

3D - Structure Graphics Capabilities with PDF-4 Database Products

Atomic Structure Information in the PDF-4 Databases

- ICDD's PDF-4 databases contain atomic structure information for a significant number of entries.
- Using the associated PDF-4 software, one can display, manipulate and analyze these structures.

	Total entries	Entries with (or cross-referenced to entries with) atomic coordinates
PDF-4+ 2013	340,653	227,110
PDF-4/Minerals 2013	40,424	28,732
PDF-4/Organics 2014	479,278	51,538

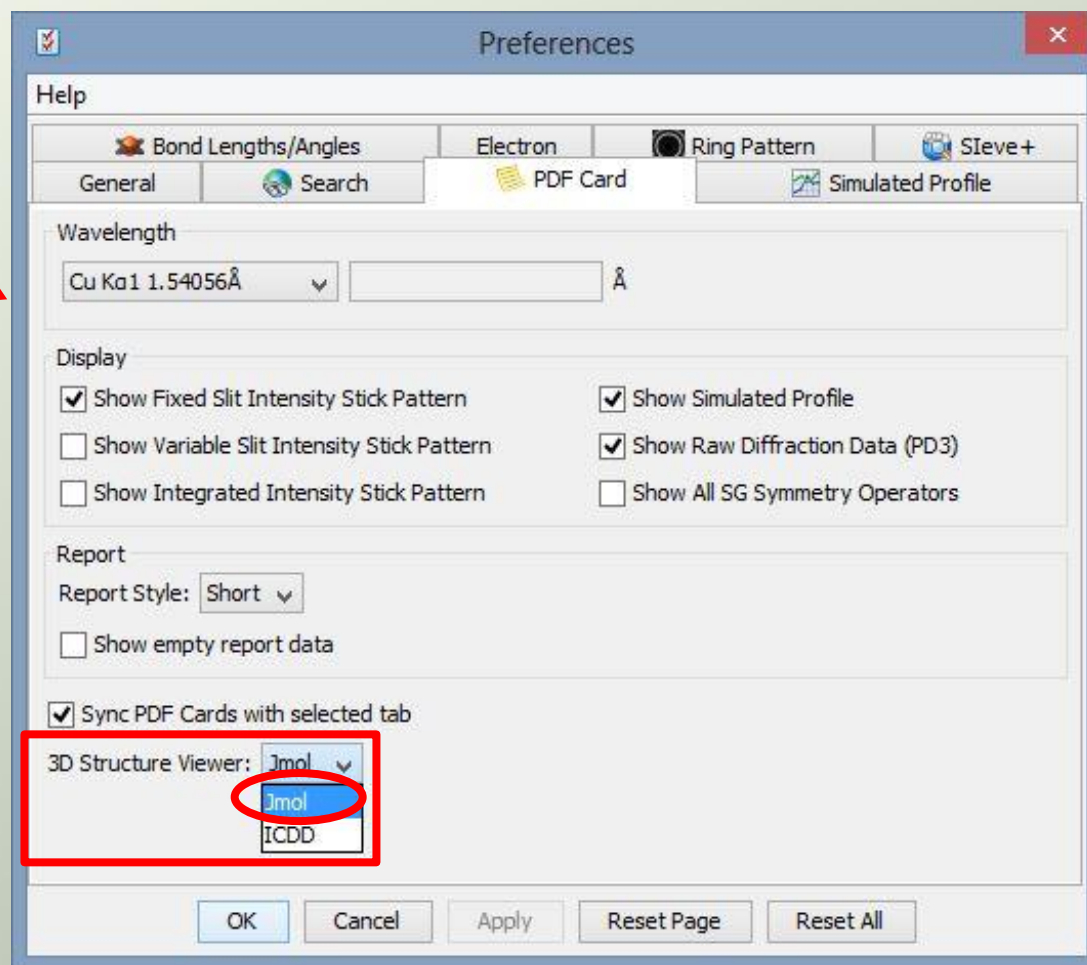
3D Structure Graphics



There are two graphics platforms available the PDF-4+ software.

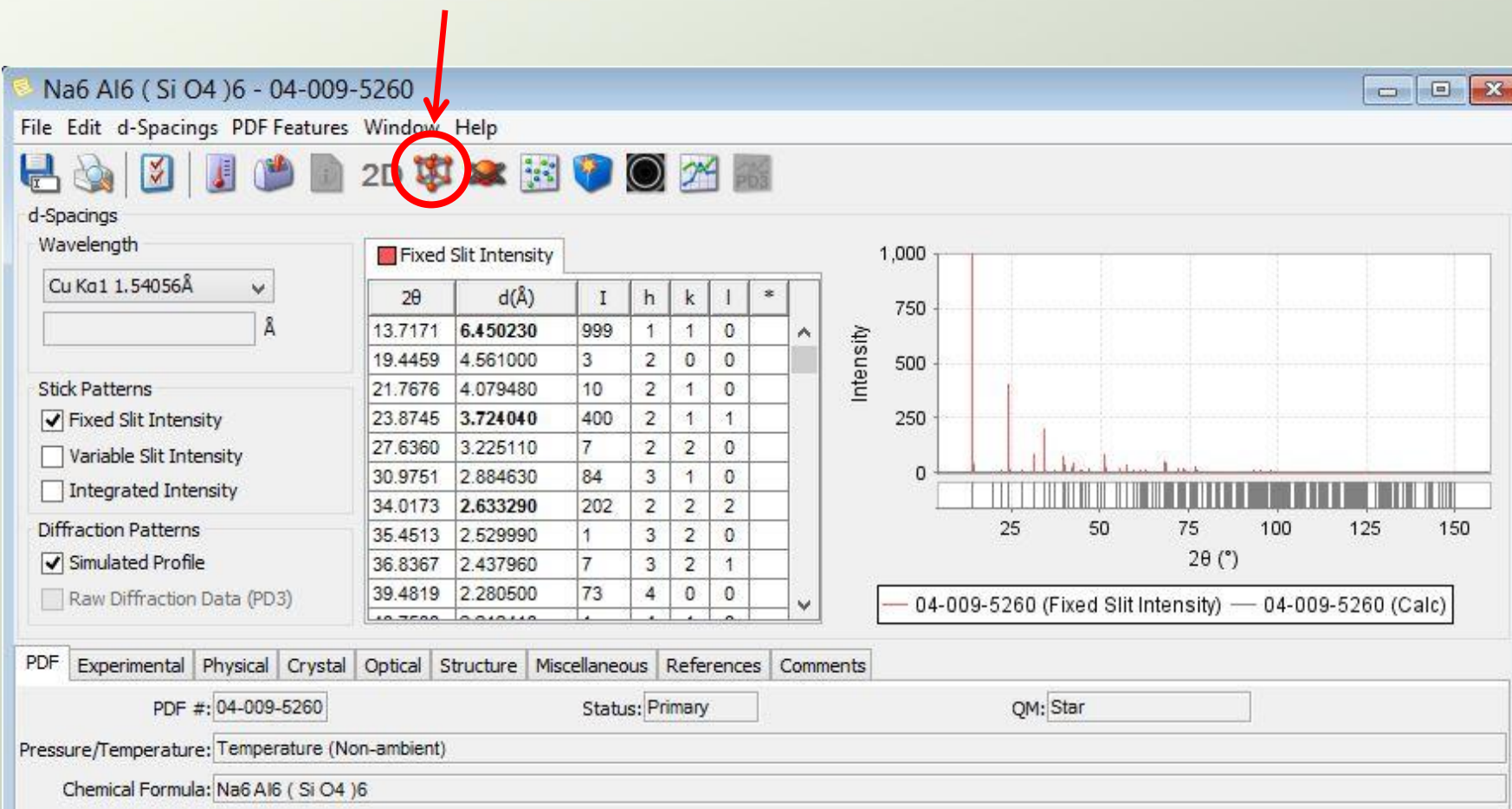
This tutorial describes the use of Jmol graphics which is the default package.

This package is selected using the PDF-4 software preferences window as shown here.



Displaying a 3D Atomic Structure

For entries with atomic structural information, the 3D-structure icon is active and can be clicked to open a 3D-structure window.



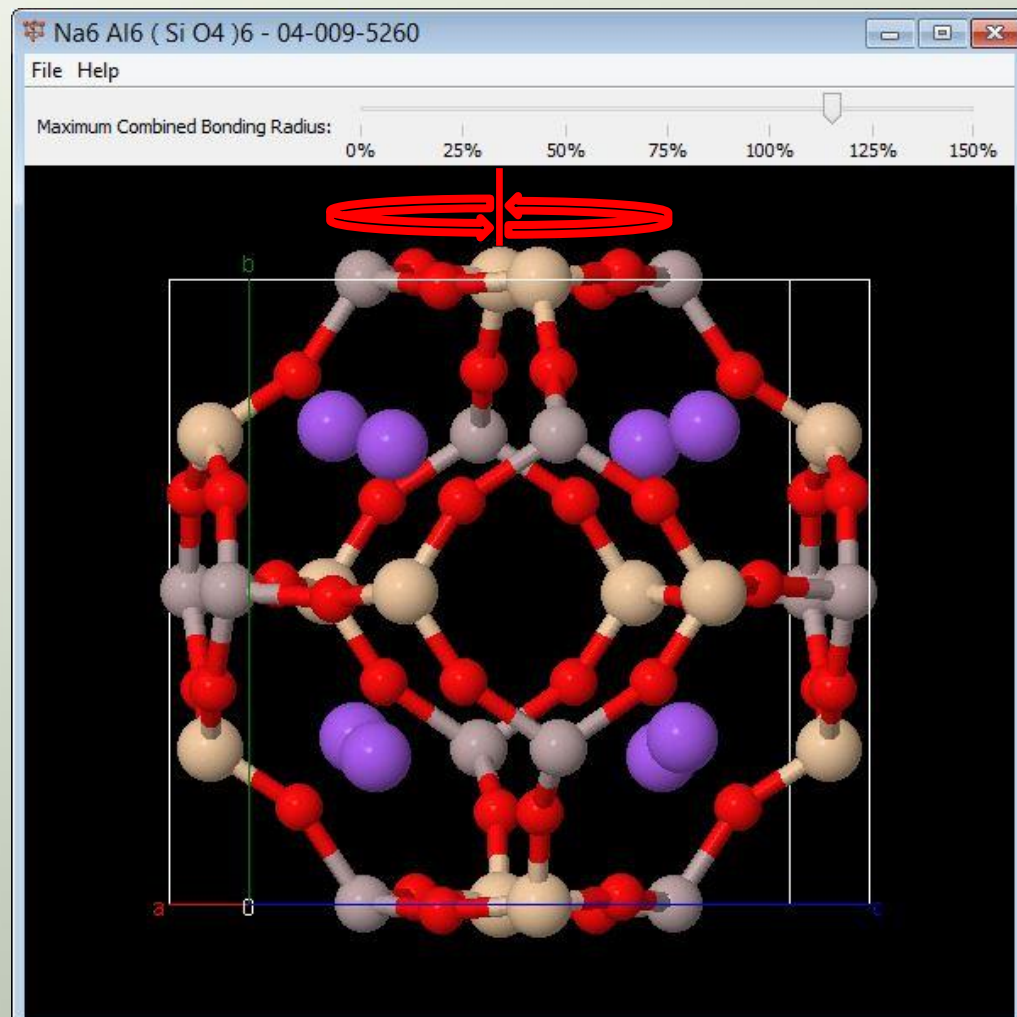
The screenshot displays the ICSD database interface for entry 04-009-5260. The title bar shows the chemical formula Na6Al6(SiO4)6. The menu bar includes File, Edit, d-Spacings, PDF Features, Window, and Help. The toolbar contains various icons, with the 3D structure icon (a ball-and-stick model) highlighted by a red circle and a red arrow pointing to it. The left sidebar shows the 'd-Spacings' section with a 'Wavelength' dropdown set to 'Cu Kα1 1.54056 Å'. Below this are 'Stick Patterns' (Fixed Slit Intensity, Variable Slit Intensity, Integrated Intensity) and 'Diffraction Patterns' (Simulated Profile, Raw Diffraction Data (PD3)). The main area features a table of d-spacings and a plot of Intensity vs. 2θ (°). The table has columns for 2θ, d(Å), I, h, k, l, and *. The plot shows experimental data (red line) and a calculated profile (black line). The bottom of the window has tabs for PDF, Experimental, Physical, Crystal, Optical, Structure, Miscellaneous, References, and Comments. The PDF tab is active, showing the PDF number 04-009-5260, Status: Primary, QM: Star, and Chemical Formula: Na6Al6(SiO4)6.

2θ	d(Å)	I	h	k	l	*
13.7171	6.450230	999	1	1	0	
19.4459	4.561000	3	2	0	0	
21.7676	4.079480	10	2	1	0	
23.8745	3.724040	400	2	1	1	
27.6360	3.225110	7	2	2	0	
30.9751	2.884630	84	3	1	0	
34.0173	2.633290	202	2	2	2	
35.4513	2.529990	1	3	2	0	
36.8367	2.437960	7	3	2	1	
39.4819	2.280500	73	4	0	0	

A Display of the Sodalite Structure

When the structure window is first opened, the structure is seen rotating about the y-axis (vertical axis).

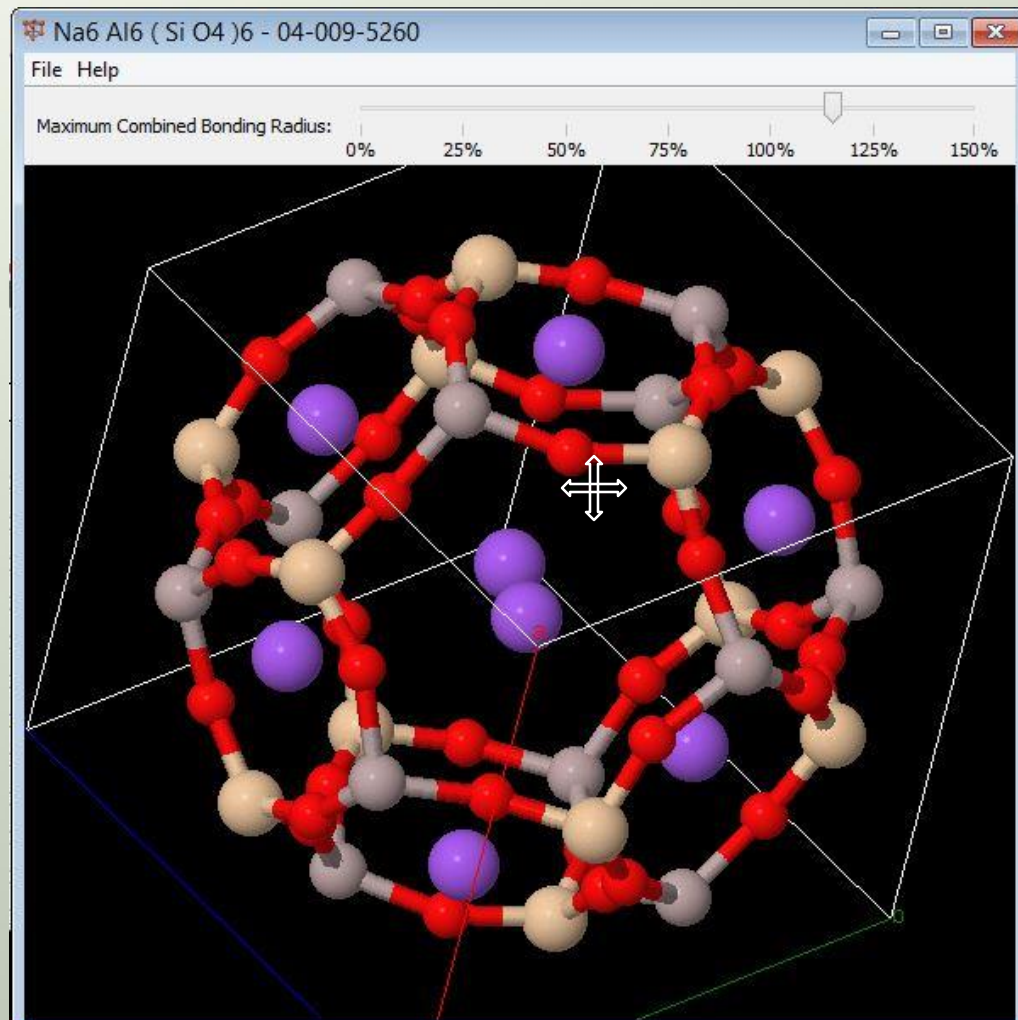
A left-mouse-click will halt this rotation.



A Display of the Sodalite Structure

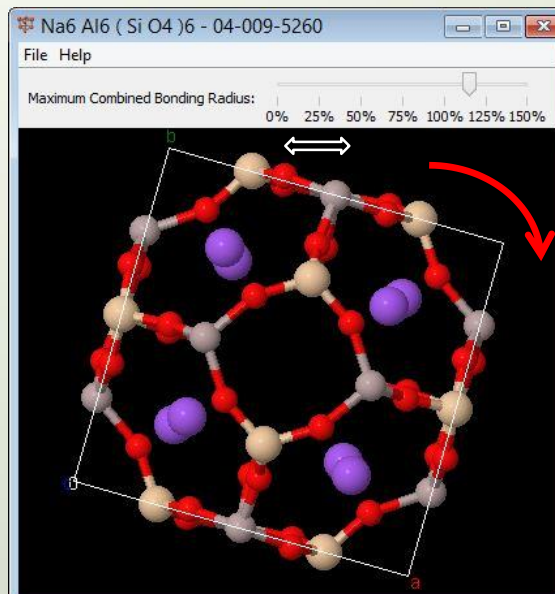
The 3D structure can be rotated manually to give the orientation of your choice.

With the left mouse button pressed, you can drag the cursor within the structure window to 'rotate' the orientation of the display about its x- or y-axis (horizontal or vertical axes respectively).



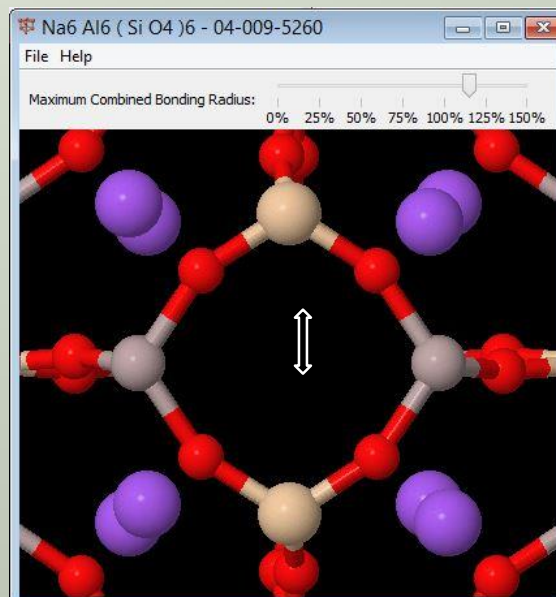
A Display of the Sodalite Structure

The 3D structure can be rotated about its z-axis (normal to the screen) by holding the 'SHIFT' key while dragging the mouse left or right with the left button pressed.



