

CCDC

Visualisations

Version 1.2 – October 2019
Teaching Subset v5.40

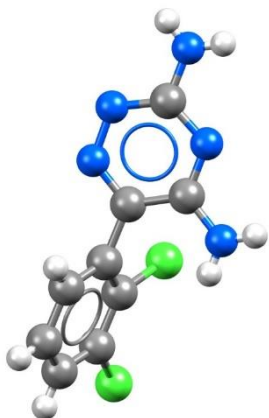


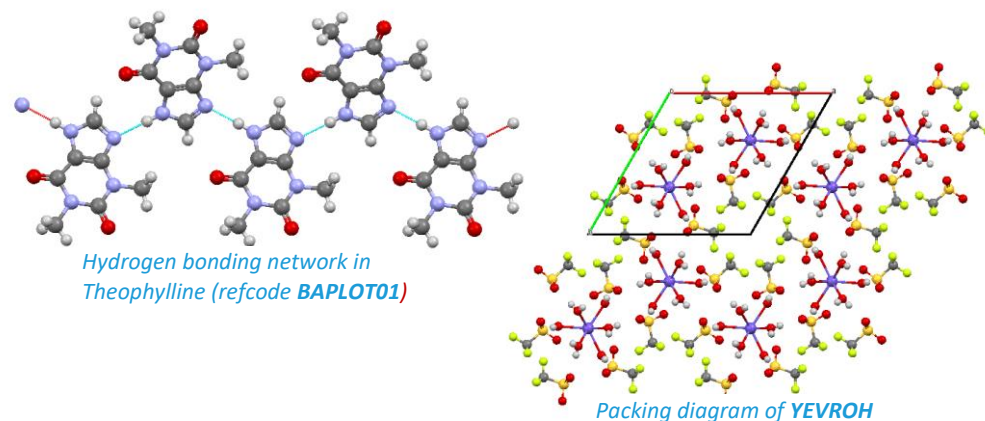
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Example 1. Generating Structure Views

In order to communicate science effectively, researchers must be able to provide clear images of structural models for inclusion in manuscripts and presentations. The program Mercury contains many features which can assist in the production of high-quality, high-resolution graphics of molecules.

This example shows you how to build structural views such as packing diagrams, void space, and intermolecular interactions, which can then be output in graphics format for use in various communications. For these examples we will be using entries in the Teaching Subset, however, the following methods can be applied to any entry in the CSD, or any of your own structure files.



Generating a Simple Molecular View

In this section, you will learn how to manipulate style options in order to generate a simple molecular view.

1. Open Mercury by clicking the desktop icon, or launching from the Start menu, Launchpad (MacOS) or command line (Linux).
2. In the **Structure Navigator** window, type the refcode CCXAPT, to bring up the structure of a cisplatin derivative.
3. The whole molecule should be displayed in the viewing window. In the **Display Options** toolbar at the bottom of the Mercury display window, tick the box for *Asymmetric Unit* and you will see half of the molecule disappear. Untick the box to bring back the whole molecule.
4. To generate the view in Step 3 above, choose *Publication* from the *Manage Styles* dropdown menu. Experiment by choosing other styles from this menu.
5. To change the style of the atoms and bonds in the structure, but to keep the white background, use the *Styles* dropdown box. Experiment with this by choosing some other options. Return to "Ball and Stick" when you are done.

