

Visualisations (MER-001)

2020.3 CSD Release

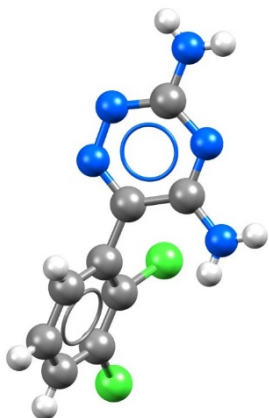


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Introduction

Mercury is the visualisation and analysis software of the Cambridge Structural Database (CSD). Mercury is used in investigating and analysing crystal structures thanks to features such as packing diagrams, display and strength assessment of intermolecular interactions networks, calculation and display of voids, calculation and display of BFDH theoretical crystal morphologies and more (features availability subject to appropriate licence). With Mercury you can visualise 3D structures from the CSD as well as your own. You can also produce high-quality publication-ready images, frames for videos and 3D print files.

Before beginning this workshop, ensure that you have installed Mercury. Please contact your site administrator or workshop host for further information.

Objectives

In this workshop we will see features of Mercury that enable an effective visualisation of crystal structures and how to produce high-resolution images. At the end of this tutorial, you should be able to:

- Explore visualisation options.
- Learn how to produce high-quality images.
- Learn how to calculate and display packing.

This workshop will take approximately 45 minutes to be completed.

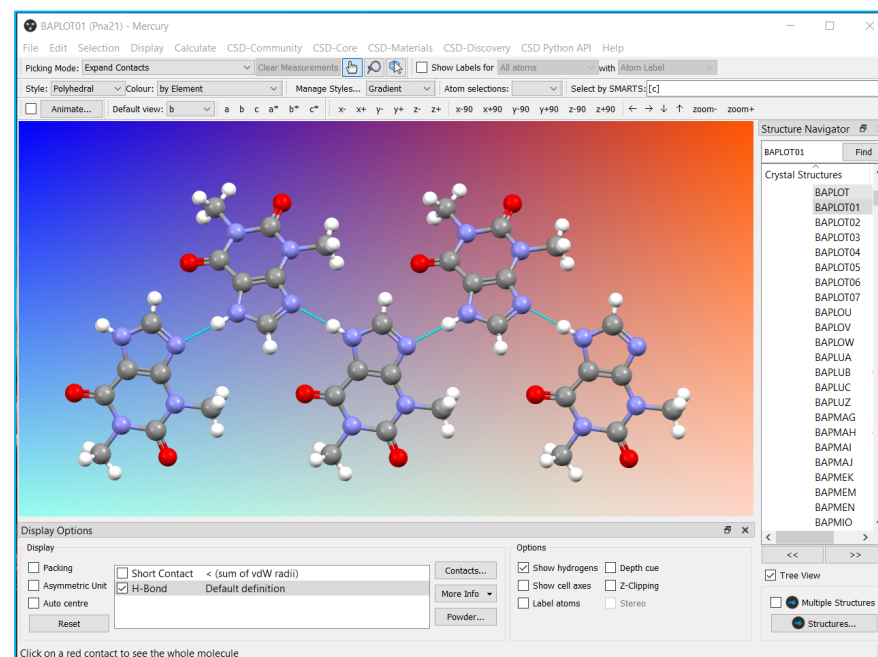
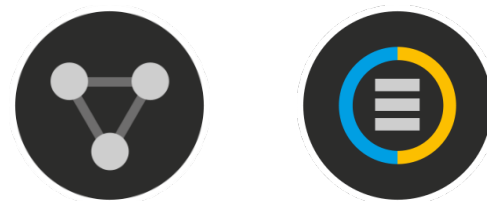
Note: The [Glossary](#) at the end of this handout contains useful terminology.

Pre-required skills

There are no pre-required skills for this workshop.