SHIFT/Left mouse button/drag left or right

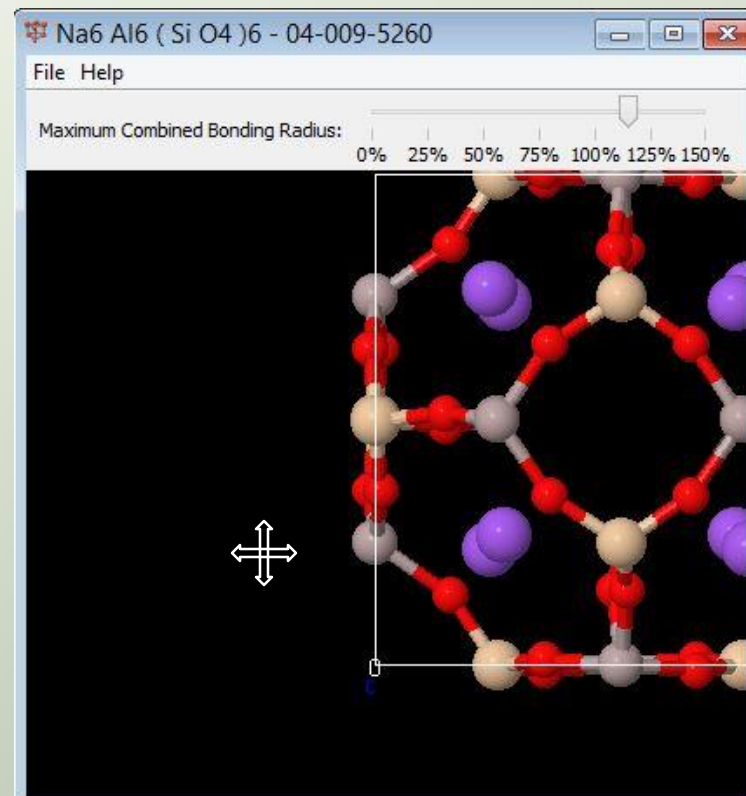
Holding the 'SHIFT' key while dragging the mouse up or down (with left button pressed) will zoom in or out of the structure display.



SHIFT/Left mouse button/drag up or down

A Display of the Sodalite Structure

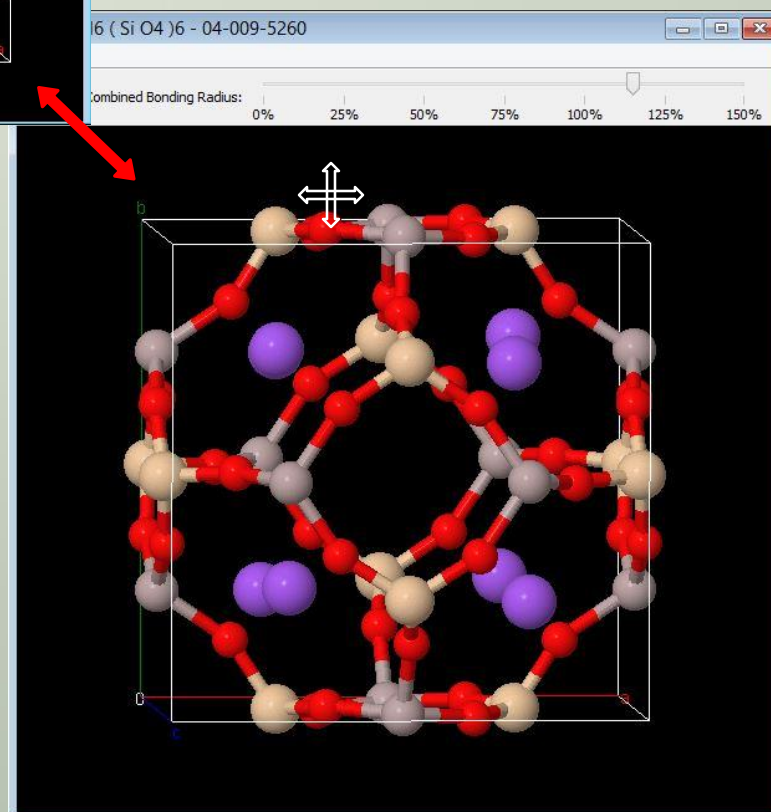
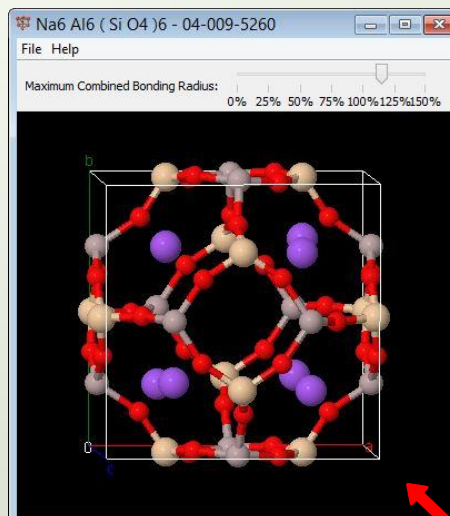
The 3D structure can be moved (translated) within the display window by holding the 'CTRL' key and dragging the mouse with the right button pressed.



CTRL / right mouse button /
drag any direction

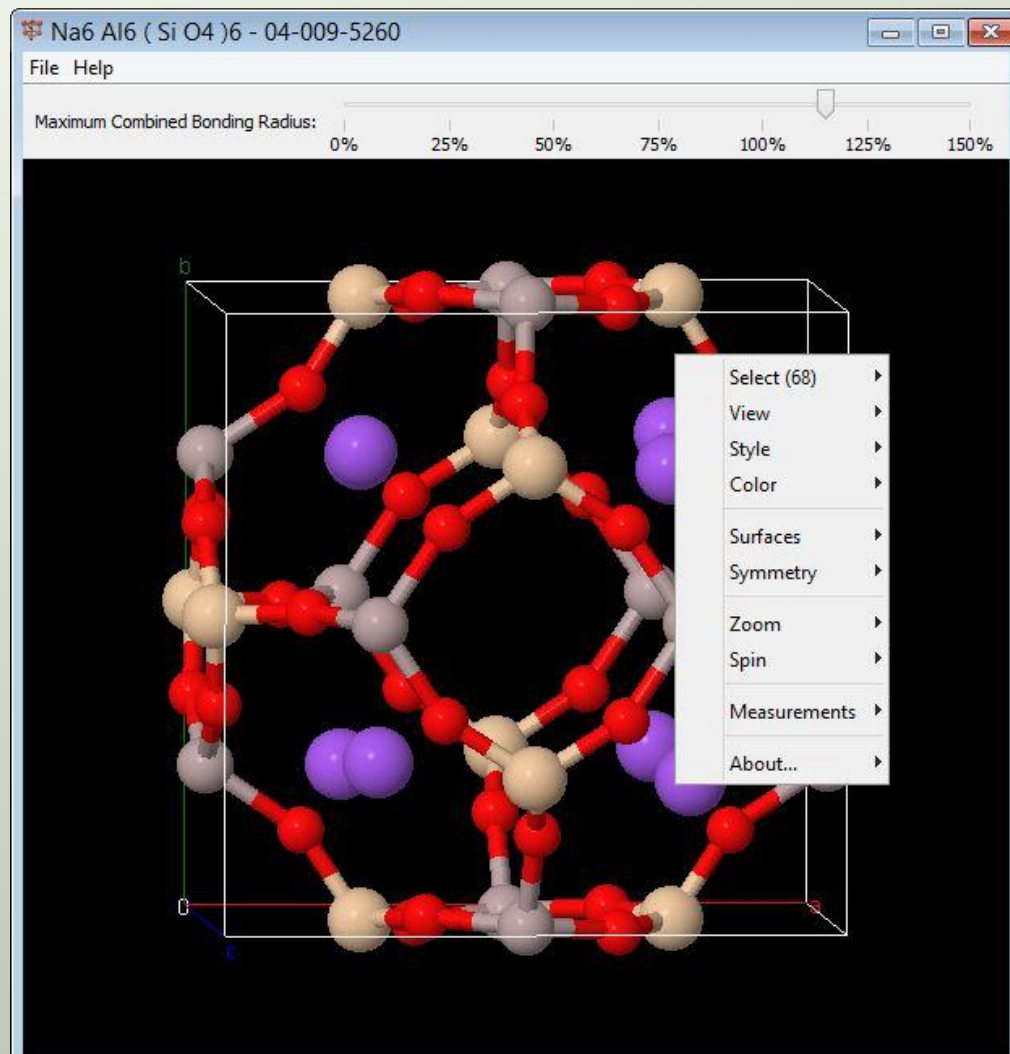
A Display of the Sodalite Structure

The display window may be re-sized by dragging the edges or corners with the left mouse button pressed. The structure will re-scale accordingly.



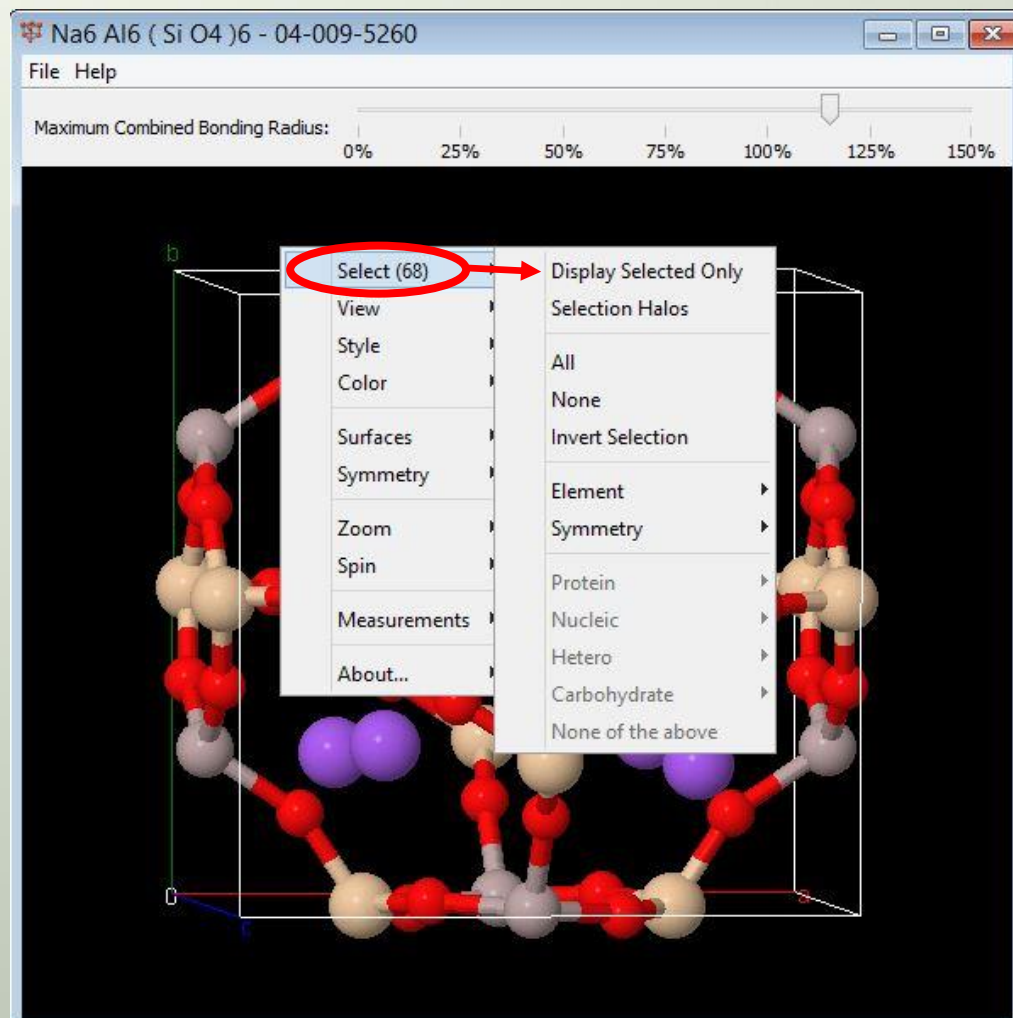
Making Adjustments to the 3D Display

- The 3D display menu is accessed with a right-mouse-button click.



Making Adjustments to the 3D Display

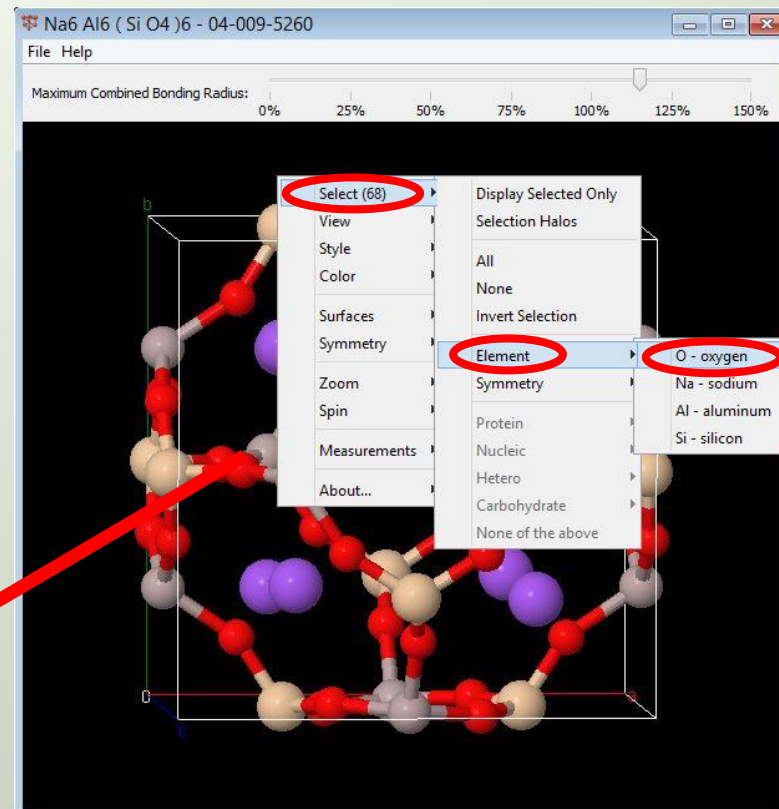
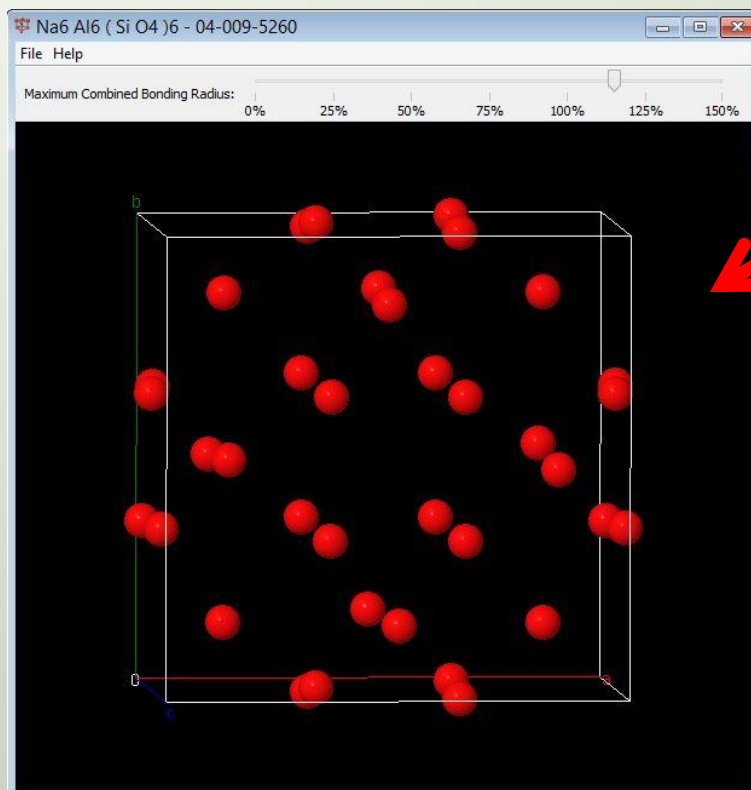
- The 'Select' menu item is used to select which atoms are displayed, or otherwise acted on. Initially, all atoms are displayed.
- To modify this, choose 'Display Selected Only' and use one of the other items on this list to choose which atoms to display.



Making Adjustments to the 3D Display

For example, to display just the oxygen atoms:

Choose 'Select' / 'Element' / 'O - oxygen' (Make sure the 'Display Selected Only' item is checked).



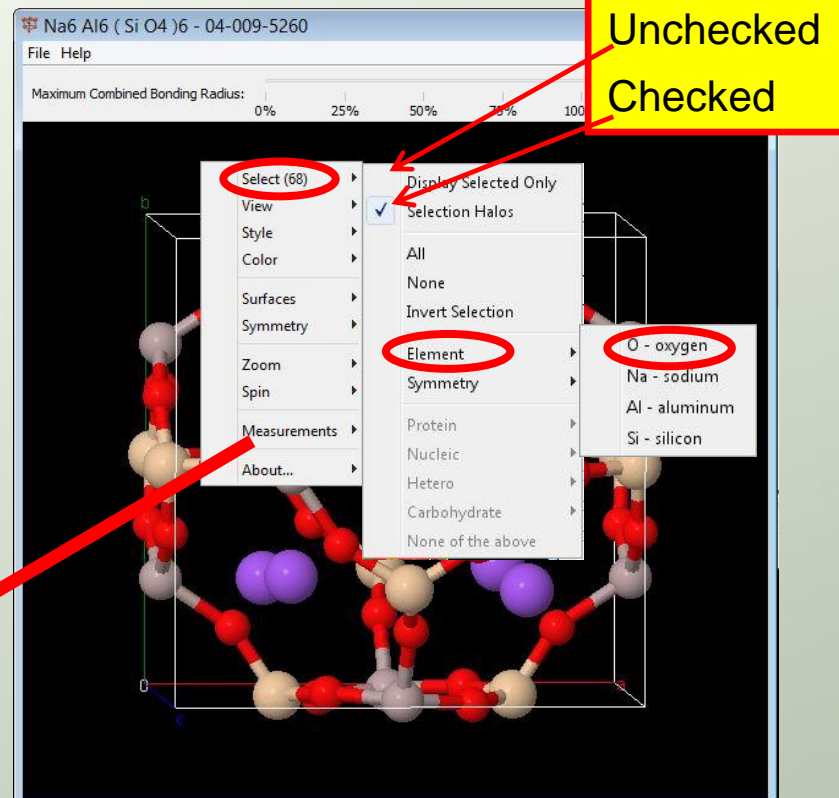
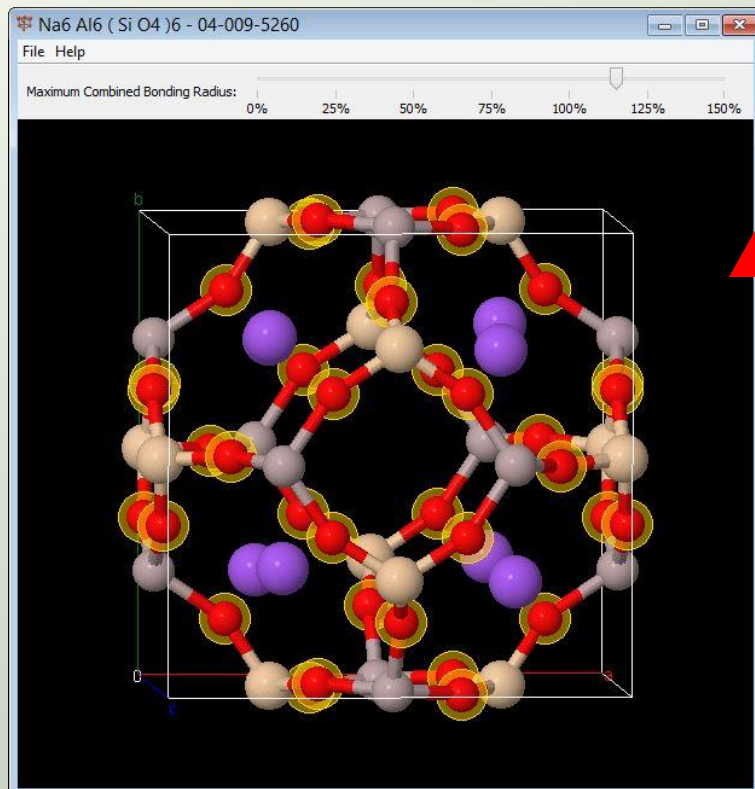
Now, just the oxygen atoms are displayed. The orientation of this display can be adjusted as before by dragging it with the left mouse button pressed.