1

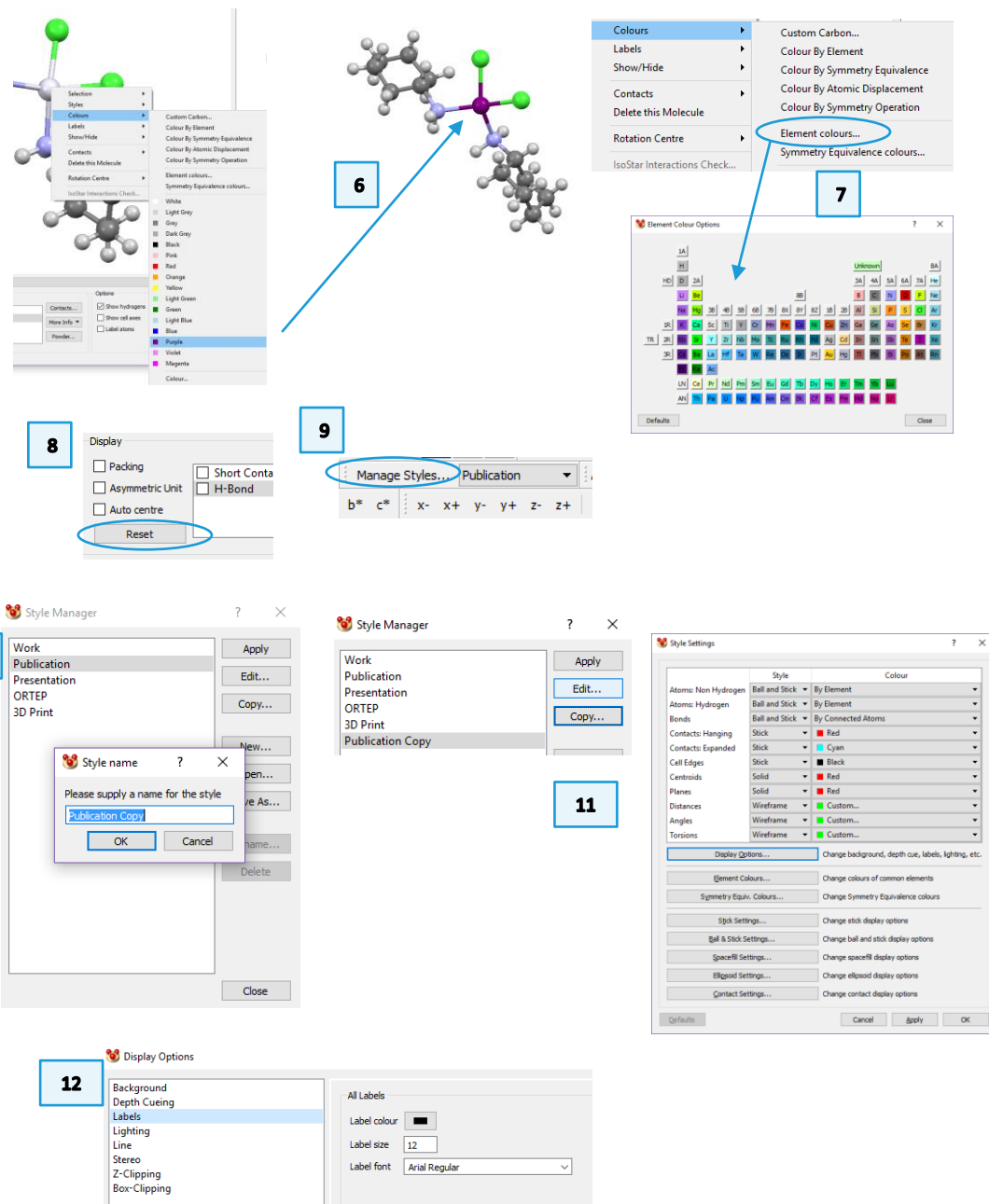
2

3

4

5

6. The white Pt atom may not stand out against a white background. To change its colour, right-click on the Pt atom and choose *Colours > Purple*. You can choose any colour in the list, depending on your preferences.
7. To change the colours of multiple elements at a time, use the *Element Colour Options* dialog, by right-clicking on any atom and selecting *Colours > Element colours...* from the drop-down menu. To restore the default "Publication" view, simply select *Publication* from the *Manage Styles* dropdown menu.
8. To orient the structure, click and drag to rotate in 3 dimensions. Shift-Click and drag to rotate the structure only in the plane of the screen. Control-Click and drag to translate the structure in the plane of the screen. Experiment with these techniques until you have the view you desire. Press the **Reset** button to return to the original view.
9. If you find that you want to create your own style type, you can access the *Style Manager* dialog by clicking on the **Manage Styles...** button.
10. It is easiest to copy and edit an existing style so we will do that here. Click the "Publications" style and then click **Copy**. Enter a name for your new style in the dialog box and click **OK**.
11. Now, select your copied style from the *Style Manager* list and click **Edit**. This will launch the *Style Settings* dialog box. Here you can change all the display properties associated with this new style type.
12. **Note:** Click the **Display Options...** button to access the style preferences for Labeling. Here you can change the font, font size and colour for labels for your new style. (You can also access this dialog from the top Mercury menu: *Display > Display Options* or *Display > Labels...* for label options only.)
13. Once you are finished adjusting your style preferences, click **OK** to save them. Click **Close** to exit the *Style Manager* dialog box. You can now access this style from the *Manage Styles...* dropdown menu.
14. You should now be able to create a structure view with your preferred styles.



