecular Unit

In CrystalMaker, this refers to an optimum view of a molecular crystal, derived by taking atoms in the *asymmetric unit* and repairing any molecular fragments. For example, the asymmetric unit for a benzene crystal shows just three carbon and three hydrogen atoms; the *molecular unit* shows an intact molecule with six carbons and six hydrogens.

### Molecule

A molecule is a distinct ensemble of atoms, connected via chemical bonds. The resulting structure has a fixed chemical composition, and provides a fundamental unit which can combine with other molecules (including the same species) to form a molecular crystal, or a fluid, or a gas.

Examples of molecules include benzene ($C_6H_6$), carbon dioxide ($CO_2$) and the water molecule ($H_2O$).

### Molecule Mode

CrystalMaker is designed to display periodic, crystal structures, with control over the range of unit cells displayed. However, sometimes details of a structure's periodic nature are not known (e.g., when dealing with an individual molecule in solution), or it may be necessary to "suspend" the periodicity of part of a structure, in order to study the effect of locally-introduced defects or distortions.

In these situations you can use CrystalMaker's "molecule mode" to display just the atoms that you define, without attempting to generate a unit cell or an extended lattice. This mode is also useful when performing "cluster" calculations.

If you are working with part of a crystal structure, and wish to convert it to a "cluster" of atoms, without large-scale periodicity, use the **Transform > Crystal to Molecule** command to convert your crystal to a "molecule".

### Primitive Lattice

The most basic type of lattice, where the unit cell has lattice points only at its corners. Since each corner is shared between eight unit cells, this gives a total of 8 × ⅛ = 1 lattice point per unit cell.

### Rhombohedral

This is a special kind of Primitive lattice, where the body diagonal has three-fold symmetry and the inter-axial angles are all non-orthogonal.

### Site Occupancy

The term "site occupancy" refers to the chemical content of a crystallographic site. In an ideal structure, a site in the crystal might contain one specific chemical element per site, e.g., a copper (Cu) atom on site 1 and a zinc (Zn) atom on site 2. Sometimes, however, crystals show disordered structures and there might be a statistical probability of different atoms occupying the same sites. For example 50% Cu and 50% Zn on sites 1 and 2. The site occupancy for both sites would then be written $Cu_{0.50}Zn_{0.50}$.

### Space Group

A space group is a three-dimensional arrangement of symmetry elements, positioned within a crystal's unit cell, which relates those atoms in the asymmetric unit ("motif") to the rest of the atoms in the unit cell.

A spacegroup is represented by a spacegroup symbol: a descriptive tag which may or may not give further information about the actual arrangement of symmetry elements. Crystallographers commonly use the "International Notation" of spacegroup symbols, examples of which include "*P* 1", "*P* 2/*c*" and "$I\,a\,\bar{3}\,d$". The first character of the symbol (e.g., "*P*" or "*I*") is the lattice type; the remaining characters relate to symmetry operators ("2" is a 2-fold rotation axis; "c" is a c-glide plane perpendicular to the 2-fold axis; etc.)

### Structure Factor

A Structure Factor, F(hkl) describes the amplitude and phase of radiation scattered by one unit cell of material for the set of lattice planes (hkl). The Structure Factor is a complex number, with real (A) and imaginary (B) parts:-

$$F(hkl) = A(hkl) + i\,B(hkl)$$

The phase angle, $\phi$, is given by the ratio of the imaginary to real parts:-

$$\tan \phi = B / A$$

The Intensity of the scattered radiation for the reflection (hkl) is proportional to the square of the amplitude, $|F|^2$.

CrystalMaker calculates structure factors, as part of its electron density calculations for a crystal.

### Synchronize

CrystalMaker's **Transform > Synchronize** command lets you apply the same model, rendering and view settings to all structures in the same window.

The Synchronize command displays a sheet/dialog letting you customize the options to be synchronized. Note that, by default, the bonding option is unselected, as the program errs on the safe side (even if you are comparing related structures, please bear in mind that bonding criteria may differ, as a result of thermal expansion or compression).

### Thermal Ellipsoid

*see* Atomic Displacement Parameter.

### Torsion Angle

The torsion angle between four atoms A–B–C–D is the angle by which the vector A–B must be rotated in order to eclipse the vector C–D, when viewed along the vector B–C.

Torsion angles are usually expressed in the range −180° to +180°. According to convention (*Klyne & Prelog, 1960, Experientia 16:521*), a clockwise rotation is positive and an anticlockwise rotation is negative.

### Unit Cell

The basic building brick of a crystal structure. This is a parallelipiped with edges parallel to the three crystallographic axes, x, y, and z. The edges along the x, y, and z directions define the crystallographic basis vectors, a, b, and c, respectively. The inter-axial angles are, by convention, called $\alpha$ (= y^z), $\beta$ (= x^z) and $\gamma$ (= x^y).

The axial dimensions and inter-axial angles uniquely define the three-dimensional periodic nature of the crystal's lattice, and are known as the lattice parameters.

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