The complete display of all atoms may be recovered by clicking 'Select' on the right-mouse-click menu and choosing 'All'.

Making Adjustments to the 3D Display

The 'Selection Halos' option allows the selected atoms to be 'highlighted' in a display of all atoms.

With 'Display Selected Only' unchecked, and having checked 'Selection Halos', the oxygen atoms can be chosen for highlighting.



Now the oxygen atoms are highlighted with yellow halos to indicate they are selected. This is useful for making color, size, or label changes to selected atoms only (as will be described).

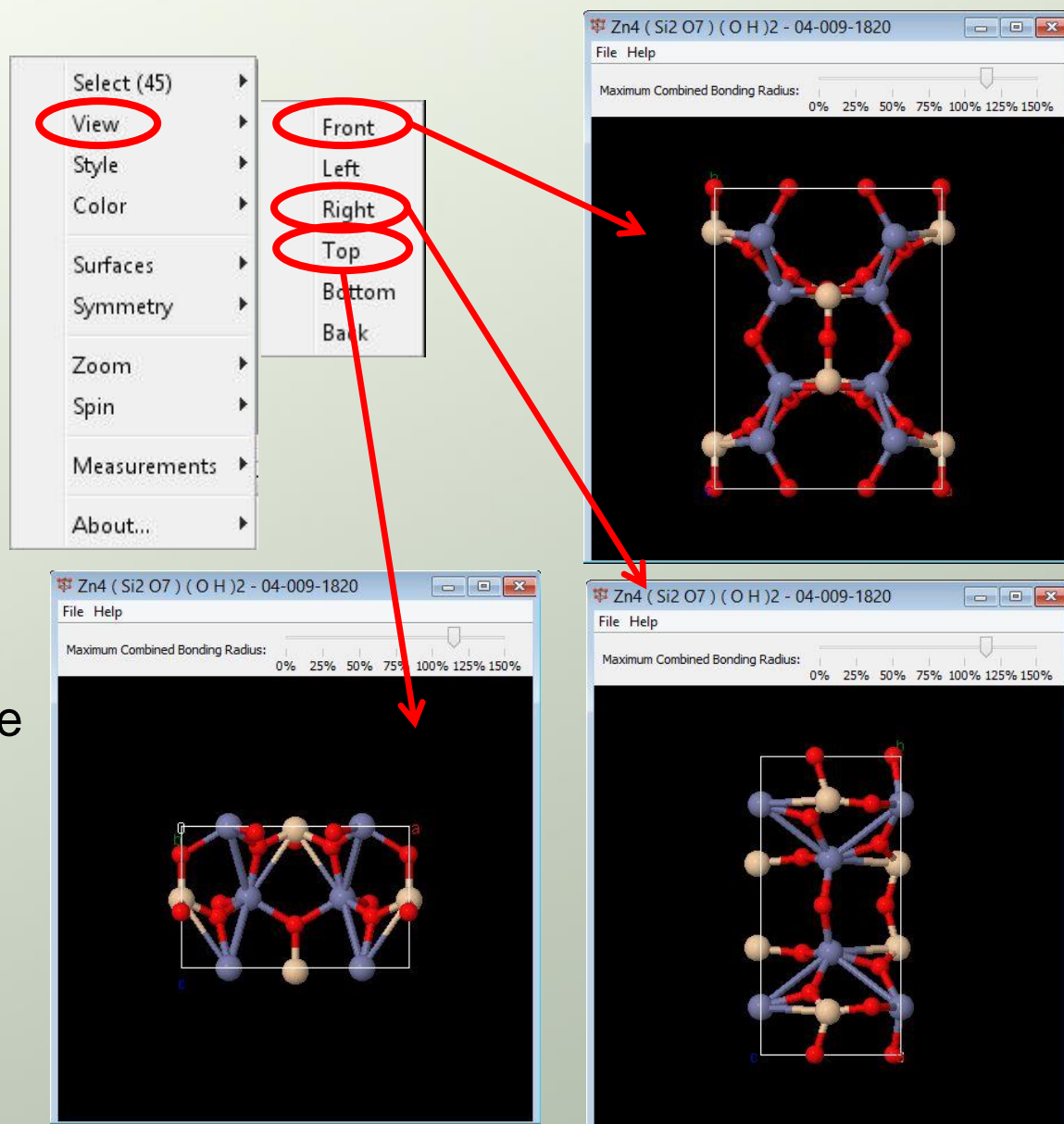
Pre-defined Orientations for 3D Structure Viewer

There are 6 pre-defined orientations that can be accessed quickly:

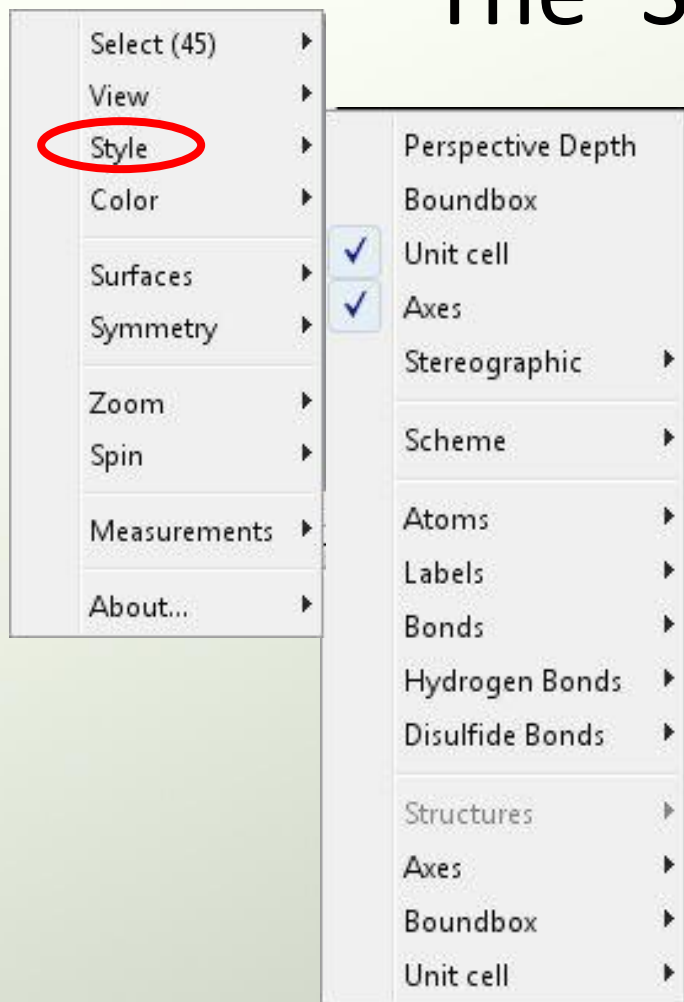
Front
Left
Right
Top
Bottom
Back

These are accessed via the 'View' item on the right-mouse-click menu.

Three of these are shown for ZnOHCl, 04-009-1820.

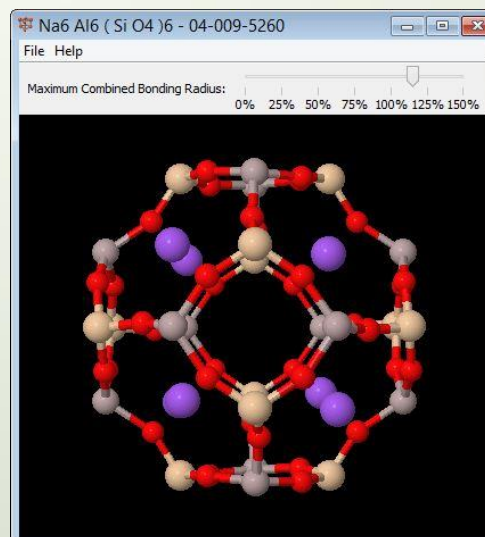
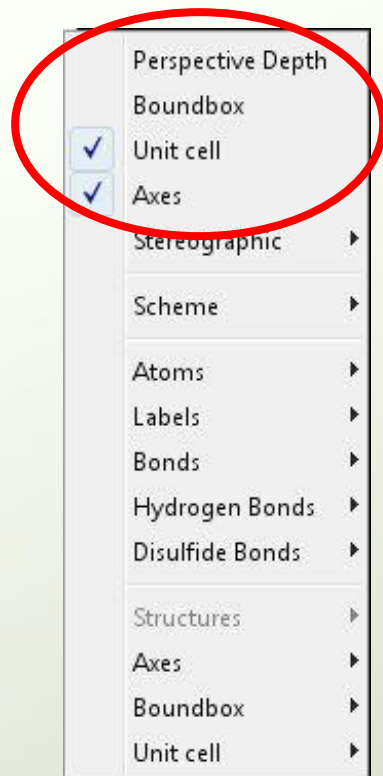


The 'Style' Menu Item

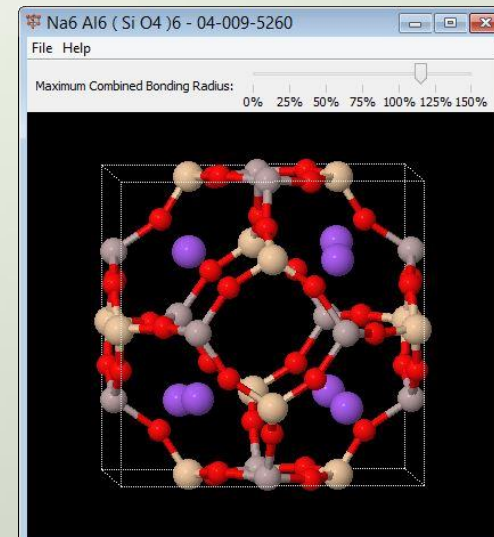


These items allow the user to decide what types of items are displayed in the 3D structure viewer, and to specify parameters affecting how these items are displayed.

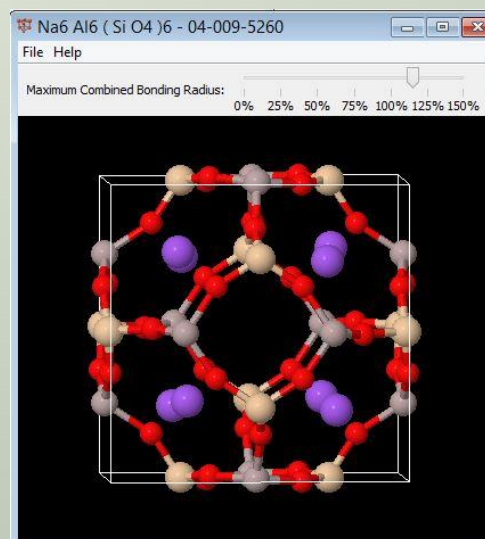
Style Menu Item Examples



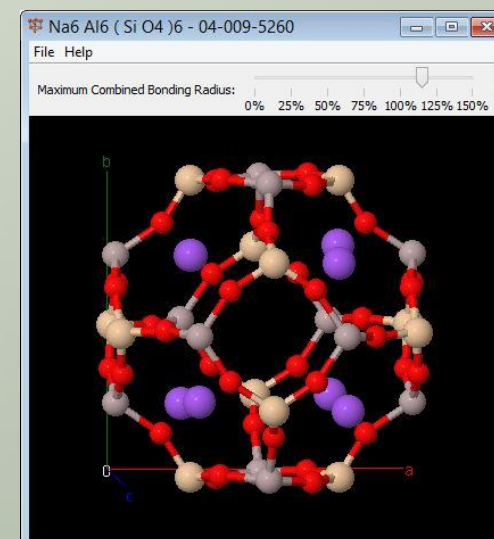
Perspective Depth



Boundbox



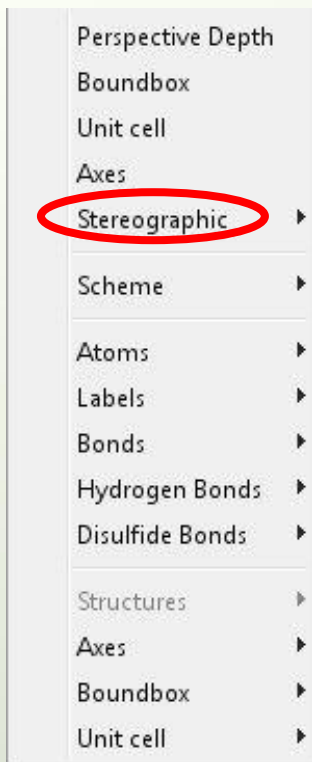
Unit cell



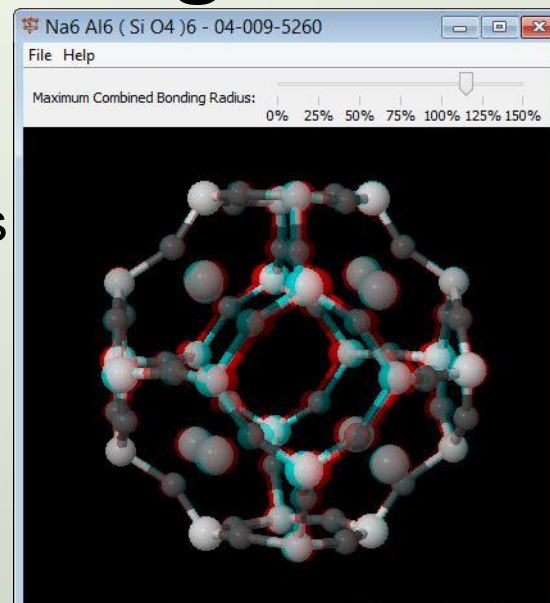
Axes

The first four items, 'Perspective Depth', 'Boundbox', 'Unit Cell', and 'Axes' can be toggled On (checked) or Off (unchecked) by clicking on them. The 'Unit cell' and 'Axes' items default to 'checked' when the viewer is launched.

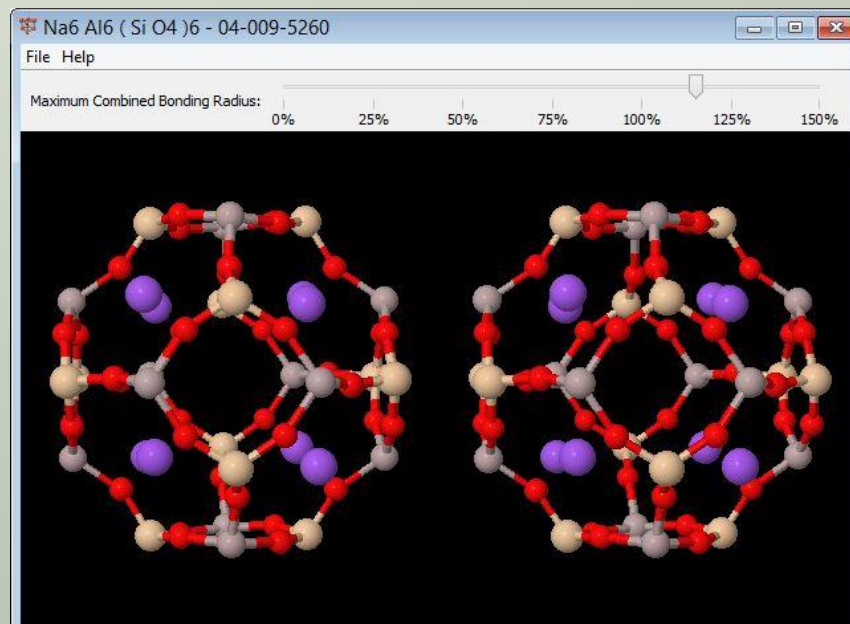
Stereographic Viewing



Stereographic →
Red + Cyan glasses



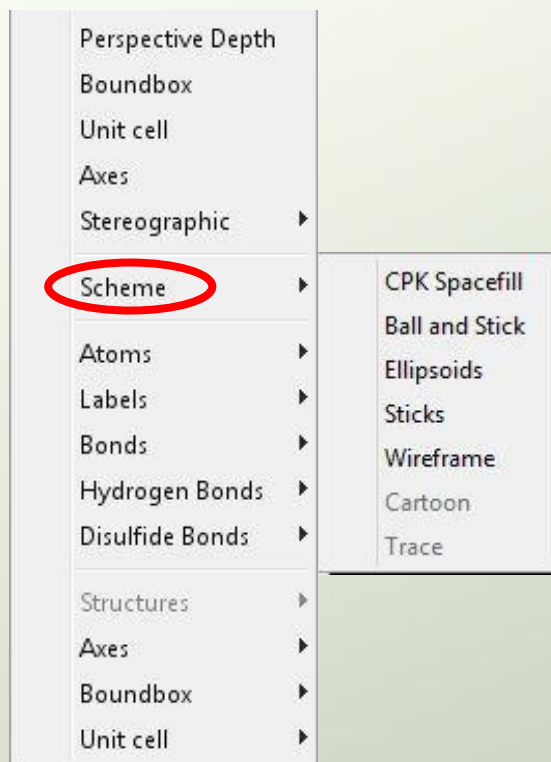
Stereographic →
Cross-Eyed Viewing



Five modes of stereographic viewing are available – two examples of which are shown here.