Generating Ellipsoid and Polyhedral Views

In this section, you will learn how to generate ellipsoid and polyhedral views. Displacement ellipsoids can be displayed for structures where the structure file contains Atomic Displacement Parameter Values. For Polyhedral displays, the “Central Elements” refers to the atoms around which the polyhedra are centred and “Ligand Elements” are the neighbouring atoms which create the corners of the polyhedron.

1. In the **Structure Navigator** window, type the refcode BIMXOK, to bring up the structure of mer-Trichloro-tris(cyclopentanone oxime)-rhodium(iii).
2. Choose *Publication* from the *Manage Styles* dropdown menu.
3. To change the style of the atoms and bonds in the structure, use the *Styles* dropdown box. Select Ellipsoid
4. We can take a closer look at the settings for Ellipsoid style. Right-click in the main window, Select *Styles* > Ellipsoid settings...
5. Click on the Draw principal ellipses box to show the principal ellipses. The default colour is black, change the colours to see how it changes the look of the molecule. The hydrogen spheres are set to 0.30 (Å), click in the Draw hydrogens box to change the radius. The bond style can be changed from Stick to Wireframe or adjust the scale to vary the thickness of the bond. The default values in the settings are adequate for this workshop. When you are ready to continue, click **Defaults** and click **Close** to exit the Ellipsoid Display Options window.
6. The molecule pictured in 5 shows the principal ellipses and wireframe bond style. The figure in 6 uses the default ellipsoid settings.

Now we are going to generate a polyhedral view of the mer-Trichloro-tris(cyclopentanone oxime)-rhodium(iii) complex. Before applying the style, **can you predict where the polyhedral corners would reside in this complex?** Your current view should be figure 6.

The figure consists of six numbered screenshots illustrating the steps to generate an ellipsoid view of a molecular structure:

- 1**: Structure Navigator window showing the search for 'BIMXOK' in the Crystal Structures list.
- 2**: Manage Styles... dropdown menu with 'Publication' selected.
- 3**: Picking Mode: Pick Atoms, Style: Ellipsoid selected.
- 4**: Right-click context menu with 'Ellipsoid settings...' selected.
- 5**: Ellipsoid Display Options dialog box with 'Draw principal ellipses' checked.
- 6**: Two views of the molecule: one with principal ellipses and wireframe bonds, and another with the default ellipsoid style.

7. To change the style of the atoms and bonds in the structure, use the *Styles* dropdown box. Select Polyhedral

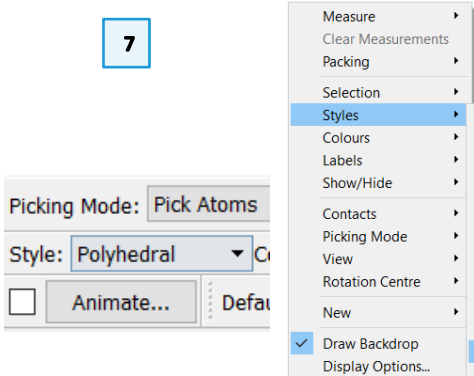
8. The polyhedral display depends on the definition of the “Central Elements” and “Ligand Elements”. We will look at these definitions in the Polyhedral Settings. Right-click in the main window, Select Styles > Polyhedral settings...