Materials

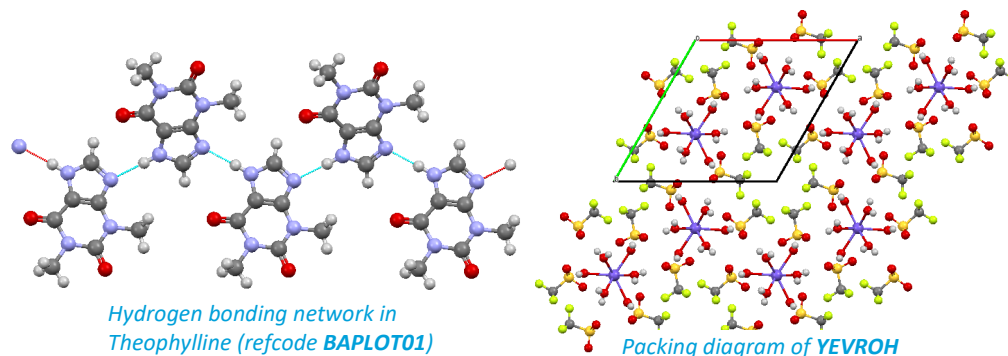
There are no additional materials required for this workshop.



Example 1. Generating Structure Views

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 select style options 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* drop-down 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. You can undo an action by clicking on Edit > Undo. Return to "Ball and Stick" when you are done.