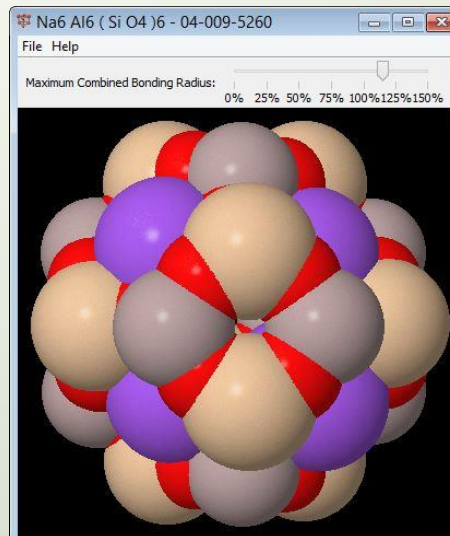
Scheme

The 'Scheme' defines the type of atom-bond construction. Four types are available.

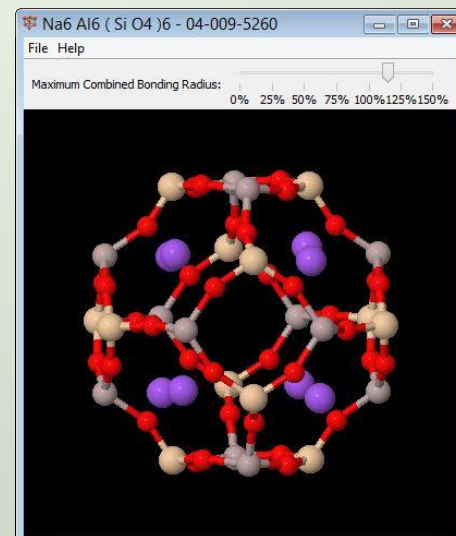


For this entry, the 'Ellipsoids' Scheme does not show ellipsoids because anisotropic displacement parameters are not provided.

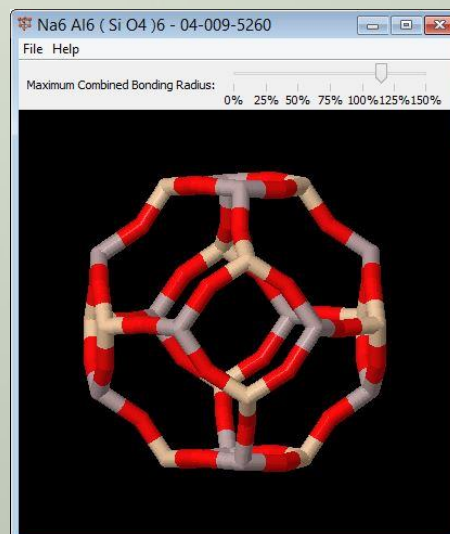
*CPK, after Robert Corey, Linus Pauling, and Walter Koltun



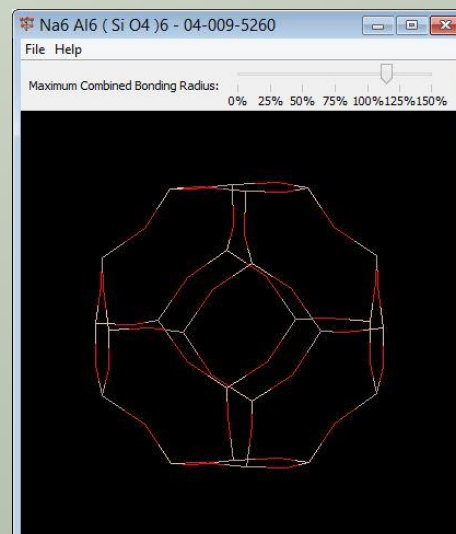
CPK* Spacefill



Ball and Stick



Sticks

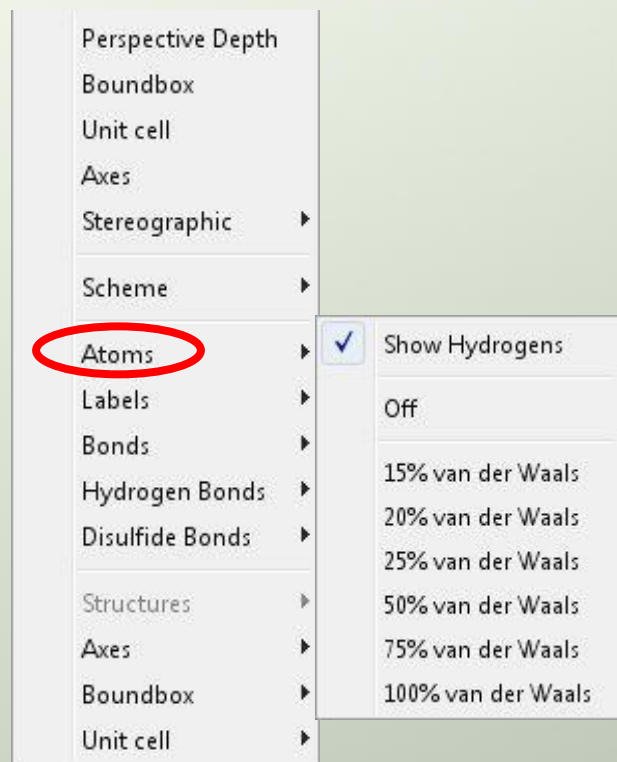
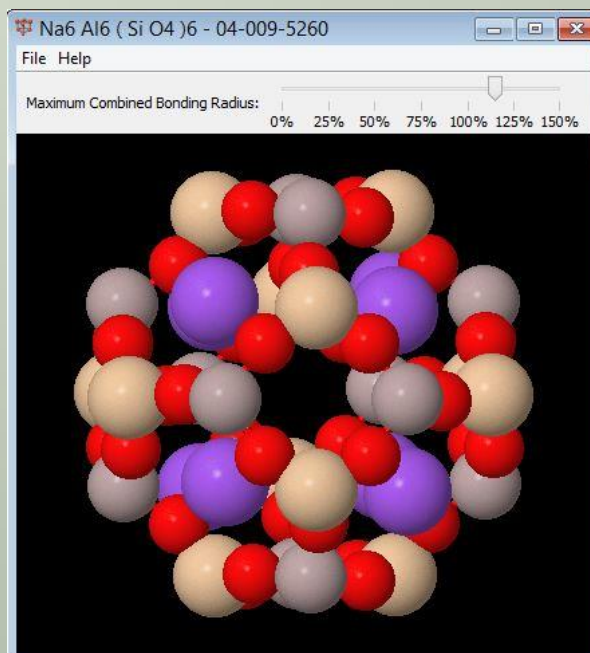
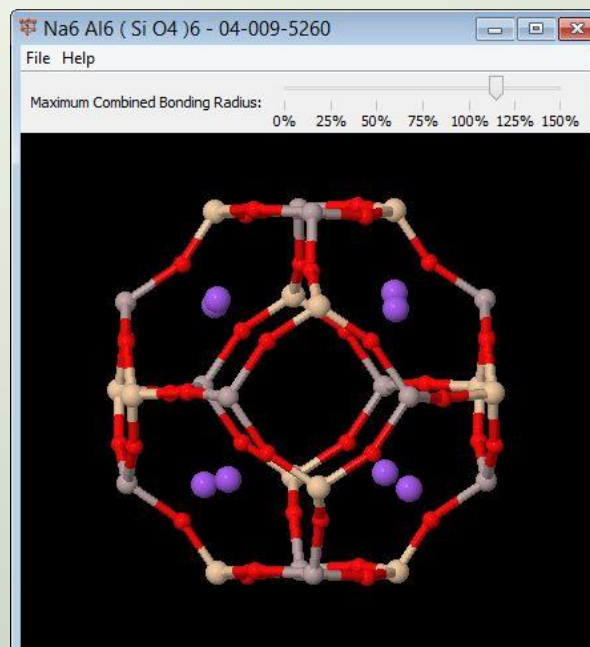


Wireframe

Atom Sizing

Atom sizing is specified in terms of van der Waals radii. The default size is 25% of the van der Waals. The 100% sizing corresponds to space-filling. If particular atoms have been 'Selected', any sizing changes will be applied only to those selected atoms.

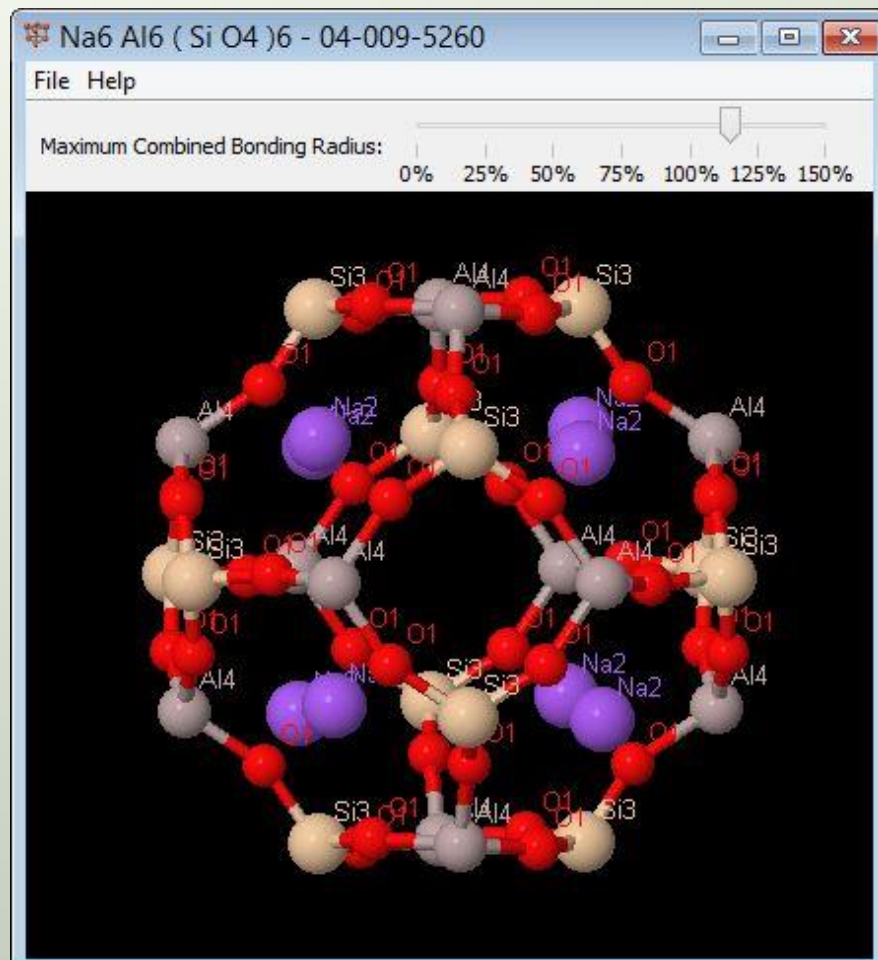
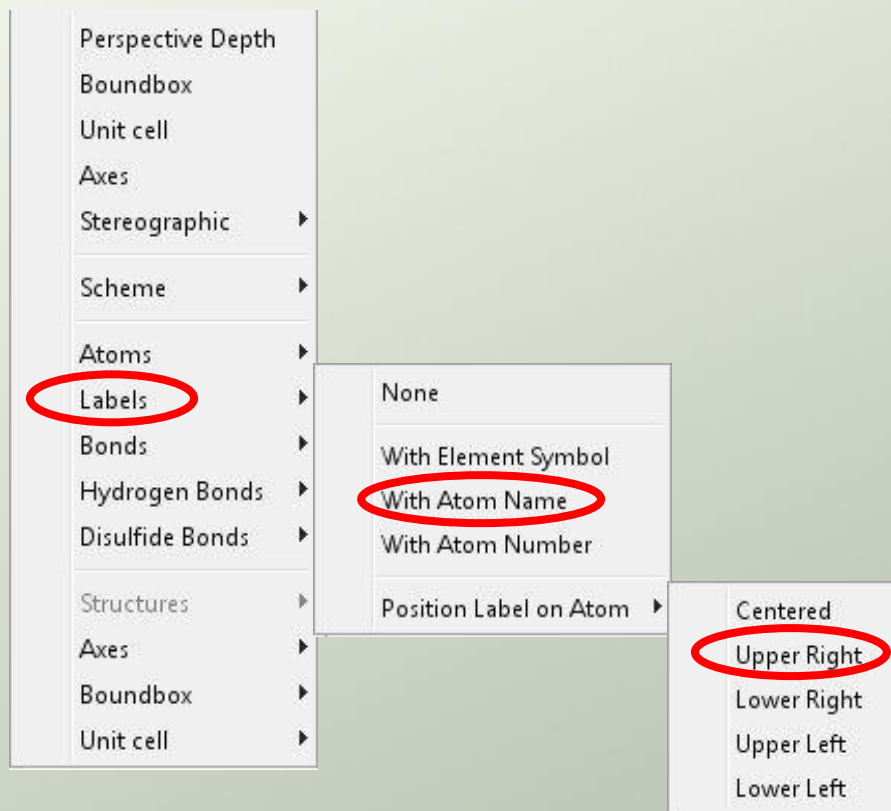
Atoms –
15% van der Waals



Atoms –
50% van der Waals

Atom Labels

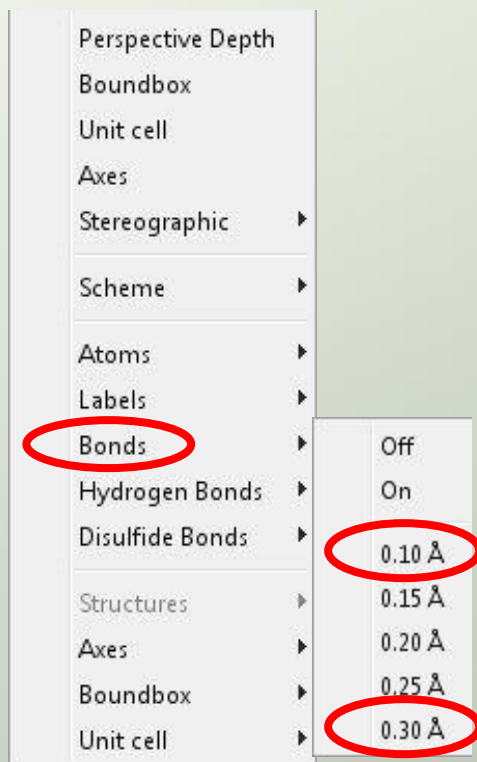
Atoms may be labeled with the element symbol, atom name, or atom number (or not at all). The position of the label relative to the atom can also be specified. As with atom sizing, if particular atoms have been 'Selected', any label changes will be applied only to those selected atoms.



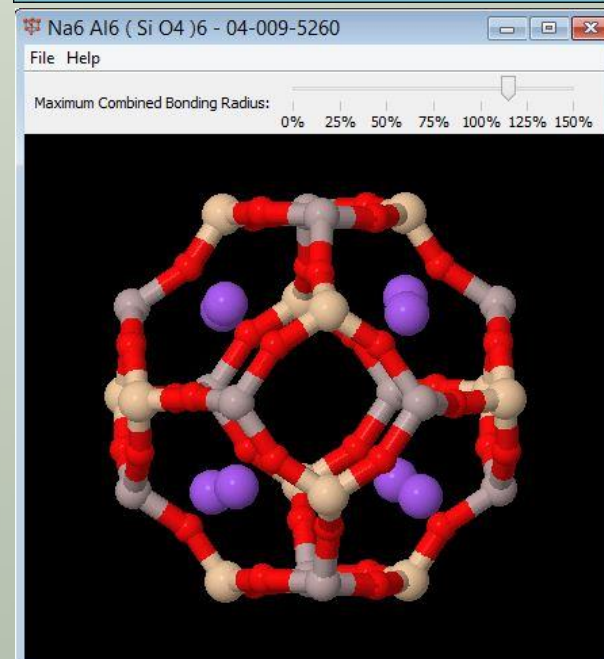
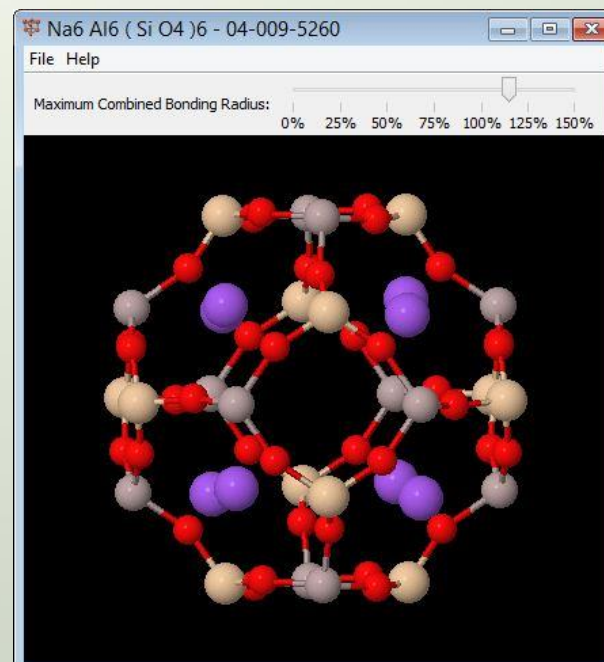
Sodalite atoms labeled with 'Atom Name' in 'Upper Right' position

Display of Bonds

Bond diameters may be specified using the 'Bonds' item on the 'Style' menu. The choices are in Angstroms and range from 0.10 to 0.30. The display of bonds may also be turned 'Off' or 'On' here.