9. Click on Central Elements to see which elements are included in this definition, click **Cancel** to return to the Polyhedral Display Options window. Click on Ligand Elements to see the defined elements for ligands. The default definitions are adequate so click **Cancel** to return to the Polyhedral Display Options window.

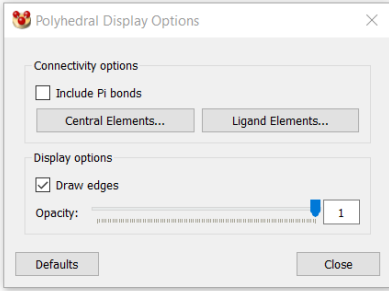
10. In the Polyhedral Display Options window, untick the box for **Draw edges** to see the effect on the display. Next, change the Opacity by clicking and dragging the slider to the left. You are now able to see the central element. The colour of the polyhedron depends on the colour of the central atom. You can change the colour by right-clicking on the polyhedron > Colours. Changing the colour of the Polyhedron will also change the colour of the central element. Once you are satisfied with the look of the complex, click **Close** to exit the Polyhedral Display Options window.

11. You should be able to create Ellipsoid and Polyhedral views for complexes. Remember, Ellipsoid style depends on the inclusion of certain parameters in the structure file or deposited entry. Polyhedral style depends on the inclusion of the central element in the Polyhedral Display Options.

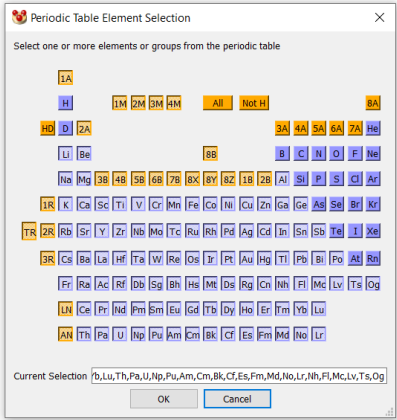
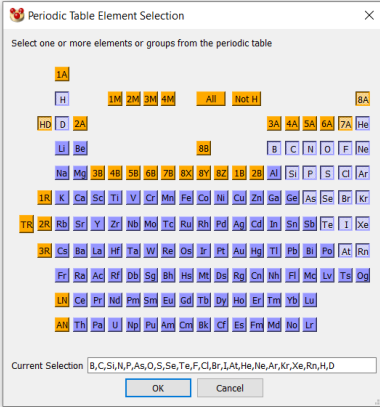
7



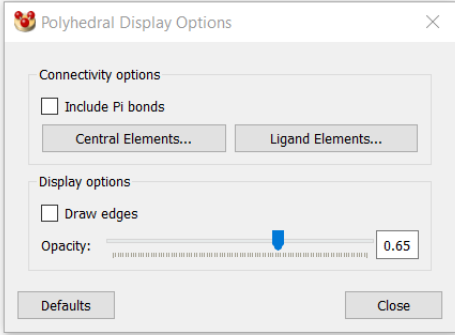
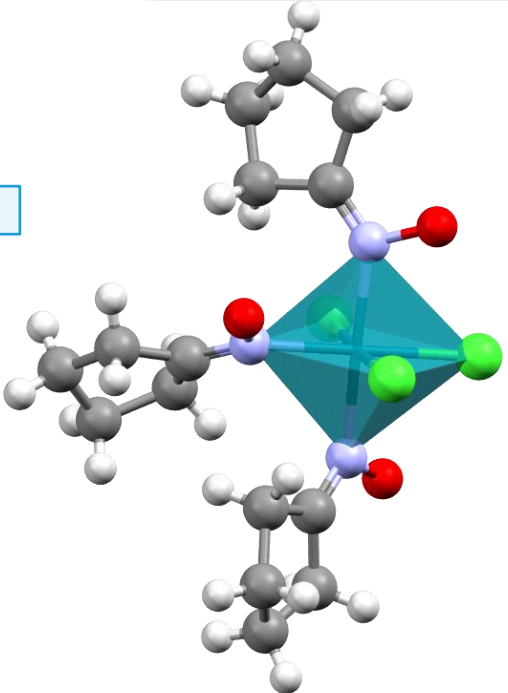
8



9

10

Generating a Packing Diagram

In this section, you will learn how to generate a packing diagram of a structure.

