

Virtual Workshop Visualisations

2020.1 CSD Release

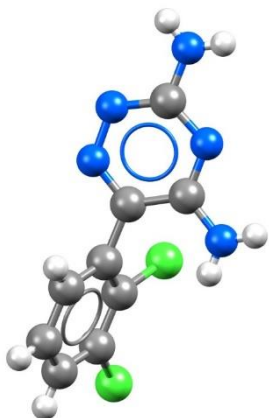


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Introduction

Mercury is the visualisation and analysis software of the Cambridge Structural Database (CSD). With Mercury you can visualise in 3D structures from the CSD as well as your own and produce high-quality publication-ready images, frames for videos and 3D print files. Mercury is also a support 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 license). You can read more about Mercury on [our website](#).

In this workshop we will see features of Mercury that enable an effective visualisation of crystal structures and how to produce high-resolution images using the POV-Ray feature in Mercury.

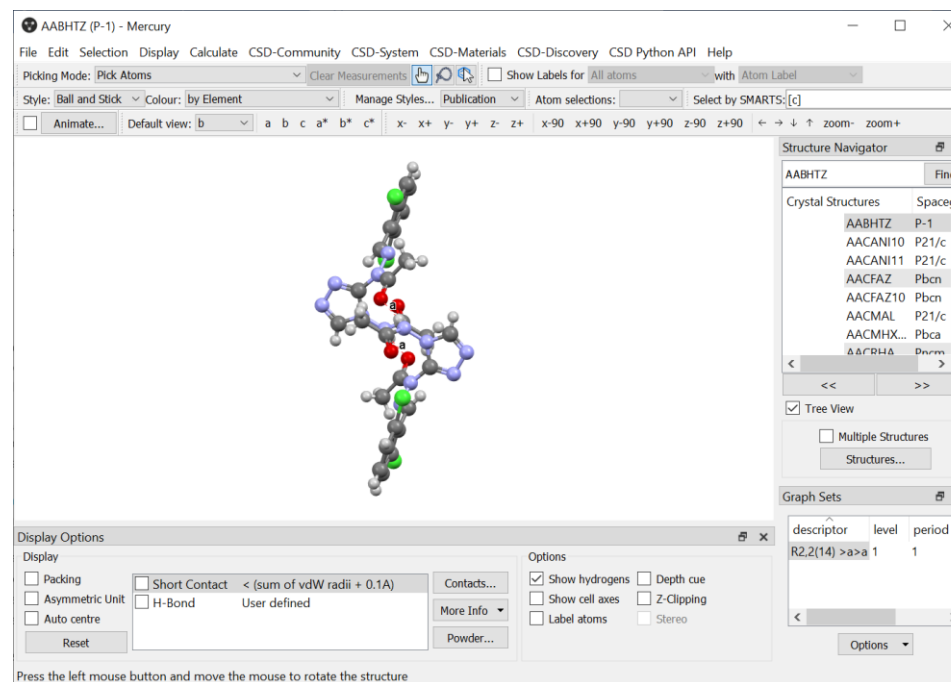
Before beginning this workshop, ensure that you have a registered copy of CSD-System or above installed on your computer. Please contact your site administrator or workshop host for further information.

Objectives

In this workshop you will:

- Familiarise with Mercury interface.
- Explore visualisation options (colour, style, ...).
- Learn how to produce high-quality images.
- Learn how to calculate and display packing.

Note: The words in *Blue Italic* in the text are reported in the Dictionary at the end of this handout, where you can also find terminology from the demo.

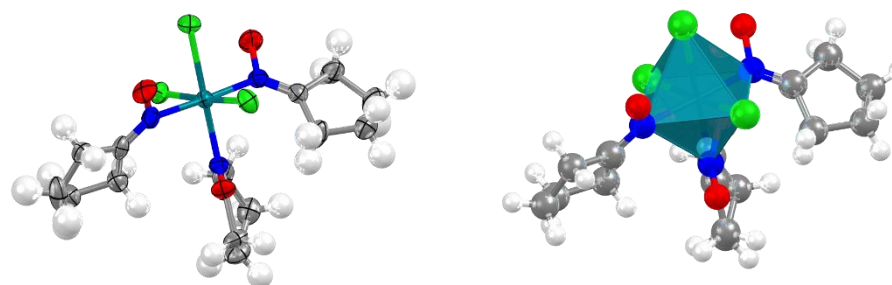


Example 1. Generating Structure Views

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.

The following exercises will introduce you to different styles and settings for visualising in Mercury.

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.