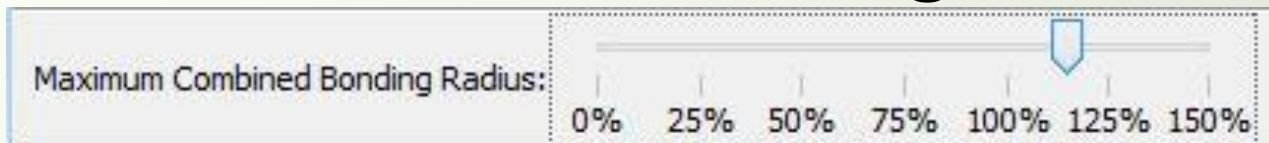


0.10 Å bonds



0.30 Å bonds

Bond Search Length

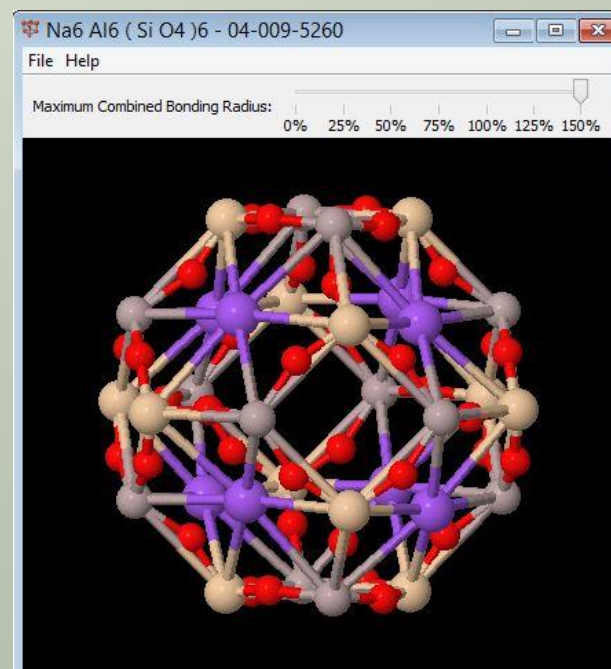
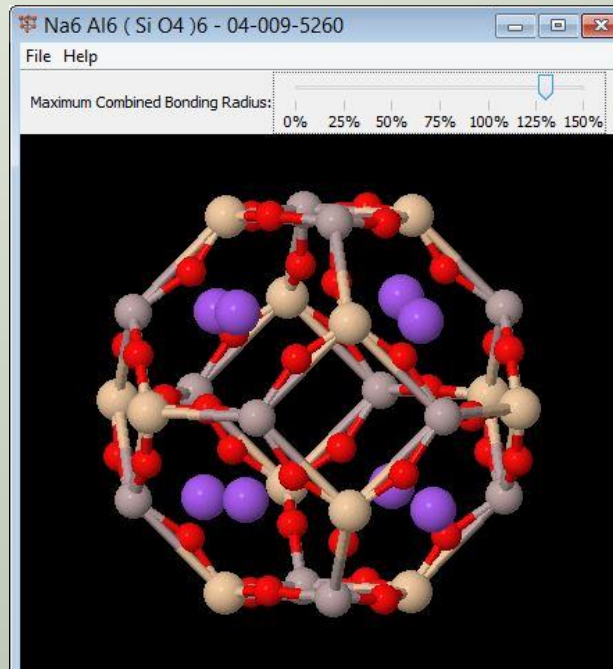
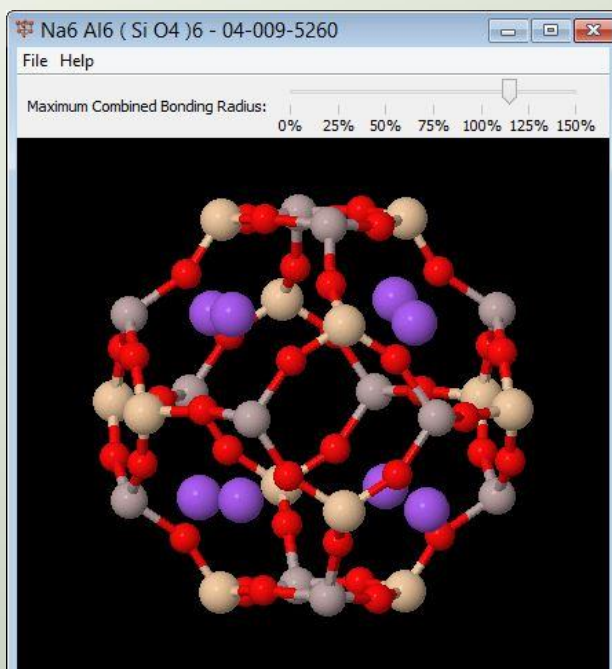


All interatomic distances in the given structure are determined and displayed according to a percentage of the combined Van der Waals radii for the two atoms involved. That percentage is user-selectable on the slider scale above the 3D structure display.

At 115%, only the covalent Si-O and Al-O bonds are shown.

At 130%, the Si – Al second-nearest neighbors are shown with connecting bonds.

At 150%, the Si-Na and Al-Na pairs are shown with connecting bonds.



Modifying Axes, Boundboxes, and Unit Cell Outlines

Perspective Depth

Boundbox

Unit cell

Axes

Stereographic

Scheme

Atoms

Labels

Bonds

Hydrogen Bonds

Disulfide Bonds

Structures

Axes

Boundbox

Unit cell

Modifications for Axes, Boundboxes, and Unit cell outlines all work similarly. They may be hidden, dotted, or solid lines of specified width. Widths specified with pixels dimensions will not scale with the display window size, those specified with Angstroms will scale.

Hide

Dotted

Pixel Width

Angstrom Width

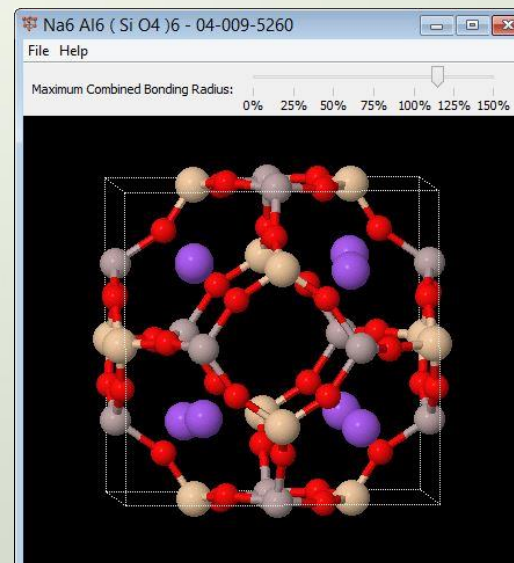
0.10 Å

0.20 Å

0.25 Å

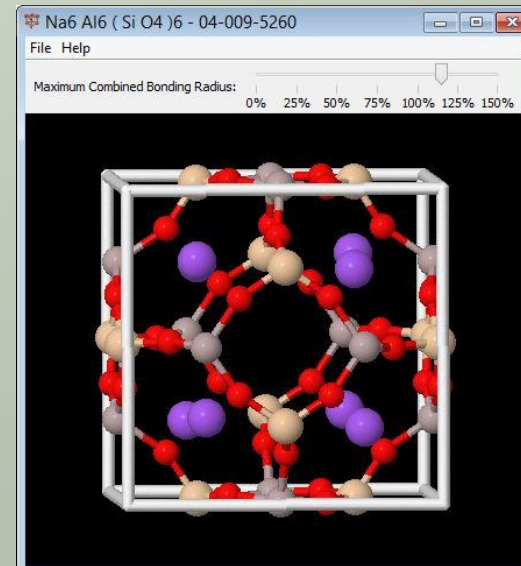
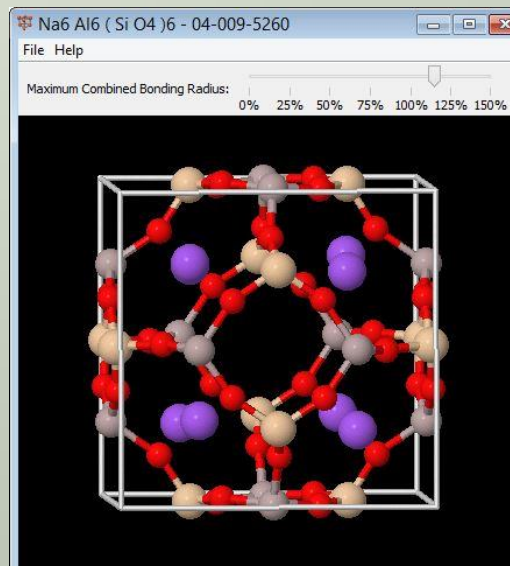
0.50 Å

1.0 Å



5 pixel Unit Cell Outline

0.20 Å Unit Cell Outline

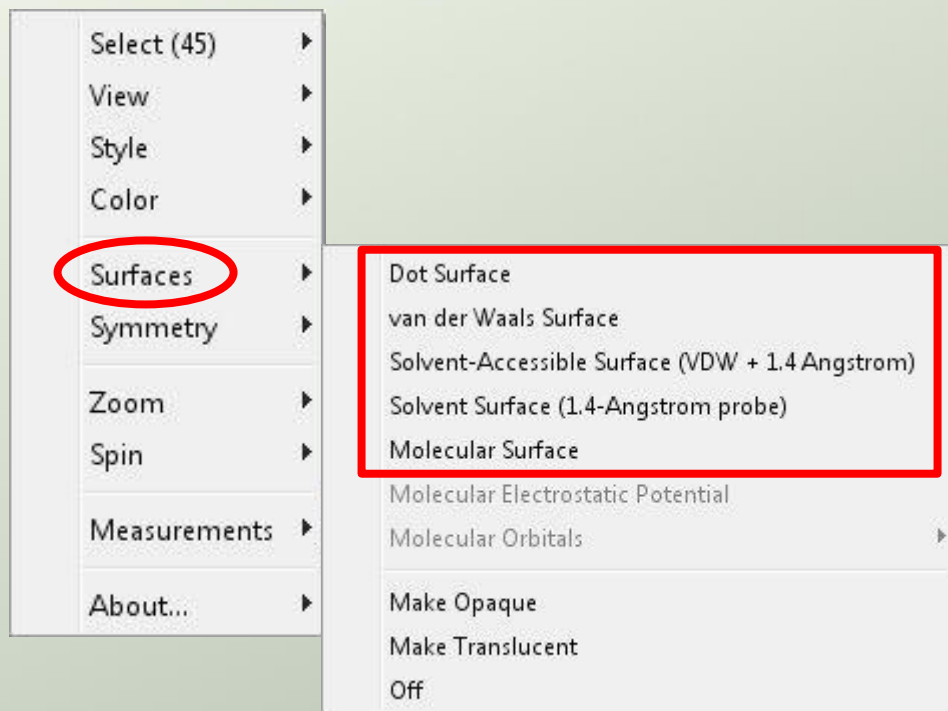


Surfaces

The visualization of structure surfaces is possible with the PDF-4+ structure viewer. Several viewing options are available as seen below in the 'Surfaces' drop-down menu below.

Any of the first five selections will display the corresponding surface, and the 'Dot Surface' can be combined with other surfaces on the list. The 'Off' choice will remove any surfaces currently displayed.

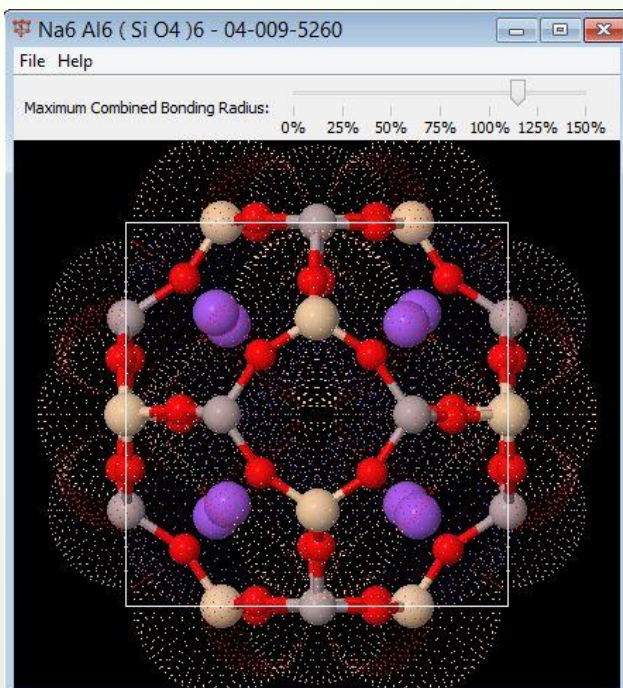
The 'Make Opaque' and 'Make Translucent' toggle whether or not the atoms and bonds are visible through the surface.



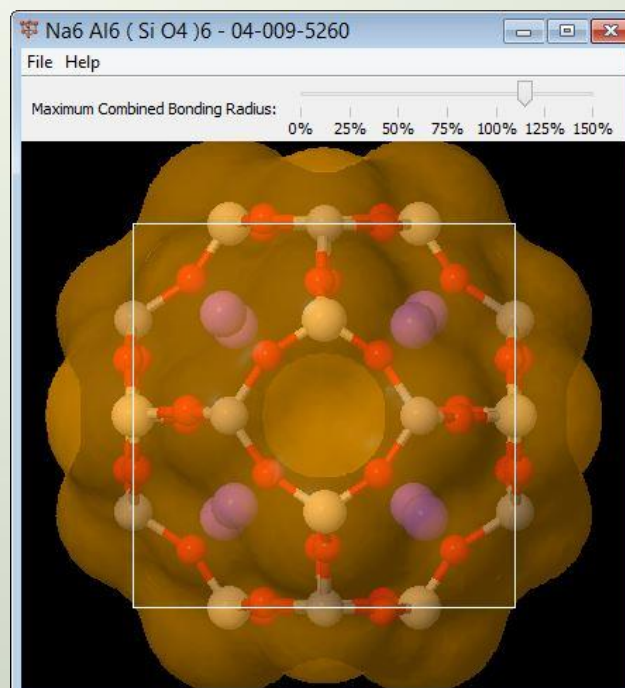
Examples of surface displays, along with their corresponding menu selection choices, are given on the following slides.

Surfaces

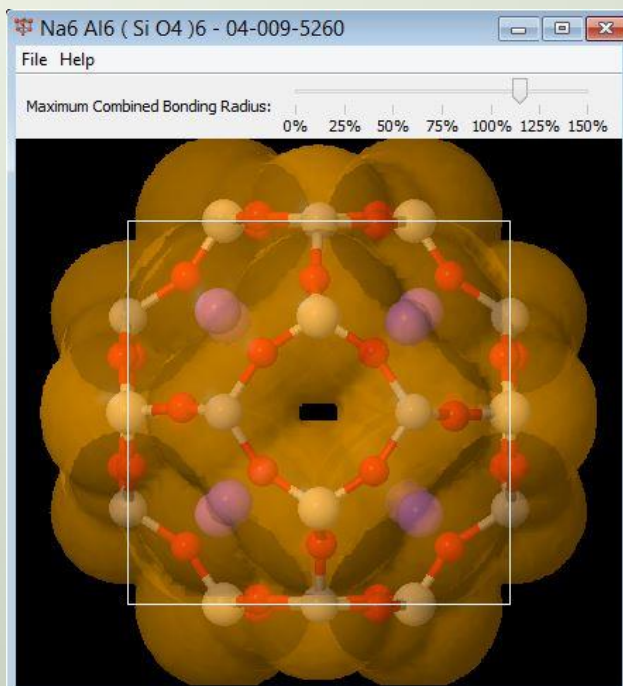
Dot Surface



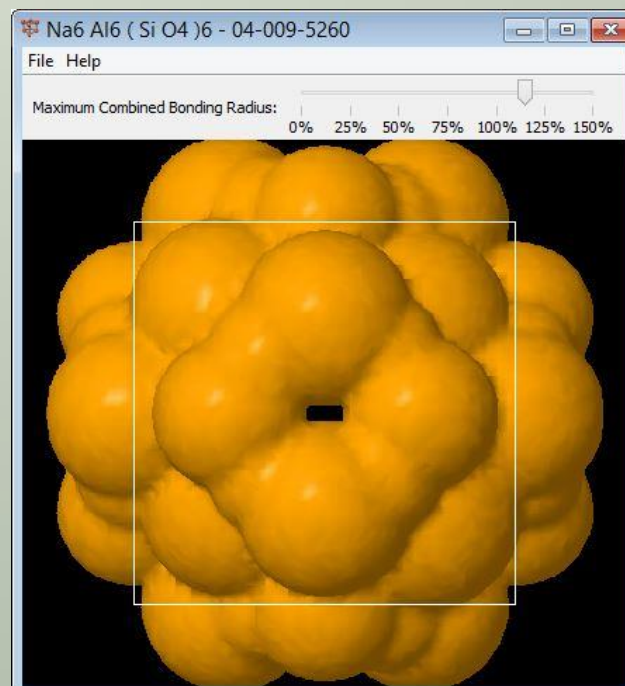
Molecular
Surface
(translucent)



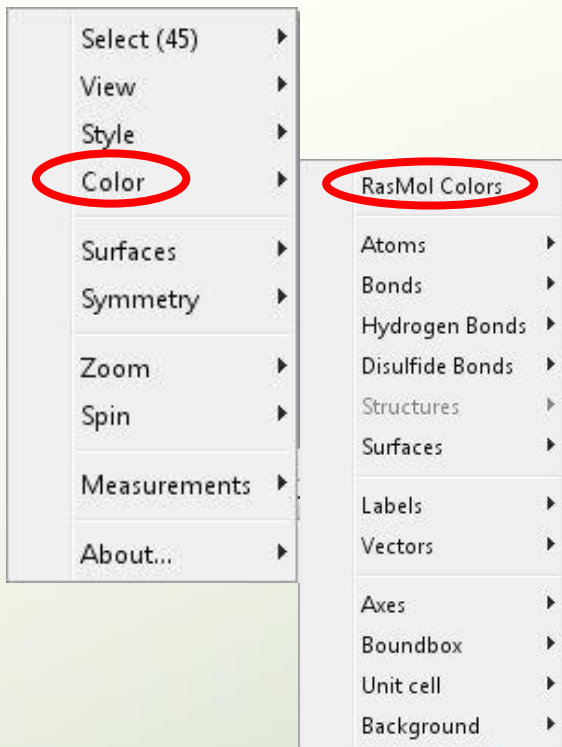
Van der Waals
Surface
(translucent)



Van der Waals
Surface (opaque)



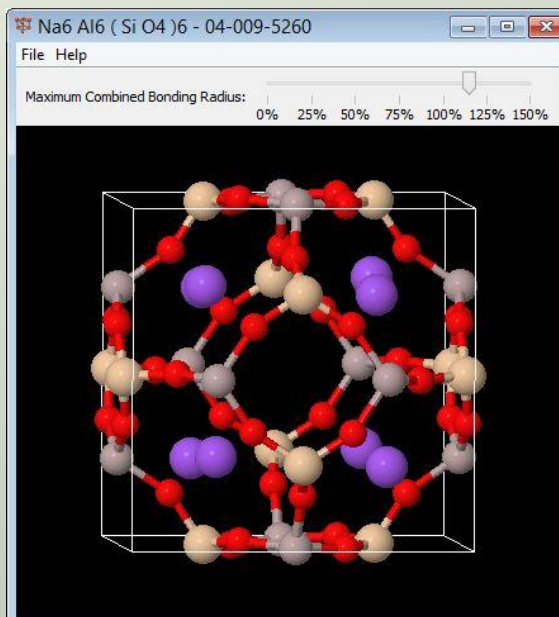
Colors



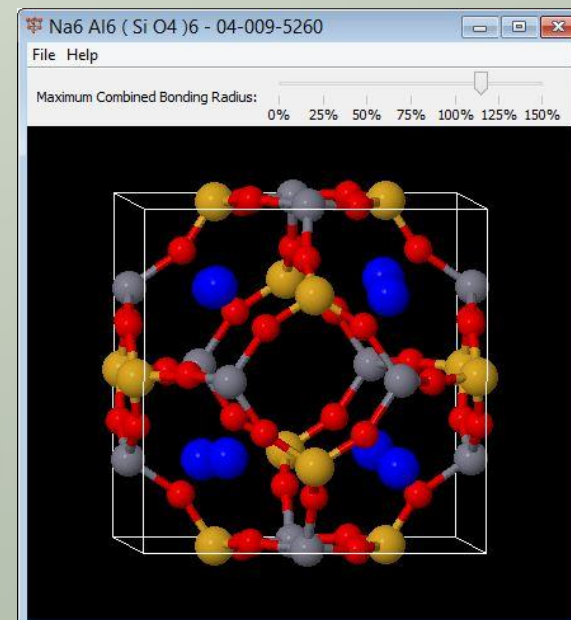
Colors for the various components of the 3D structure display can be assigned from choices on this menu.