1. In Mercury, type the refcode **YEVROH** in the **Structure Navigator** toolbar.
2. This will display the metal-organic salt compound, nona-aqua-curium(iii) tris(trifluoromethanesulfonate) which crystallizes in the space group $P6_3/m$. Tick and untick the *Asymmetric Unit* box to see what atoms are generated by symmetry (Step 3 above).
3. Tick the *Packing* box in the **Display Options** toolbar to generate a packing diagram.
4. To change the settings of the packing diagram, choose *Calculate > Packing/Slicing* from the top menu. This will launch the *Packing and Slicing* dialog box.
5. The top half of this window contains the packing preferences. Click the radio button next to “...in molecules where Any atoms fits” and see how this changes the packing diagram in the Mercury window. Notice how two more metal-hydrate complexes appear in the center of the view and triflate anions appear at the edges.
6. To change the range of the packing diagram along any individual axis, click the **+ 0.5** buttons by the corresponding axis. Or type a specific range in the text boxes. This example is $-1.0 - 2.0$ along the *b* axis.
7. Alternatively, click the **2x2x2** or **3x3x3** buttons to make an expanded packing diagram along all three axes at once.
8. To orient the view along the crystallographic *c* axis, click the **c** button just above the viewing window.
9. When you are done, click the **OK** button at the bottom of the *Packing and Slicing* dialog box to exit.

The figure consists of eight numbered screenshots illustrating the steps to generate a packing diagram in Mercury:

- 1**: Structure Navigator window showing the refcode **YEVROH** entered in the search field.
- 2**: 3D ball-and-stick model of the molecule, nona-aqua-curium(iii) tris(trifluoromethanesulfonate).
- 3**: Display Options toolbar with the **Packing** checkbox checked.
- 4**: The **Calculate > Packing/Slicing...** menu path.
- 5**: Packing and Slicing dialog box. The radio button for “...in molecules where Any atoms fits” is selected.
- 6**: Packing diagram showing the expanded packing along the *b* axis, with the range set to $-1.0 - 2.0$.
- 7**: Packing diagram showing the expanded packing along the *c* axis.
- 8**: Final packing diagram view.

Displaying Intermolecular Contacts

This example will show you how to display hydrogen bonds and short contacts in a crystal structure.

1. In Mercury, type the refcode **BAPLOT01** in the **Structure Navigator** toolbar to load the structure of theophylline into the viewer. Click **Reset** to restore the view to the default (i.e. no packing) arrangement.
2. To see if theophylline exhibits any hydrogen bonds, tick the box next to H-Bond in the **Display Options** toolbar. Now you will see two red dashed lines indicating hydrogen bonding interactions to nearby atoms.
3. Click each atom to generate the complete molecule. Keep doing this until you have generated a network of 4 or 5 molecules.
4. Once you have a nice hydrogen-bonded chain of molecules, right click the red dashed lines and choose *Delete Hanging Contacts* to remove these dangling bonds.
5. Now type the refcode **CAFINE** in the **Structure Navigator** toolbar. This will load caffeine hydrate in the viewer.
6. We want to know if there are hydrogen bonding interactions to the water molecule, but this crystal structure does not include the hydrogen atoms on this water. Tick the box next to H-Bond and contacts might not appear.
7. To see hydrogen bonding contacts without hydrogen atoms present, double click the row for H-Bond to access the *Define H-Bonds* dialog window. Make sure the box next to "Require hydrogen atoms to be present" is unticked and then click **OK** to exit the window.
8. Now you will see hydrogen interactions between the caffeine and water molecules. Follow steps 3 and 4 above to generate the hydrogen bonding network.

1 Structure Navigator
BAPLOT01 Find

2 Display Options
Display
 Packing
 Asymmetric Unit
 Auto centre
 Short Contact < (sum of vdW radii - 0.15Å)
 H-Bond User defined
Contacts...
More Info
Reset
Powder...