1

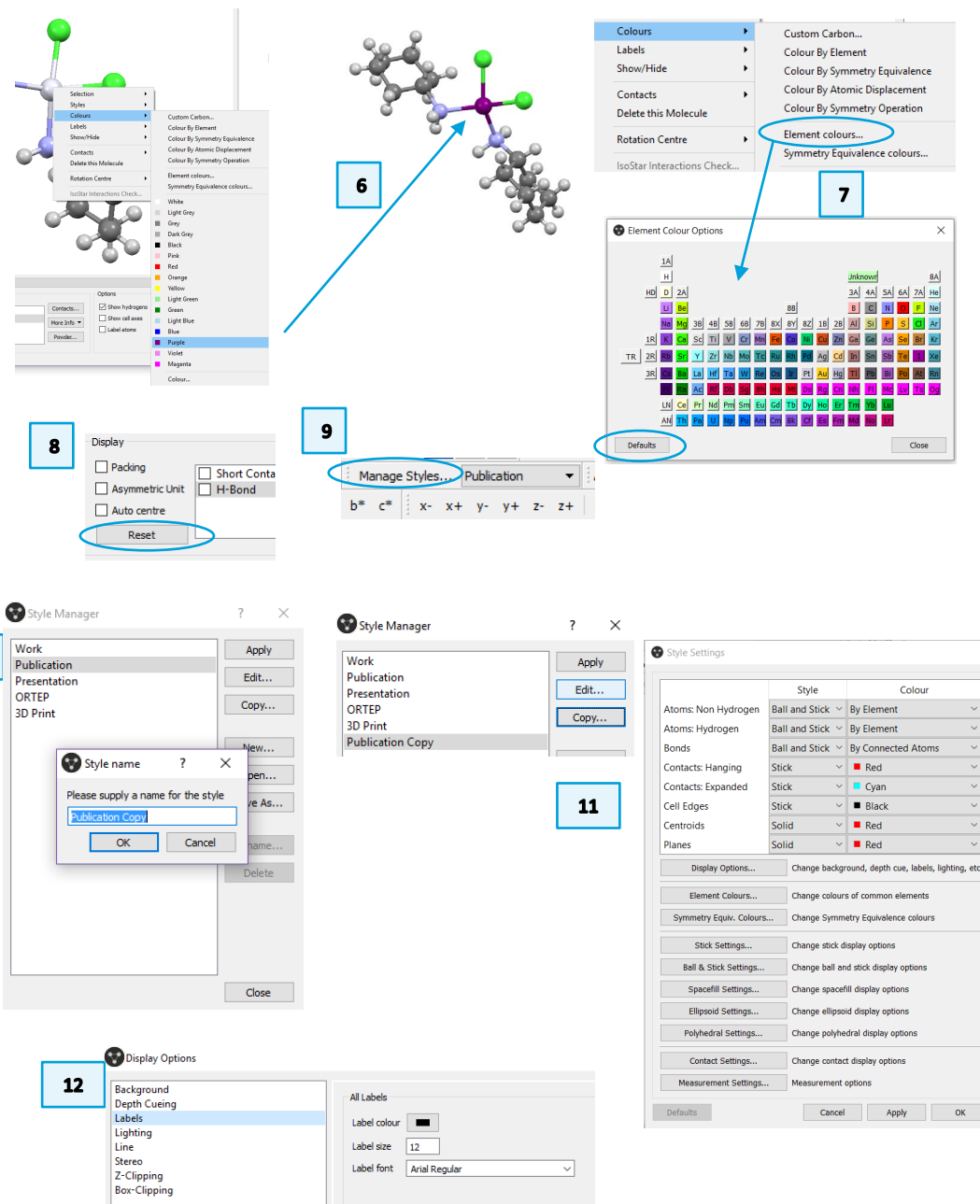
2

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 colours, click "Defaults" in the Element Colour Options box and click Close.
8. To orient the structure, click and drag to rotate in 3 dimensions. Shift-Click and drag left to right or up and down 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 "Publication" 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'.
- 2**: Manage Styles dropdown menu with 'Publication' selected.
- 3**: Picking Mode dropdown menu with 'Style: Ellipsoid' selected.
- 4**: Right-click context menu with 'Ellipsoid settings...' selected.
- 5**: Ellipsoid Display Options dialog box. The 'Draw principal ellipses' checkbox is checked. The 'Bond style' is set to 'Stick'.
- 6**: Two molecular views. The left view (labeled 6) shows the molecule with principal ellipses and wireframe bonds. The right view (labeled 5) shows the molecule with principal ellipses and stick bonds.

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. Note that the central atom should be selected, you can see the central atom clearer if you adjust the opacity first. 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 Picking Mode: Pick Atoms
Style: Polyhedral
Animate... Default

8 Measure
Clear Measurements
Packing
Selection
Styles
Colours
Labels
Show/Hide
Contacts
Picking Mode
View
Rotation Centre
New
Draw Backdrop
Display Options...

9 Polyhedral Display Options
Connectivity options
☐ Include Pi bonds
Central Elements... Ligand Elements...
Display options
☒ Draw edges
Opacity: 1
Defaults Close

10 Periodic Table Element Selection
Select one or more elements or groups from the periodic table
Current Selection: b,Lu,Th,Pa,U,Np,Pu,Am,Cm,Bk,Cf,Es,Fm,Md,No,Lr,Nh,Fi,Mc,Lv,Ts,Og
OK Cancel

10 Polyhedral Display Options
Connectivity options
☐ Include Pi bonds
Central Elements... Ligand Elements...
Display options
☐ Draw edges
Opacity: 0.65
Defaults Close

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 crystallises in the space group $P6_3/m$. Tick and untick the *Asymmetric Unit* box to see what atoms are generated by symmetry (Step 3 in Generating a Simple Molecular View 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 atom 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 to 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**: The Structure Navigator toolbar with the refcode **YEVROH** entered in the search field.
- 2**: A 3D ball-and-stick model of the molecule, nona-aqua-curium(iii) tris(trifluoromethanesulfonate).
- 3**: The Display Options toolbar with the **Packing** checkbox checked.
- 4**: The top menu showing the path **Calculate > Packing/Slicing...**.
- 5**: The **Packing and Slicing** dialog box. The "Include atoms" section has the radio button for "... in molecules where Any atom fits" selected.
- 6**: The packing diagram view with the **b** axis range expanded to -1.0 to 2.0. The dialog box is open, showing the **b** axis range set to -1.0 to 2.0.
- 7**: The packing diagram view with the **c** axis selected in the Default view dropdown.
- 8**: The final packing diagram view, showing the molecules packed in the unit cell.

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 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. Click *Reset* in the bottom left corner to return to the default view.
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 Powder... Reset