The atom colors initially default to a CPK scheme based on atom type. Another scheme, familiar to protein crystallographers, is RasMol colors, which can be easily selected by clicking on it directly.

CPK Color Scheme (default)



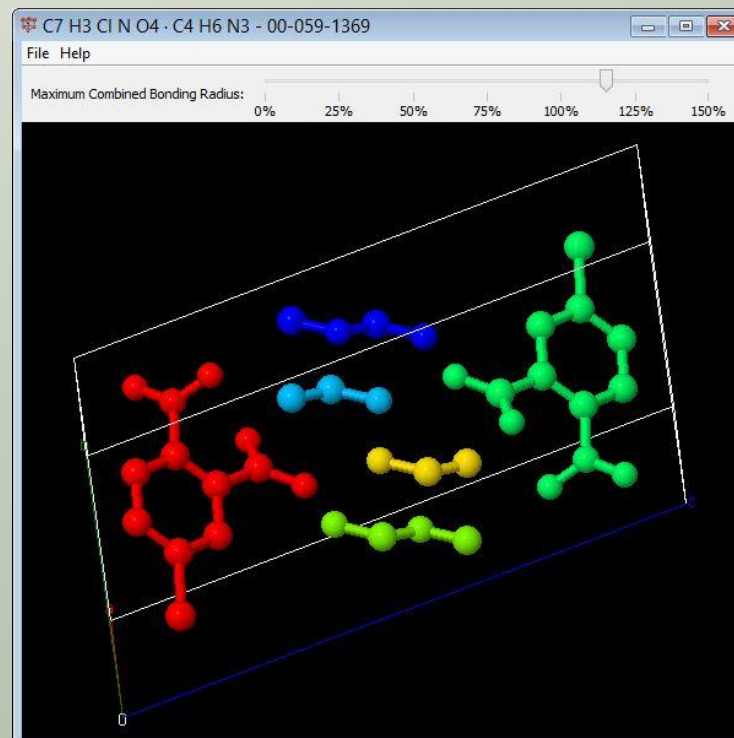
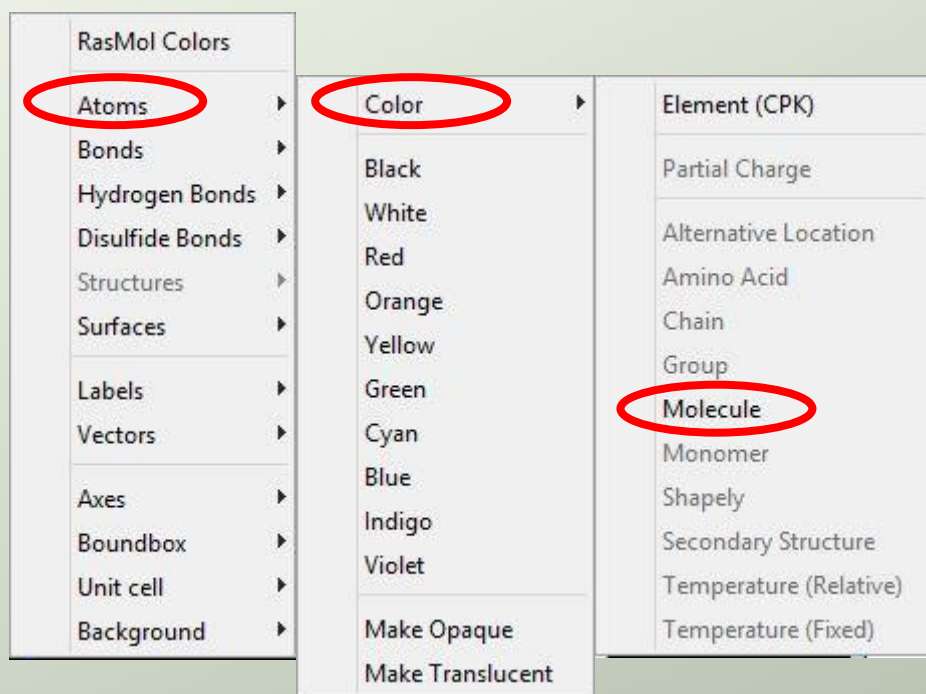
RasMol Color Scheme



Colors - Atoms

The menu for coloring atoms contains 'Schemes' as well as specific colors.

- The 'Element (CPK)' scheme is the default for all 3D displays.
- The 'Formal Charge' scheme currently displays structures as if all atoms were neutral, but future development is planned.
- The 'Molecule' scheme gives a different color to each isolated molecule or unconnected atom. An example for 2-Aminopyrimidin-1-ium 5-chloro-2-nitrobenzoate (00-059-1369) is shown using this scheme.

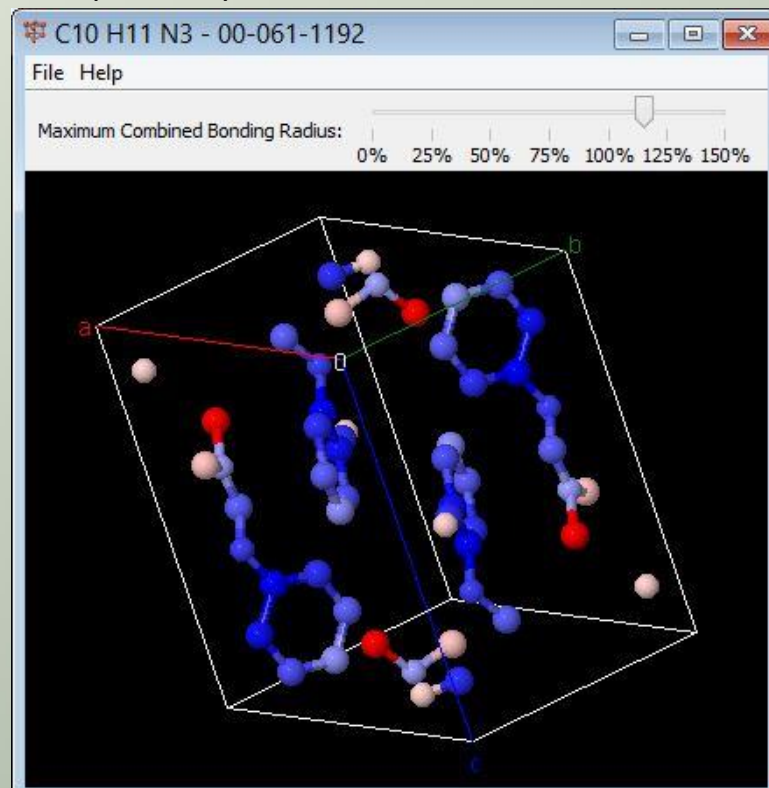
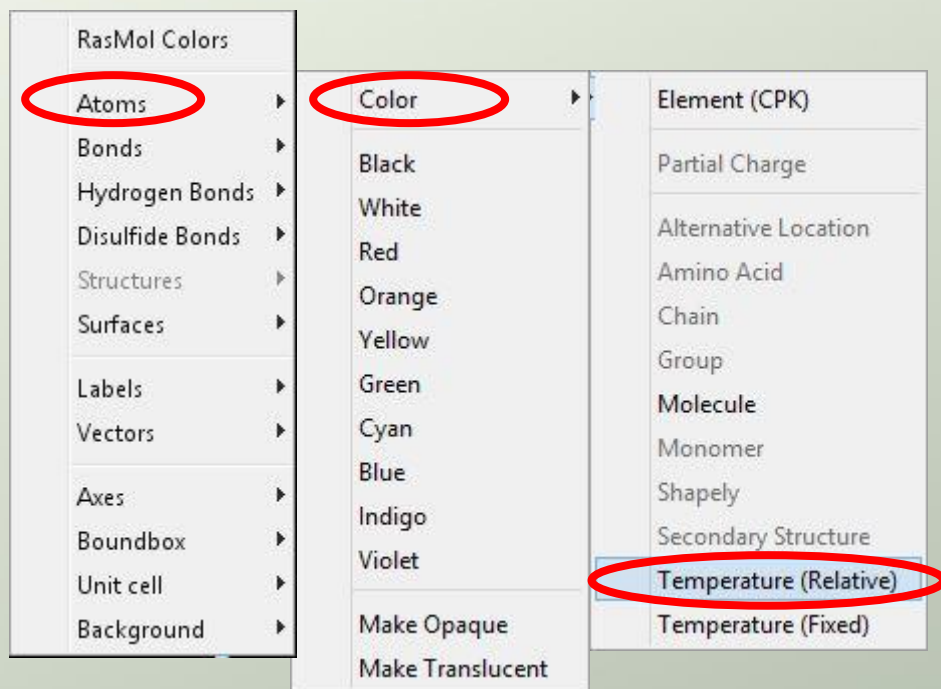


Colors - Atoms

Two additional schemes, 'Temperature (Relative)' and 'Temperature (Fixed)' are based on the thermal displacement parameters of the atom sites and become selectable for entries that contain anisotropic thermal displacement parameters with their atomic coordinates.

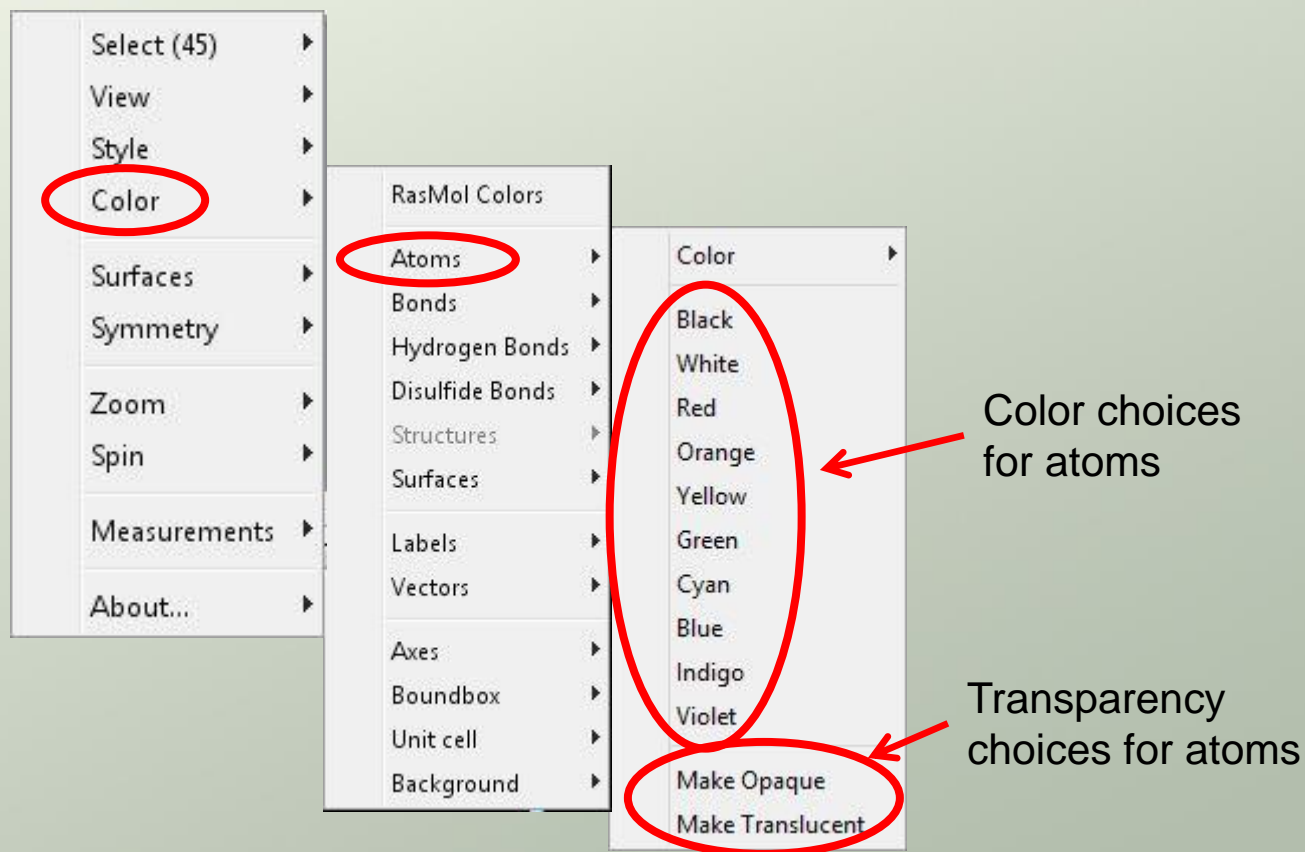
An example is given for N'-(2-Cyanophenyl)-N,N-dimethylimidofornamide using the 'Temperature (Relative)' scheme.

Atoms with smaller thermal displacement parameters (colder) are bluish tinted, those with larger thermal displacement parameters (hotter) are reddish tinted.



Colors - Atoms

- Beyond the 'Schemes' there are specific colors available for atoms. There is also the option to make atoms opaque or translucent.
- When any of these choices are selected, that color (or transparency option) is applied to all atoms or to just selected atoms if particular atoms have been previously 'Selected'.

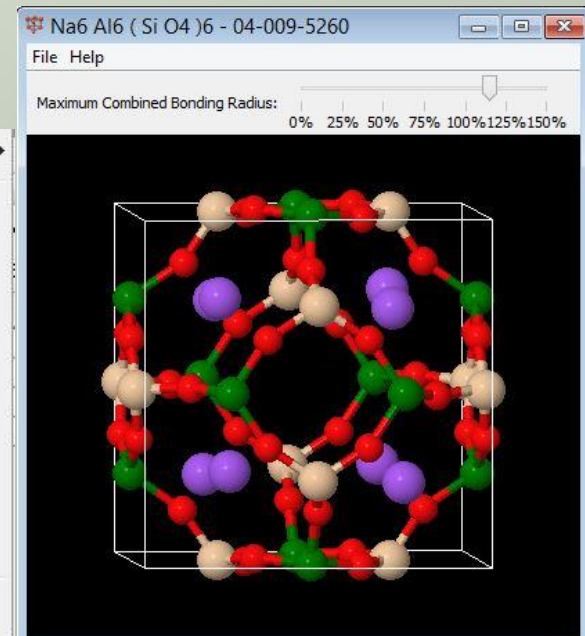
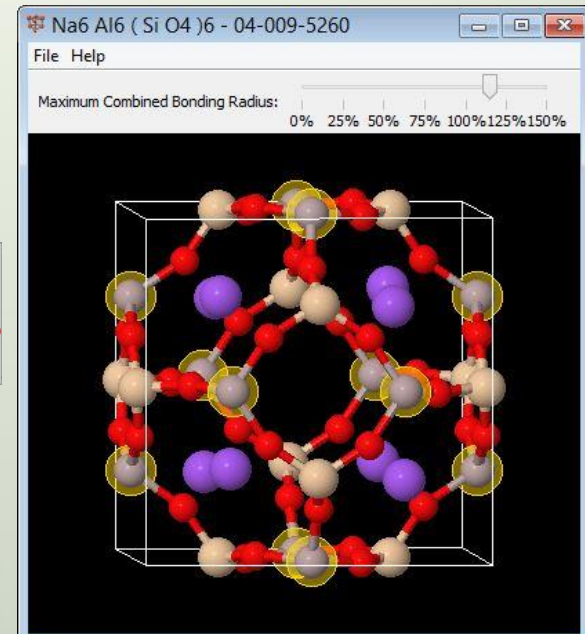
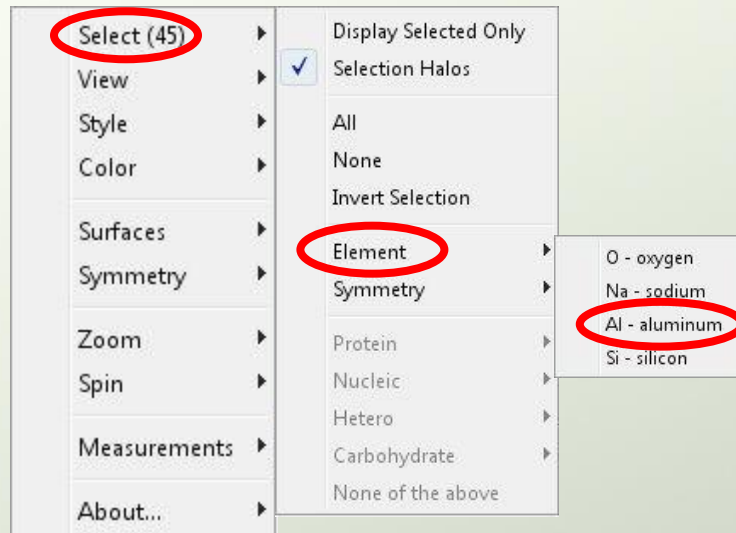


Colors - Atoms

Using the previous sodalite example, to make just the aluminum atoms green:

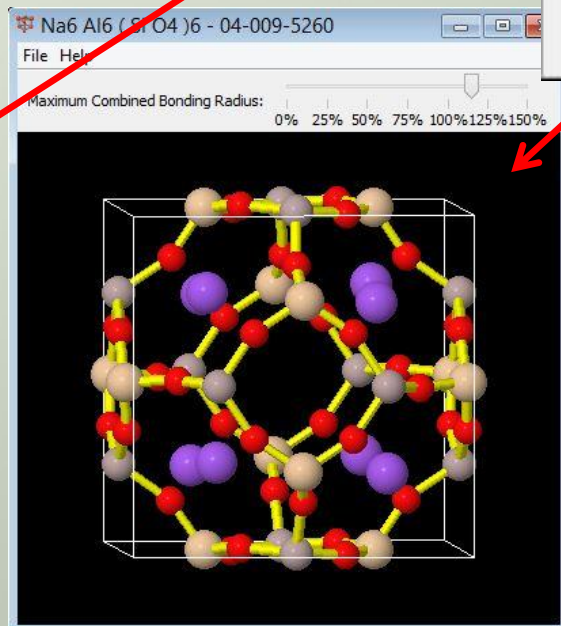
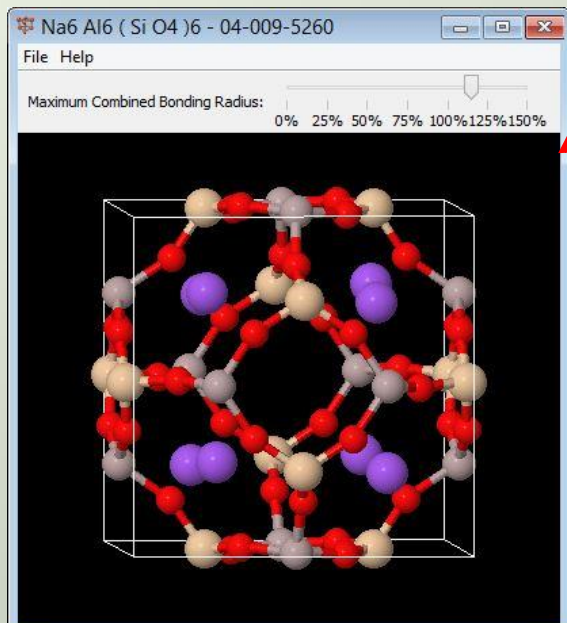
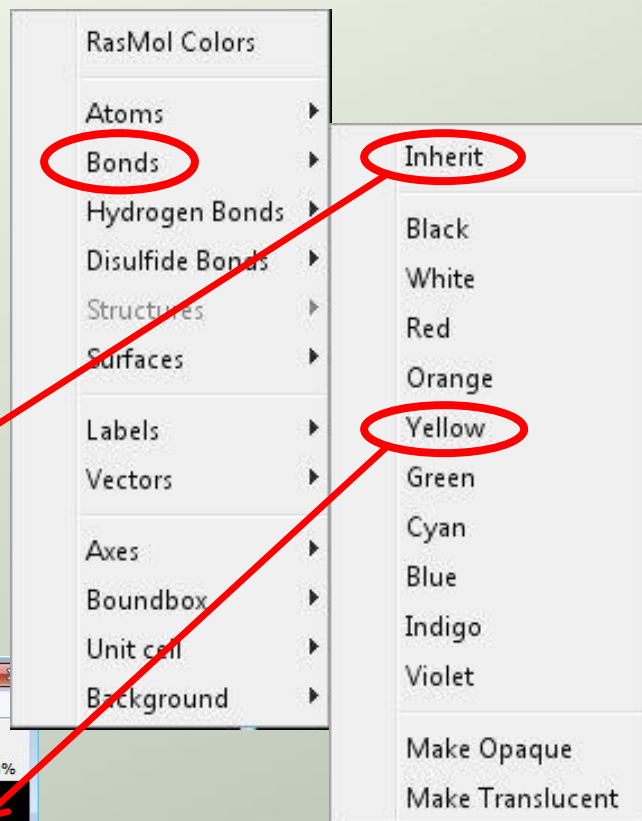
- first select the Al atoms ('Select' / 'Element' / 'Aluminum')
- then apply the color ('Color' / 'Atoms' / 'Green').