3

4 Expand All
Expand Contact
Expand Contacts from this Atom
Expand Contacts from this Molecule
Find Contacts from this Atom
Find Contacts from this Molecule
Delete Hanging Contacts
Delete Contact
Delete Contacts from this Atom
Delete Contacts from this Molecule
Delete this Molecule

5

7 Define H-bonds
Select options and click OK or Apply when done
 Require hydrogen atom to be present
D-H...A angle >= 120.0 degrees
Donor atom types:
 all donors
 nitrogen
metal bound N
imine N
aromatic (6-ring) N
amide or thioamide N
planar N
pyramidal N
ammonium N (NH4+, RNH3+ ...
 unclassified N
 oxygen
Acceptor atom types:
 all acceptors
 nitrogen
metal bound N
terminal N (cyano, etc.)
aromatic (6-ring) N
other 2-coordinate N
3-coordinate N
unclassified N
oxygen
metal bound O
carboxylate O
WARNING: atom types may not be classified properly for non-Cambridge Structural Database structures
Contact distance range:
 Actual distance vdW distance
Minimum = sum of vdW radii minus 5.00
Maximum = sum of vdW radii plus 0.00
 Intermolecular
 Intramolecular: Donor and Acceptor separated by > 3 bonds
Default Cancel Apply OK

8

Generating a Graph Set View

Graph set analysis of hydrogen-bonding patterns is based on a set of descriptors which specify the type of pattern along with the numbers of hydrogen-bond donors and acceptors, written as $G^a_d(n)$. G represents the type of pattern (C for chain, S for intramolecular hydrogen bonds, R for ring, D for finite), a is the number of acceptors, d is the number of donors and n the number of atoms in the pattern. This example will show you how to calculate the graph set notation and display hydrogen bonding patterns in Mercury.

1. In Mercury, type the refcode **GLYCIN** in the **Structure Navigator** toolbar to load the structure of glycine into the viewer. This simple molecule has many available hydrogen bonding patterns. Click **Reset** to restore the view to the default (i.e. no packing) arrangement.
2. From the top menu choose *Calculate > Graph Sets...* which will launch the **Graph Sets** window. This may appear as a separate window, as a tab hidden behind or beneath the **Structure Navigator** toolbar.
3. Click on any of the descriptors to see the corresponding motif. To generate a nice view, click on the **R4,4(16) >a>b<a<b** motif. This will bring up a view of four glycine molecules in a ring.
4. The *Options* dropdown menu includes features to *Edit* the type of motif that is displayed in the list, define the geometry of hydrogen bonds and donor/acceptor atom types (*H-bond definition...*), change the *Highlighting* of motifs, and *Save* the list of graph set descriptors. Choose *Highlighting...*
5. The H-bond colour should be set to “By symmetry equivalence” and the Style should be set to “Ball and stick.” Click these dropdown menus to change colours and see different styles, but ultimately remain with “Ball and stick.” In the *Style* dropdown in the main Mercury window, choose *Capped Sticks*.
6. Select the atoms in Ball and Stick mode – the ones involved in the motif – and right-click to change their colour as in Step 6 of the first example to highlight the motif even more.

1

Structure Navigator

GLYCIN Find

2

Calculate CSD-Community

- Centroids...
- Planes...
- Packing/Slicing...
- Contacts...
- Molecular Shell...
- Graph Sets...
- Powder Pattern...
- Structure Overlay...
- Molecule Overlay...

3

Graph Sets

descriptor	level	period	# molecules
C1,1(5) a	1	1	2
C1,1(5) b	1	1	2
C1,1(5) c	1	1	2
C1,1(5) d	1	1	2
C2,2(6) >a<b	2	2	3
C2,2(10) >a>b	2	2	3
R4,4(16) >a>b<a<b	2	4	4
R6,6(26) >a>a>b<a<a<b	2	6	6
R5,5(20) >a>a>b<a<b<b	2	5	5
C2,2(6) >a<c	2	2	3
C2,2(10) >a>c	2	2	3

4

Options

- Edit options...
- H-bond definition...
- Highlighting...
- Save...