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

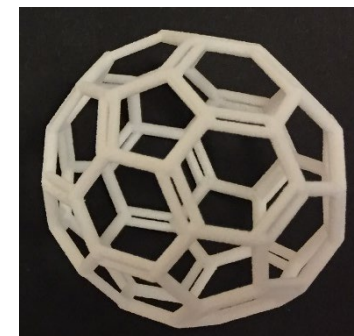
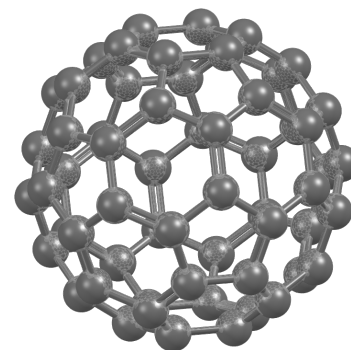
7 Define H-bonds
Select options and click OK or Apply when done
☐ Require hydrogen atom to be present
D-H...A angle >= 120.0 degrees
Donor atom types:
☐ all donors
☒ nitrogen
 ☒ metal bound N
 ☒ imine N
 ☒ aromatic (6-ring) N
 ☒ amide or thioamide N
 ☒ planar N
 ☒ pyramidal N
 ☒ ammonium N (NH4+ R)
Acceptor 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
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

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 classroom 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 image shows a sequence of four steps for generating a high-resolution image using POV-Ray in Mercury:

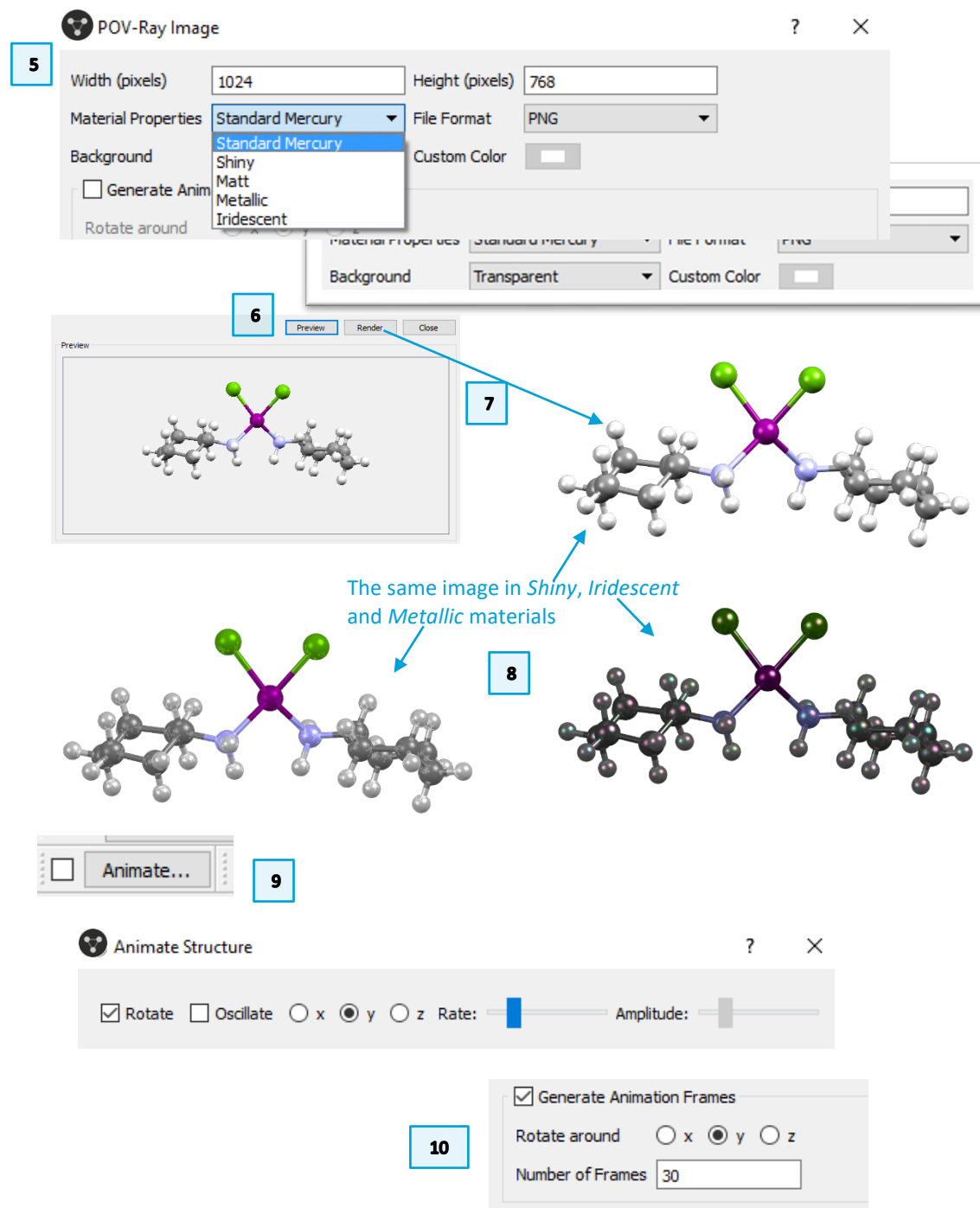
- Step 1:** The Mercury icon is shown.
- Step 2:** The Structure Navigator window is shown with 'CCXAPT' entered in the search bar.
- Step 3:** The resulting molecular structure is shown in the Mercury interface.
- Step 4:** The POV-Ray Image dialog box is shown. The 'File' menu is open, and 'POV-Ray Image...' is selected. The dialog box shows settings for Width (1024), Height (768), Material Properties (Standard Mercury), File Format (PNG), Background (As Mercury), and a 'Browse...' button for the Output Directory.