During the selection process, it may be helpful to have the 'Halos' option checked so the atoms selected are noted in the display.

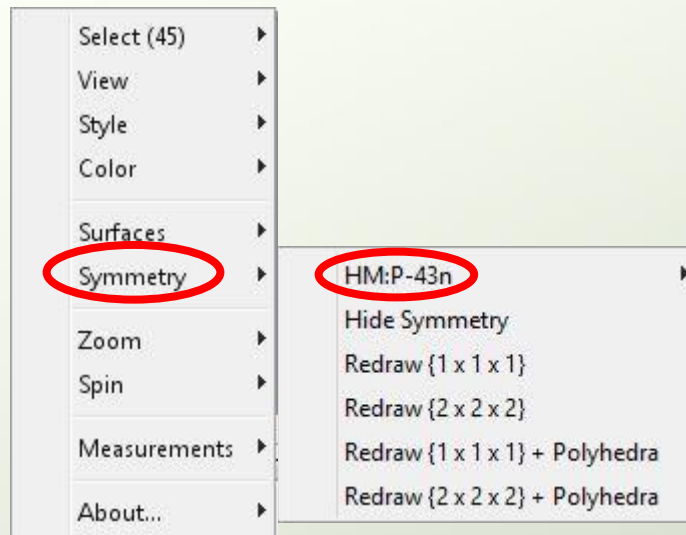


Colors

- Other items for which colors can be specified are found on the 'Color' sub-menu. (For 'Bonds', the associated atoms must be 'Selected' before any bond color specifications can be applied.)
- In addition to the menu colors, 'Bonds' and 'Labels' can be set to 'Inherit' their color from their associated atoms. This is the default for both Bonds and Labels. For 'Bonds', one half of the bond length will be colored like the atom at that end, the other half like the atom at the other end.



Symmetry



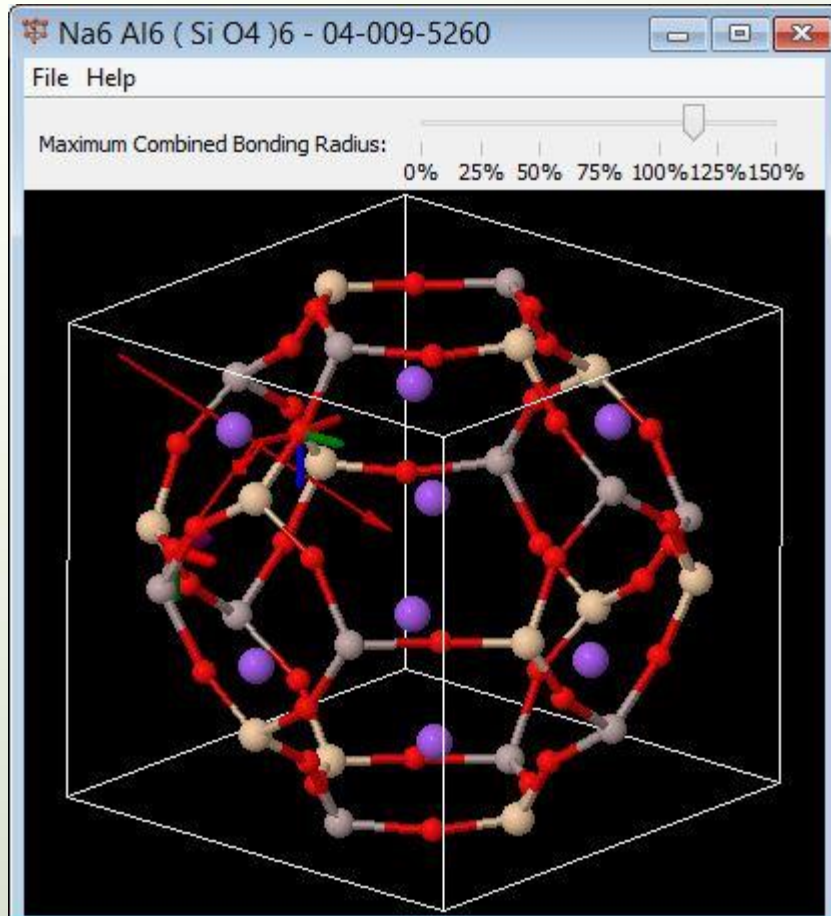
With the 'Symmetry' item, one can display various space group symmetry elements in the 3D display or expand the structure display to a 2 x 2 x 2 block of unit cells.

The first item on the 'Symmetry' menu is the space group of the structure being displayed. This item brings up a list of the symmetry elements that exist for this space group. Left-clicking on any one of these will illustrate it within the displayed structure.

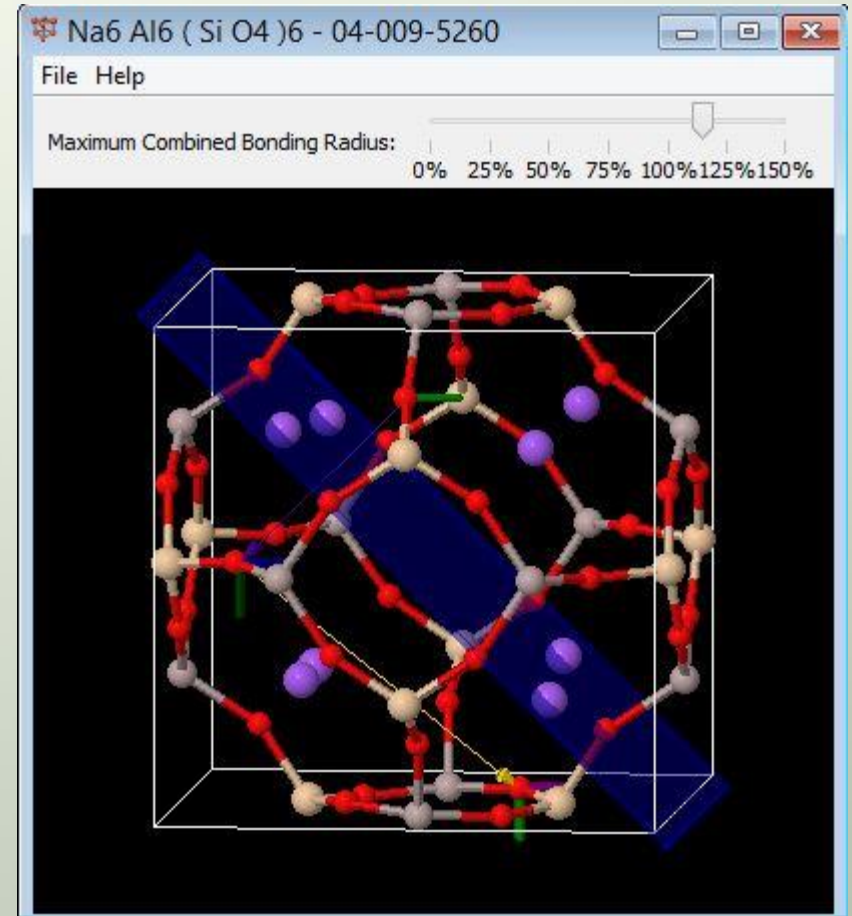
Two of these are shown for the sodalite structure on the next slide.

1 identity (x,y,z)
2 C3 axis (z,x,y)
3 C3 axis (y,z,x)
4 C2 axis (-x,y,-z)
5 C3 axis (-z,x,-y)
6 C3 axis (-y,z,-x)
7 C2 axis (x,-y,-z)
8 C3 axis (z,-x,-y)
9 C3 axis (y,-z,-x)
10 C2 axis (-x,-y,z)
11 C3 axis (-z,-x,y)
12 C3 axis (-y,-z,x)
13 d-glide plane translation: 1/2 1/2 1/2 (x+1/2,z+1/2,y+1/2)
14 d-glide plane translation: 1/2 1/2 1/2 (y+1/2,x+1/2,z+1/2)
15 d-glide plane translation: 1/2 1/2 1/2 (z+1/2,y+1/2,x+1/2)
16 a-glide plane translation: 1/2 0 0 (x+1/2,-z+1/2,-y+1/2)
17 4-bar axis inversion center at 1/2 0 1/4 (y+1/2,-x+1/2,-z+1/2)
18 4-bar axis inversion center at 1/2 1/4 0 (z+1/2,-y+1/2,-x+1/2)
19 4-bar axis inversion center at 1/4 1/2 0 (-x+1/2,z+1/2,-y+1/2)
20 4-bar axis inversion center at 0 1/2 1/4 (-y+1/2,x+1/2,-z+1/2)
21 b-glide plane translation: 0 1/2 0 (-z+1/2,y+1/2,-x+1/2)
22 4-bar axis inversion center at 1/4 0 1/2 (-x+1/2,-z+1/2,y+1/2)
23 c-glide plane translation: 0 0 1/2 (-y+1/2,-x+1/2,z+1/2)
24 4-bar axis inversion center at 0 1/4 1/2 (-z+1/2,-y+1/2,x+1/2)

Symmetry



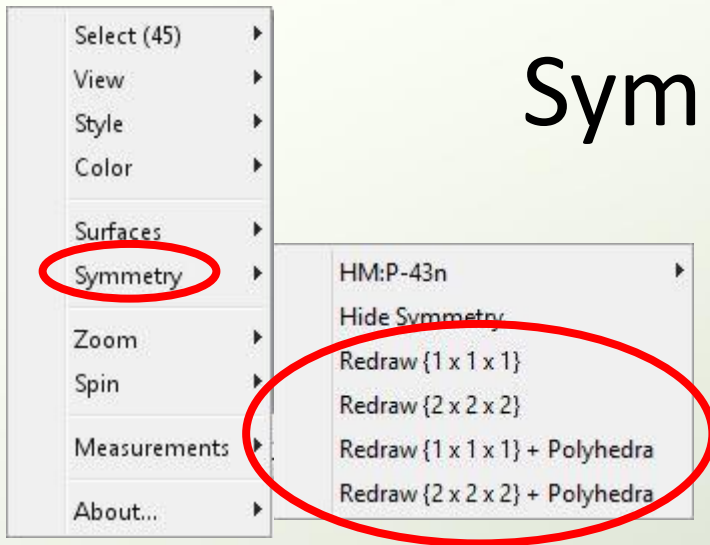
C3 axis shown (structure rotated for clarity)



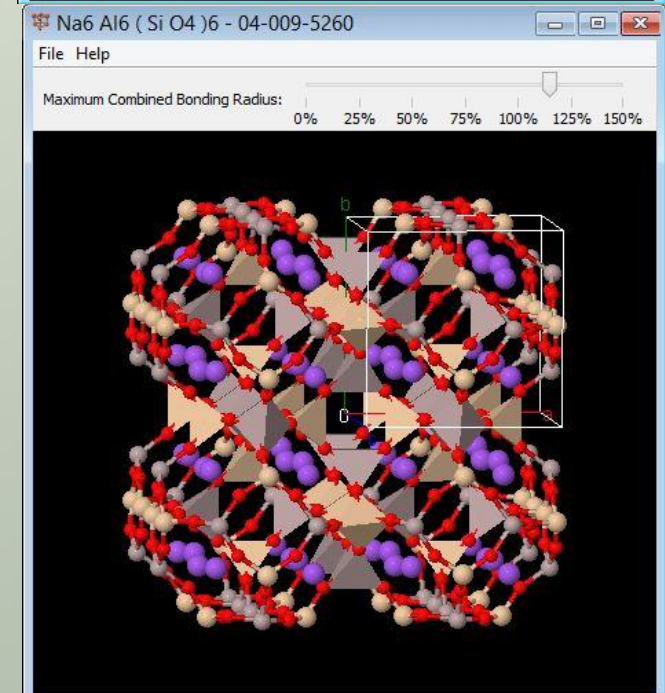
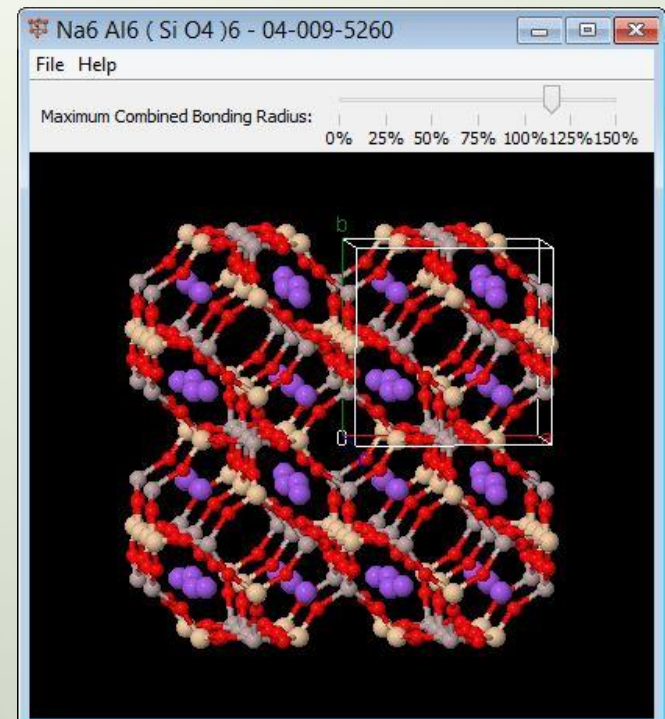
d-glide plane shown

These items may be removed from display by clicking the 'Hide Symmetry' item on the 'Symmetry' menu.

Symmetry

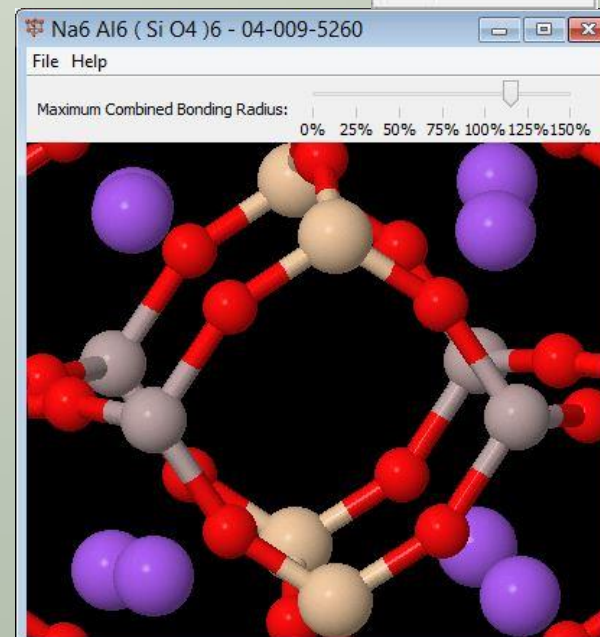
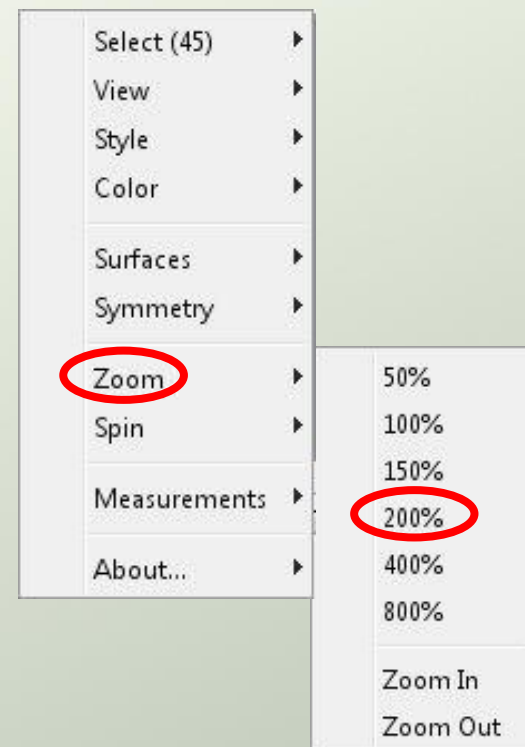


- By default, the 3D display module renders one unit cell of the structure.
- Using this menu, a block of 8 unit cells ($2 \times 2 \times 2$) can alternatively be shown.
- The user also has the choice of displaying all complete polyhedra in either the single or $2 \times 2 \times 2$ block of unit cells.
- The use of polyhedra can often clarify silicate and ceramic structures.