5

Highlight Options

Highlight options

H-bond colour: By symmetry equivalence

Style: Ball and stick

Show H-bond labels

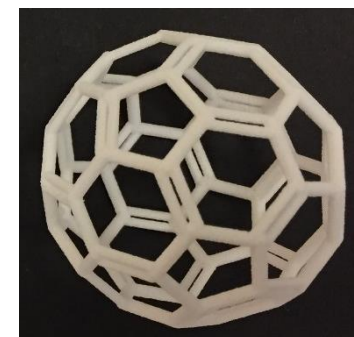
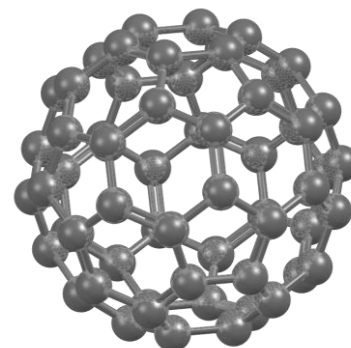
Close

6

Example 2. Generating Images and 3D Print Files

There are many ways to visualise the structure views created in Mercury, including high-resolution static views, animated rotating images, and 3D printed models. Each of these formats has its place in manuscripts, lecture presentations, websites, and tactile class-room displays.

The following exercises will show you how to generate high-resolution graphics files, the files needed to produce an animated rotating GIF, and files that can be sent to a 3D printer to produce a structural model directly from Mercury.



High-resolution POV-Ray image (left) and 3D printed model (right) of fullerene (refcode: FULLER).

High-resolution images

POV-Ray, or Persistence of Vision Raytracer, is a program which can be used to create very high-resolution and stylistic images. This example is not a definitive guide to POV-Ray, but will show you how to create a high-resolution image *via* the POV-Ray plug-in in Mercury.

1. Open Mercury by clicking the icon or launching from the start menu.
2. In the **Structure Navigator** window, type the refcode CCXAPT, to bring up the structure of a cisplatin derivative.
3. Change colours and styles as in previous examples to obtain your desired view. Make sure the image appears in Mercury exactly how you want it to appear in your manuscript or presentation. Here the colours of the Pt and Cl atoms have been changed, and the molecule rotated to a new orientation.
4. From the top menus, choose *File > POV-Ray Image...* to launch the **POV-Ray Image** dialog box. The upper section of this window includes information on the resolution and style of the POV-Ray generated image. The bottom section includes a path to the POV-Ray executable and an Output directory. You should not need to change the POV-Ray executable location, but you may want to change the Output Directory location. Click **Browse...** to do this.

The screenshots illustrate the workflow:

- 1:** Mercury application icon.
- 2:** Structure Navigator window showing the search for refcode 'CCXAPT'.
- 3:** The resulting 3D ball-and-stick model of cisplatin with Pt and Cl atoms highlighted.
- 4:** The POV-Ray Image dialog box, showing settings for resolution (1024x768), file format (PNG), and the location of the POV-Ray executable and output directory.

- Change the *Material Properties* to the desired setting by clicking in the dropdown box and clicking the appropriate type. Select *Transparent* from the *Background* dropdown menu. Leave all other default values the same.
- For complicated or large images, or on slow computers, POV-Ray may take a while to create the image file. Click **Preview** to check what the image will look like before rendering the full-size file. The POV-Ray window will briefly appear as the rendering proceeds.
- When you are satisfied with the output, click **Render** to create the file. You can find the .png file in the output directory shown in the bottom of the window.
- Using different *Material Properties* creates different image styles. Try different materials to see the effects.

Generating Rotating Images.

For presentations or websites, you may want to display a rotating image of your molecule, to highlight stereochemistry, or other spatial effects that are not obvious in static images. This section will show you how to generate images that can be used to make animated (rotating) molecule graphics.