5. 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.
6. 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.
7. 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. A .pov file is also generated and can be open with POV-Ray.exe.
8. 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.

9. 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.
10. 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.



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](https://www.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 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.

The image contains several numbered screenshots (12-18) showing the software interface for generating a 3D print model:

- 12:** The **Structure Navigator** window showing 'SUCROS01' loaded.
- 13:** The **Manage Styles...** dropdown menu with '3D Print' selected.
- 14:** The **Ball and Stick Display Options** dialog box with default settings (Atom Size: 0.25, Bond Radius: 0.2).
- 15:** The **File** menu with 'Print in 3D...' highlighted.
- 16:** The **3D Printing** dialog box with 'VRML (colour)' selected as the file format.
- 17:** A 3D model of sucrose with a support framework (a grey base and vertical pillars) for printing.
- 18:** A final 3D model of sucrose without the support framework.

Conclusions

This workshop introduced the Mercury interface. You should now be familiar with:

- The Mercury interface and exploring options and functions.
- Changing between different visualisation options, selecting styles and colours to display your structure of interest effectively.
- Creating publication-ready high-quality images, selecting resolution, material and background
- Calculating and display the packing of a crystal structure, and the asymmetric unit.
- Creating your own style (or styles), with settings defined by you to make more effective fitting your structures and visualisation necessities.

Next steps

The Mercury user guide and other available Mercury documents can be found [here](#). There is an intermediate level Mercury self-guided workshop that can be found [here](#).

Feedback

We hope this workshop improved your understanding of Mercury and you found it useful for your work. As we aim at continuously improving our training materials, we would love to get your feedback. Click on [this link](#) to a survey, it will take less than 5 minutes to complete. The feedback is anonymous. You will be asked to insert the workshop code, which for this self-guided workshop is MER-001. Thank you!

Glossary

Asymmetric unit

The asymmetric unit is the smallest part of a crystal structure from which the complete structure can be built using space group symmetry.

The asymmetric unit may consist of only one molecule or ion, part of a molecule, or several molecules that are not related by crystallographic symmetry. (This is why you sometimes see more than one molecule in Mercury when you first display a structure from the Cambridge Structural Database.)

Atomic Displacement Parameters (ADPs)