Zoom

- The 'Zoom' menu allows you to set the magnification level of the displayed structure relative to the display window size.
- A 'Zoom' of 100% will approximately fill the current window with the displayed structure (and is the default).
- Specific zoom values are given in the menu, as well as the ability to 'Zoom In' or 'Zoom Out' in a step-wise fashion.
- The sodalite structure at a 'Zoom' of 200% is shown here.

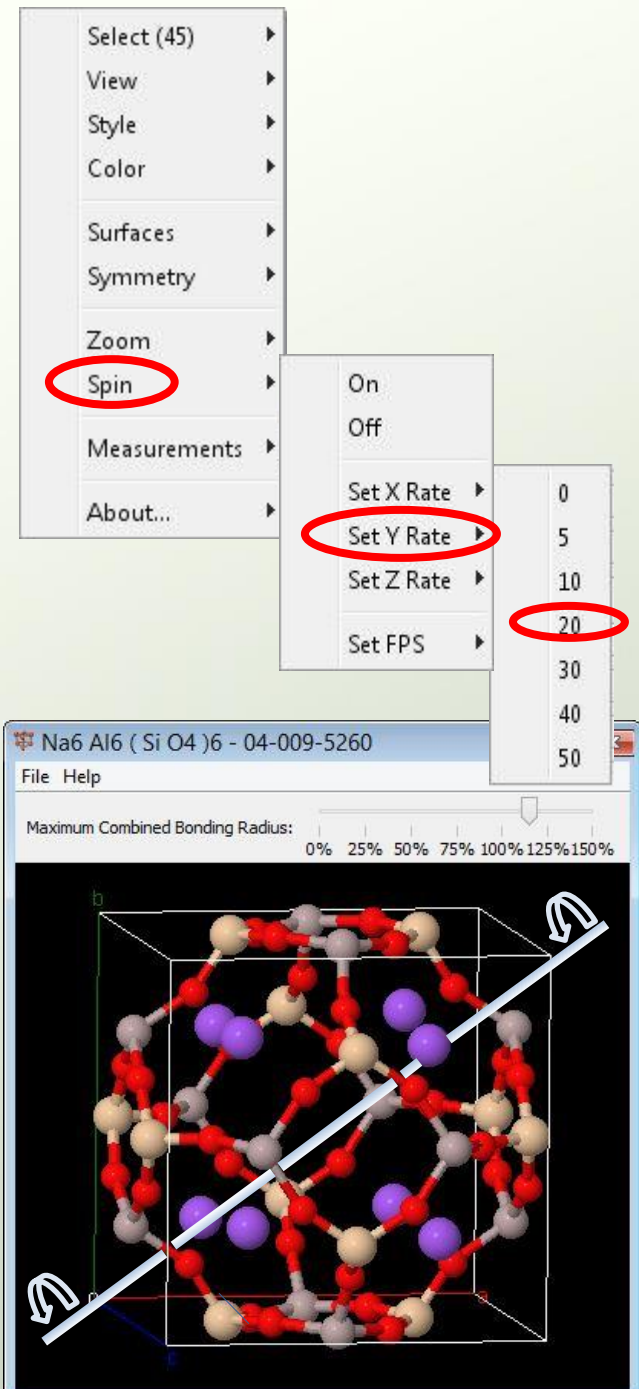


Spin

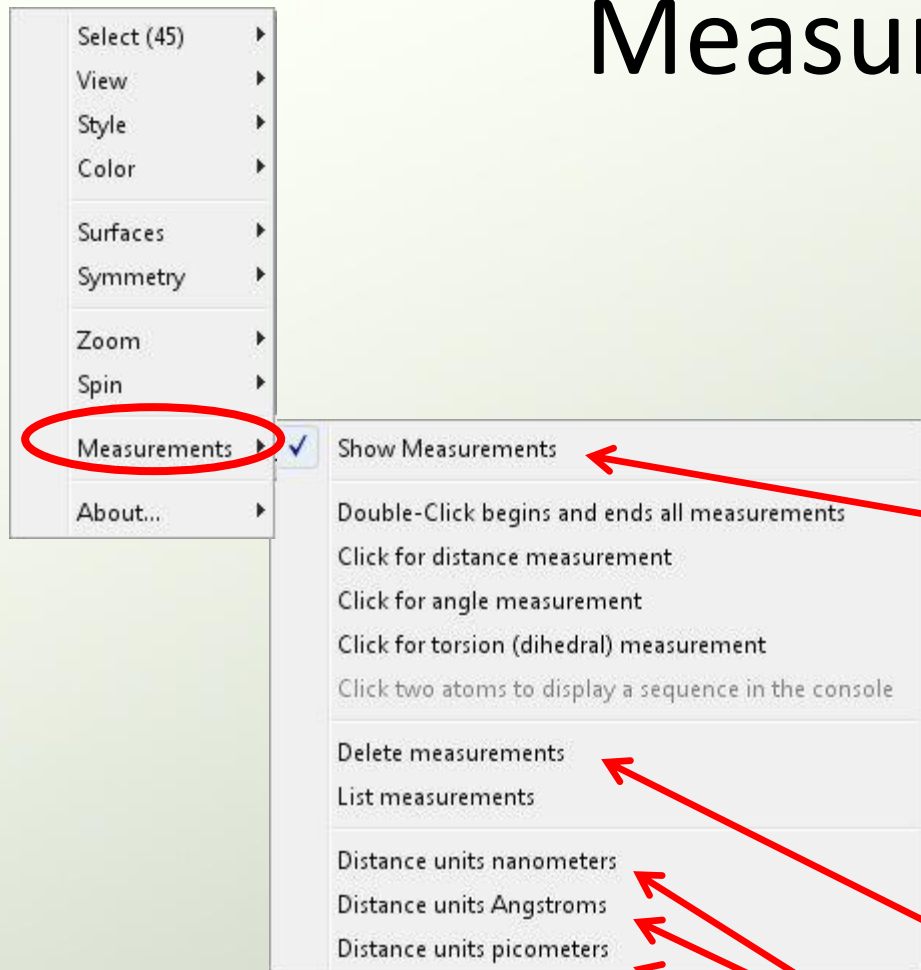
The 3D structure display can be animated via the 'Spin' menu. The spin rate is defined by setting individual rates of rotation around the three major axes: X = horizontal axis, Y = vertical axis, and Z = axis normal to screen. The original, default rate is to spin the structure around the Y-axis at a rate of 20°/second.

Spinning is activated by left-clicking the 'On' menu item, and halted by either left-clicking the 'Off' menu item or left-clicking anywhere on the display window.

One can enter combinations of rates to get other spin directions. For example, specifying the same X-axis and Y-axis rate (leaving the Z-axis rate at 0) will cause the structure to spin around a 45° axis that is in the plane of the screen. For the sodalite structure, viewed face-on, if all three axis rates are specified equal, the axis of rotation will be a 'body-diagonal' passing through the upper-near-right corner and continuing to the lower-far-left corner.



Measurement



Bond distances and angles can be calculated and displayed on the structure display itself. This is accomplished through the 'Measurements' menu item.

By default, the 'Show Measurements' item is checked. If you want to hide measurements temporarily, uncheck this item. If you want to permanently remove measurements, click the 'Delete measurements' item.

Measurements may be specified in units of nanometers, Angstroms, or picometers by checking the appropriate item at the end of the list. The default is nanometers.

Measurement

Three types of measurements may be specified:

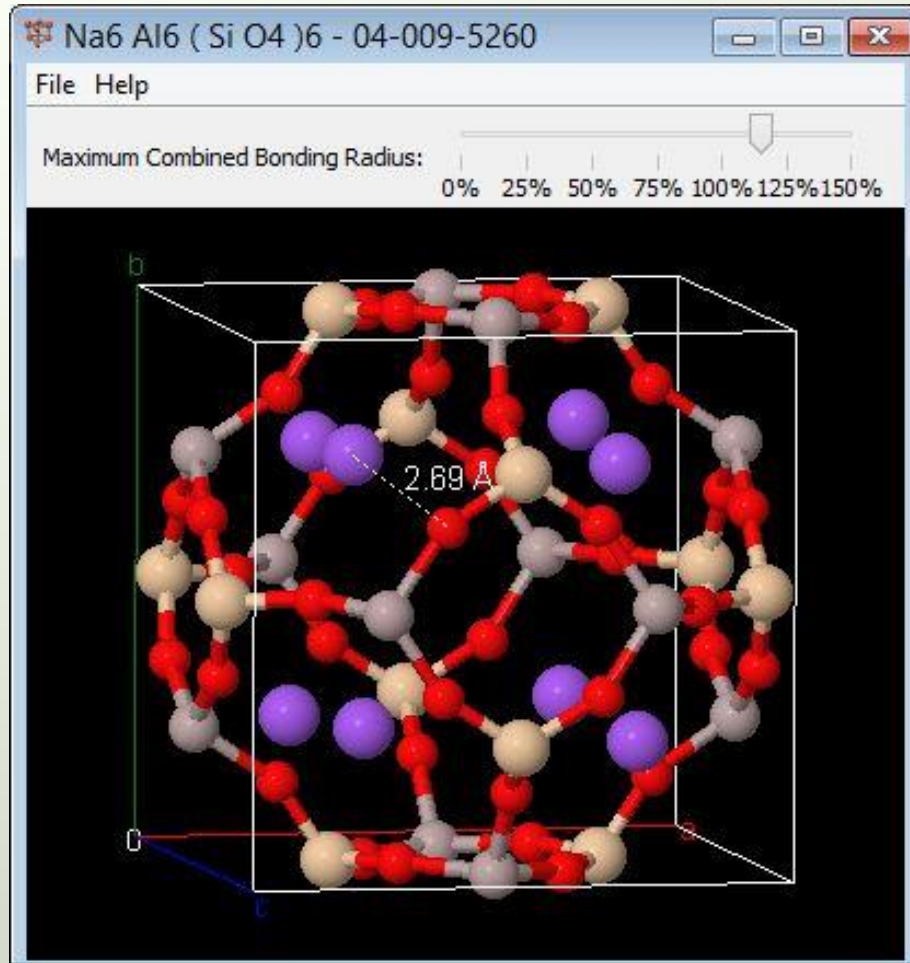
1. A distance measurement between any two atoms that may or may not be bonded.
2. An angular measurement using any three atoms. The second atom specified will be defined as the vertex of the angle.
3. A tortional angular measurement using four atoms. This measurement specifies the angle between two planes – the first containing atoms 1, 2, and 3, the second containing atoms 2, 3, and 4. (See examples to follow)

There are two ways to specify these measurements:

1. Choose the type of measurement from the 'Measurement' menu, then left-click on the atoms needed to define the measurement.
2. Without choosing the type of measurement, double-left-click on the first atom and the last atom, but single-left-click on any needed atoms in between. For example, to specify a tortional angular measurement, double-left-click on the first atom, single-left-click on atoms 2 and 3, then double-left click on the fourth atom.

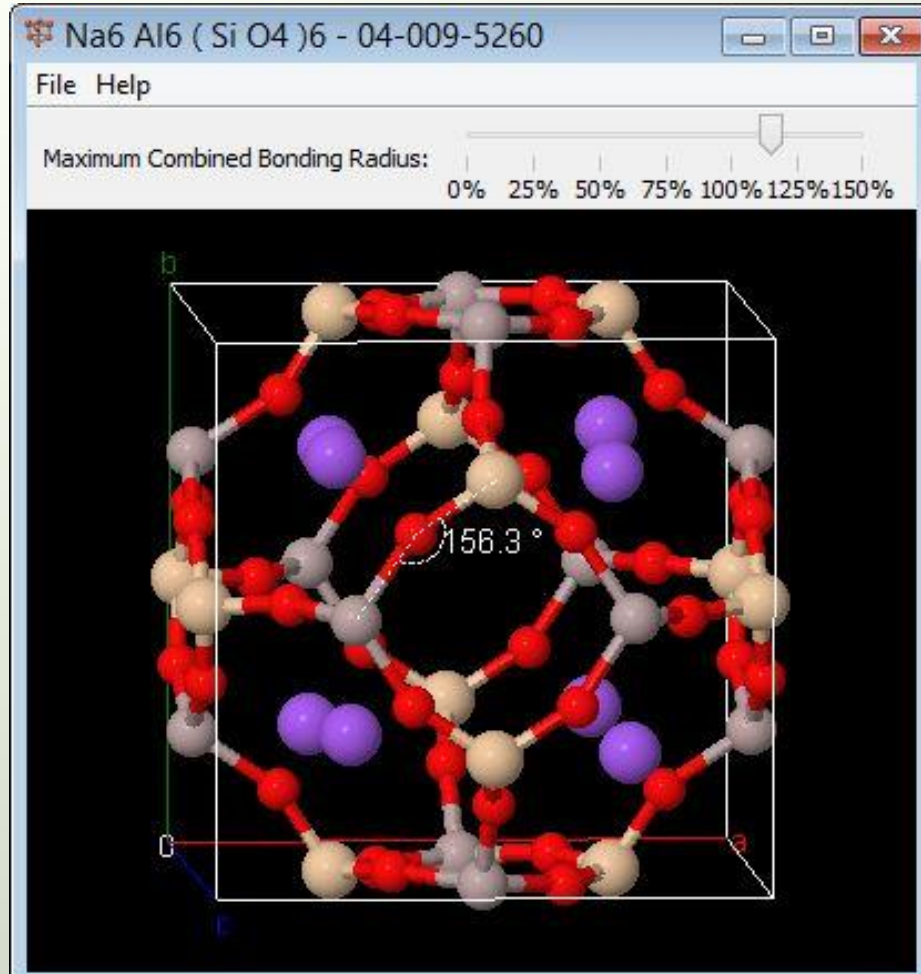
Tip: The linear components of the measurement are depicted with white dashed lines. You may have to rotate the structure to see the measurement value.

Measurement



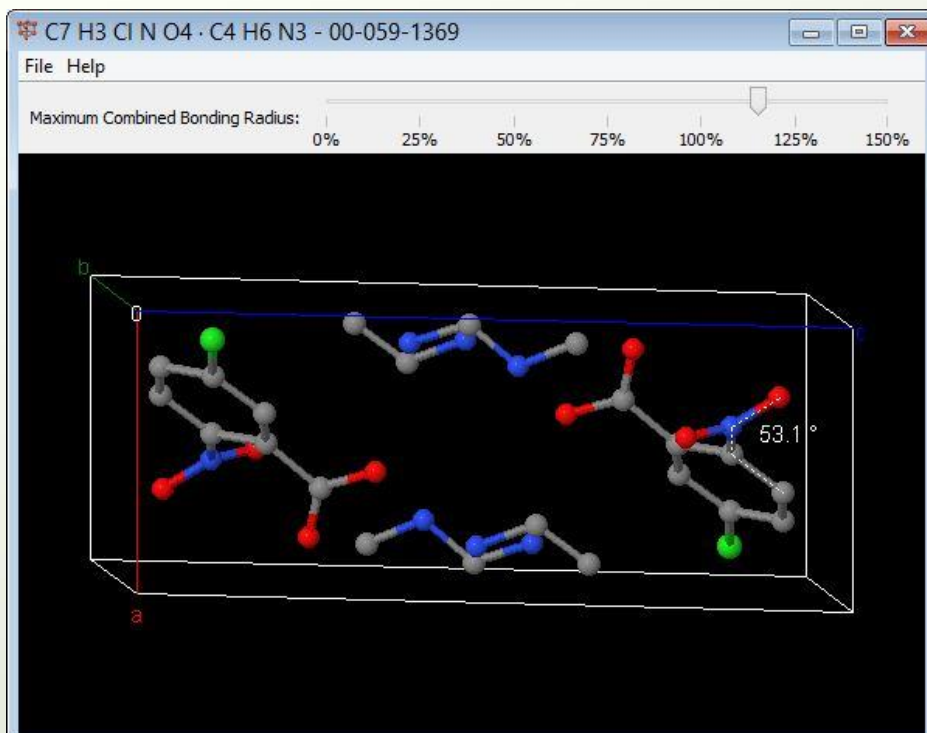
A distance measurement between a sodium ion and an oxygen atom in the sodalite structure: 2.69 Å.

Measurement



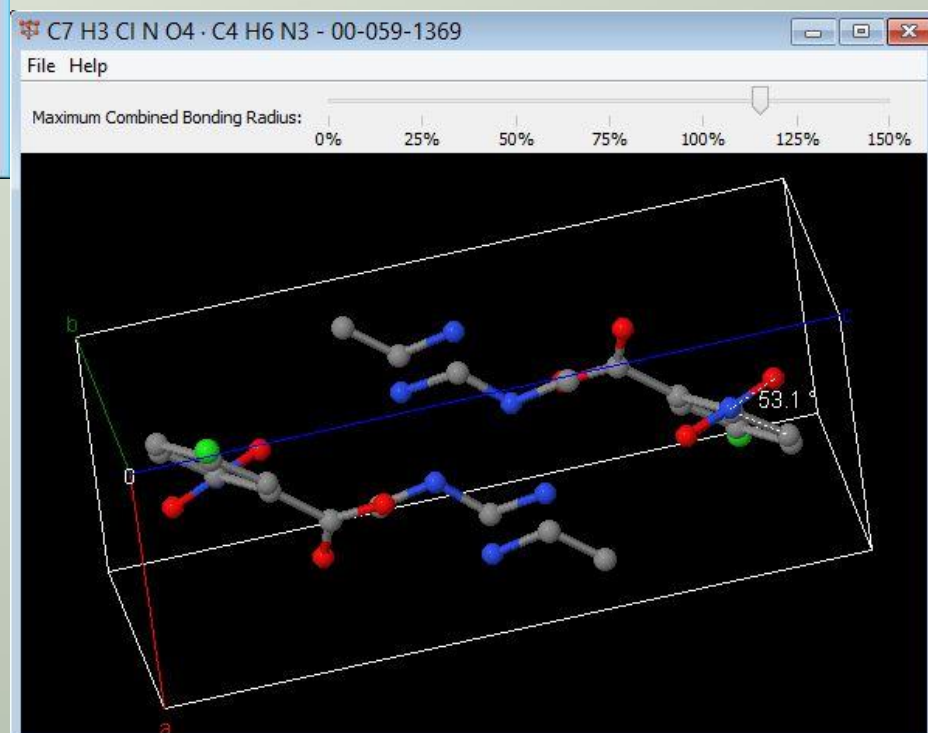
An angular measurement between the bonds on either side of an oxygen atom in the sodalite structure. Si – O – Si, 156.3°

Measurement



A torsional angular measurement on a nitro- substituent on a benzoate molecule. The measurement indicates an angle of 53.1° between the benzene ring plane and the NO_2 plane.

The perspective shown at the right more clearly illustrates the angle being measured.



PDF-4+ Structure Graphics Summary

- Over 225,000 entries with structures available for display in the PDF-4+ 2013 database and over 50,000 entries available in the PDF-4/Organics 2014 database.
- Flexibility of display styles and colors for atoms and bonds.
- Stereographic display capability.
- Retrieval of bond distances and angles directly from the structure display.
- Animation of structure displays with specifiable axes and speeds.