- To see how the rotation will look, click the **Animate...** button in the Mercury window. Tick the box next to **Rotate** and select the radio button for the “y” axis. This will start the molecule rotating in the Mercury viewer. Select different axes (one at a time) and note how the molecule rotates.
- Once you have decided on the orientation of your molecule and the axis of rotation, return to the **POV-Ray Image** dialog box. Tick the box next to “Generate Animation Frames.” Now specify the axis of rotation (x, y, or z) and the “Number of Frames” to generate. The structure will always rotate through 360 degrees, so the higher number of frames, the higher the “resolution” of the rotating image. The default value of **30** is typically a good compromise between file size and resolution. Click **Render** to generate the 30 images. This may take a long time depending on your computer speed.

5 POV-Ray Image

Width (pixels) 1024 Height (pixels) 768

Material Properties Standard Mercury File Format PNG

Background Standard Mercury Custom Color

Shiny
Matt
Metallic
Iridescent

Generate Anim
Rotate around

Width (pixels) 1024 Height (pixels) 768

Material Properties Standard Mercury File Format PNG

Background Transparent Custom Color

6 Preview Render Close

Preview

7

The same image in Shiny, Iridescent and Metallic materials

8

Animate... **9**

Animate Structure ? X

Rotate Oscillate x y z Rate: Amplitude:

10 Generate Animation Frames

Rotate around x y z

Number of Frames 30

11. The series of images will be saved in their own folder in your specified output directory. There are many web-based applications which can be used to convert a series of images into an animated gif, for instance gifmaker.me.

Generating a 3D Print Model File

Making 3D printed models of crystal structures can highlight interesting features of the molecules as well as help explain many chemical and crystallographic concepts. This section shows you how to create the files used by 3D printers to make 3D objects.

12. To make a 3D print model file, simple choose the structure you want from the **Structure Navigator** or upload your own 3D coordinate file (e.g. CIF, RES, PDB, etc.). For this example, we will load **SUCROS01** for sucrose.

13. For 3D models, the orientation is not important. However, most 3D models work best when the cylinders for bonds and are thicker than normal graphics. From the *Manage Styles...* dropdown menu, choose **3D Print** and notice how the bonds become thicker.

14. To edit these settings, right-click an atom or bond in the molecule and choose *Styles > Ball and Stick settings...* This will launch the **Ball and Stick Display Options** dialog window. Leave the defaults for now, and click **Close** to exit.

15. To generate the file, from the top menu choose *File > Print in 3D*. This launches the **3D Printing** dialog window.

16. In the **3D Printing** dialog window, click the *File Format* dropdown menu to choose either STL (monochrome) or VRML (colour) formats, depending on the type of printer you have and the type of model you wish to make.

17. If we had more than one molecule in our structure, or a particularly long and unstable molecule, we might wish to *Generate a Support Framework* by ticking this box. Leave it unchecked for now.

18. Click **Generate** to save the file to the specified folder. Click **Close** to exit.

12 Structure Navigator

SUCROS01 Find

13 Manage Styles... Publication
Work
Publication
Presentation
ORTEP
3D Print

14 Selection
Styles
Colours
Labels
Show/Hide
Contacts
Delete this Molecule

Wireframe
Capped Sticks
Ball and Stick
Spacefill
Ellipsoid
Stick settings...
Ball and Stick settings...
Spacefill settings...
Ellipsoid settings...
Contact settings...
 Display Bond Types
 Display Aromatic Rings
 Highlight Acyclic Aromatic Bonds

Ball and Stick Display Options

Atom Size (times van der Waals radius)

Non-metals: 0.25

Metals: 0.25

Bond Radius (Angstroms): 0.2

Defaults Close

15 File Edit Selection Display Calculate

Open... Ctrl+O
Recent Files
Sketch Molecule... Ctrl+K
Auto Edit Structure on Load
Save As... Ctrl+S
POV-Ray Image...
Print in 3D...
Exit Ctrl+Q

16 3D Printing

File Format: STL (monochrome)
Scale (mm/Å): STL (monochrome) VRML (colour) Output Size (mm):
 Generate Support Framework
Plinth Thickness (Å): 0.8
Column Radius (Å): 0.1
Generate Close
Settings
Output Directory: C:\Desktop\3DPrints Browse...

17