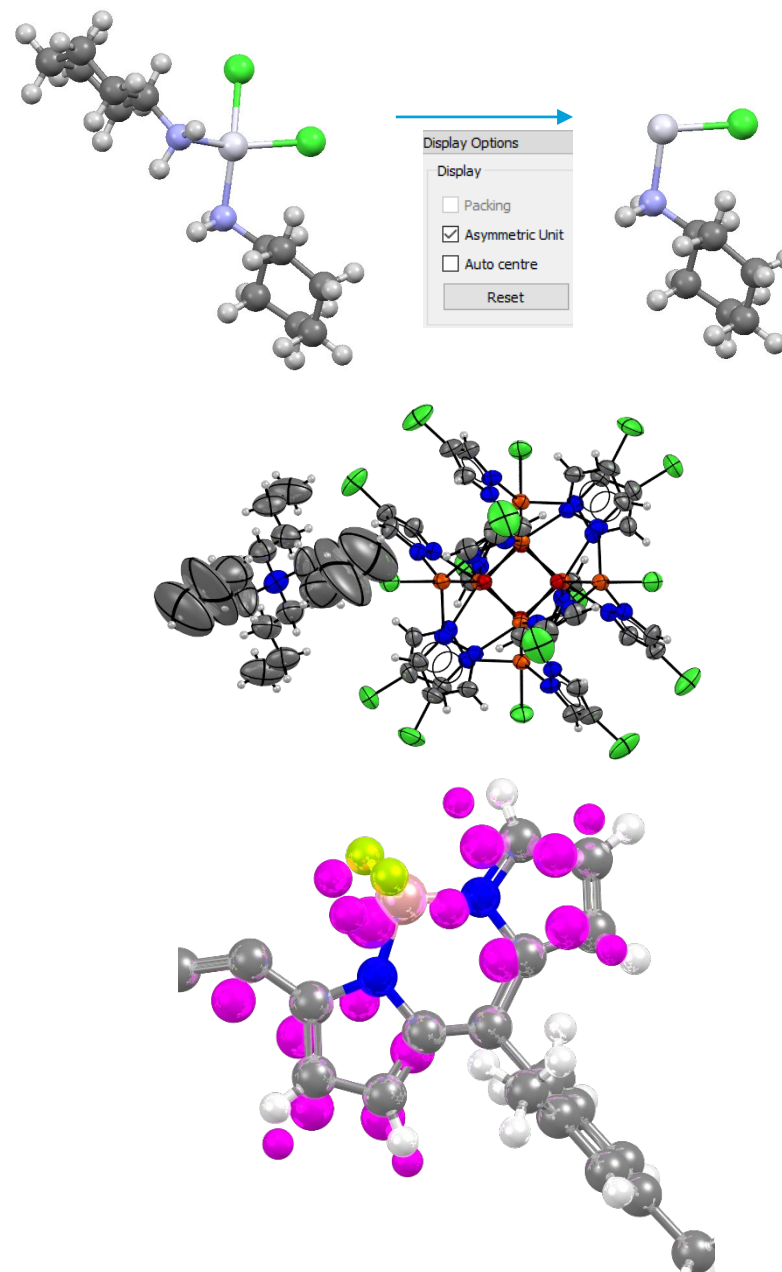
Atomic Displacement Parameters (also known as *atomic vibration parameters* and *thermal parameters*) are used to generate displacement ellipsoids. Displacement ellipsoids represent atomic motion and can be either isotropic or anisotropic. The shape and size of ADPs can be used to highlight potential errors with the data; the smaller and more spherical the ellipses for anisotropic atoms, the better the data (see Troublesome Crystal Structures: Prevention, Detection and Resolution, R. L. Harlow, J. Res. Natl. Inst. Stand. Technol., 101(3), 327, 996).

Suppressed Atoms

In Cambridge Structural Database (CSD) structures one or more atoms may be suppressed. A common example is when the author reports two sets of atomic coordinates, for major and minor sites, in a disordered structure. In most cases the atoms of the minor site will be suppressed.

Disordered Structures

Disordered structures display a lack of regularity. For example, each of the F atoms in a trifluoromethyl group, $-\text{CF}_3$, might be randomly distributed between two sites. This means that the crystallographer will report two sets of coordinates for each F atom. In some cases, two alternative sites are occupied equally; in other cases, there is a major site and a minor site. Disorder can involve more than two sites and it can also involve a whole molecule. Disordered structures in the Cambridge Structural Database may have been treated in one of two ways. In older structures, only one position is kept for each disordered atom. When such a structure is read into Mercury, it will therefore appear as if it is not disordered at all. In more recent structures, all positions of disordered atoms are kept but only one set is connected by bonds to form a complete molecule. When a



Suppressed atoms of PIYDEI are in pink.

structure like this is displayed in Mercury, it will have the appearance of a complete molecule with disconnected atoms at various points to indicate alternative sites for the disordered atoms.

Unit cell

The unit cell is the basic building block of a crystal, repeated infinitely in three dimensions.