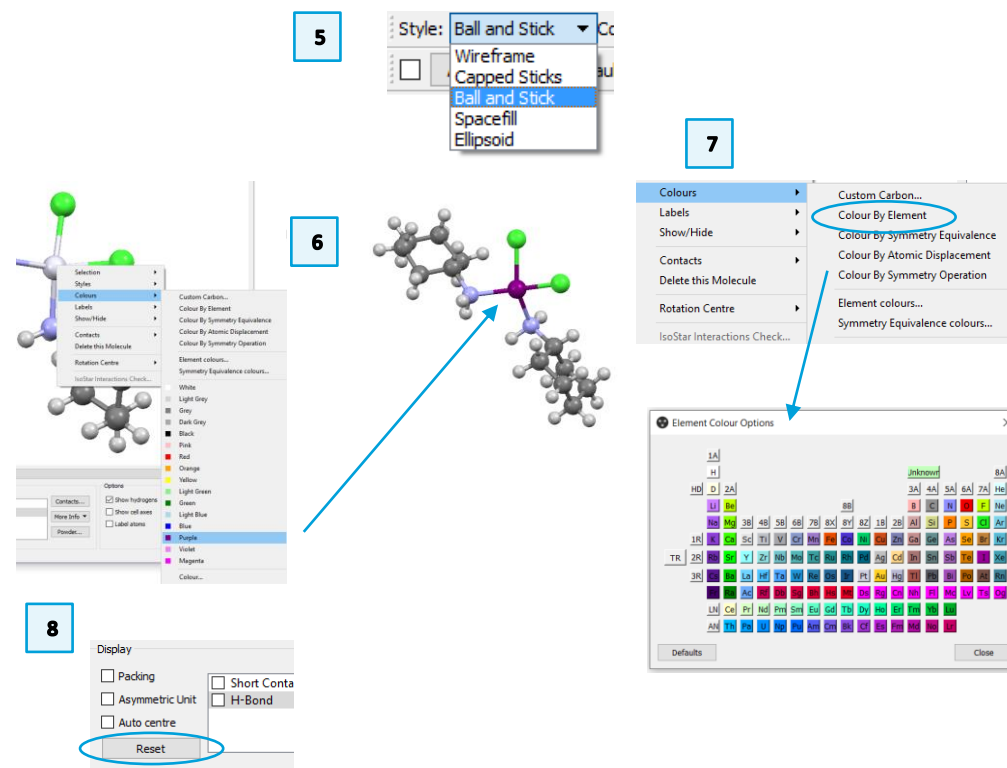
*Ellipsoid View (right) and Polyhedral view (left)
for structure with refcode **BIMXOK***

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. Return to "Ball and Stick" when you are done.

6. The white platinum (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* drop-down 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 (Cmd-Click for macOS) 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.



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. Polyhedral displays are possible for metal-organic molecules, where the metal is the central element.

Ellipsoid View

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.

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

- 1**: The **Structure Navigator** window showing the search for the refcode **BIMXOK** under **Crystal Structures**.
- 2**: The **Manage Styles...** dropdown menu with **Publication** selected.
- 3**: The **Picking Mode: Pick Atoms** window with **Style: Ellipsoid** selected and the **Animate...** button highlighted.
- 4**: The **Styles** dropdown menu with **Ellipsoid settings...** selected.
- 5**: The **Ellipsoid Display Options** dialog box. The **Probability level (%)** is set to 50. The **Display options** section shows **Draw principal ellipses, in colour:** (checked), **Draw hydrogens as fixed-size spheres, of radius (Å):** 0.30, and **Draw Non-Positive-Definite atoms as cubes** (checked). The **Bond style:** is set to **Stick** and the **Radius (Å)** is 0.06.
- 6**: Two molecular models side-by-side. The left model shows the molecule with principal ellipses and wireframe bond style. The right model shows the molecule with principal ellipses and stick bond style.

Polyhedral View

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.

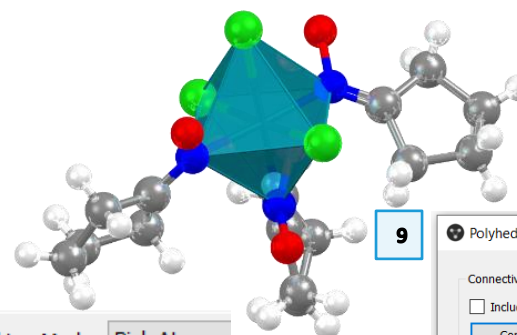
7. To change the style of the atoms and bonds in the structure, use the *Styles* dropdown box. Select Polyhedral

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...*

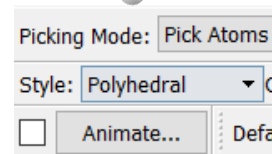
9. Click on Central Elements to see which elements are included in this definition, click **Cancel** to return to the Polyhedral Display Options window. Click on Ligand Elements to see the defined elements for ligands. The default definitions are adequate so click **Cancel** to return to the Polyhedral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

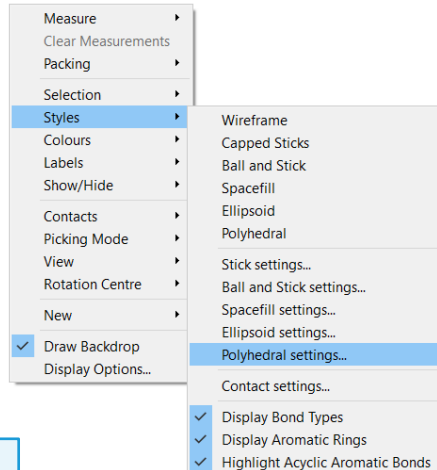
11. You should be able to create Ellipsoid and Polyhedral views for complexes. Remember, Ellipsoid style depends on the inclusion of certain parameters in the structure file or deposited entry. Polyhedral style depends on the inclusion of the central element in the Polyhedral Display Options.



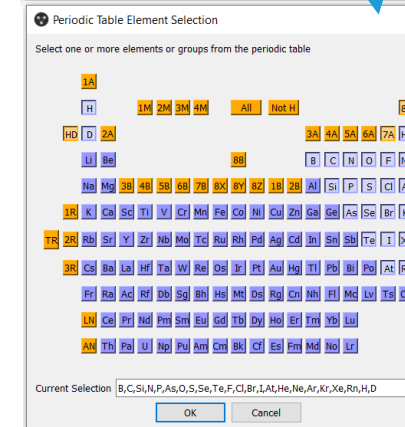
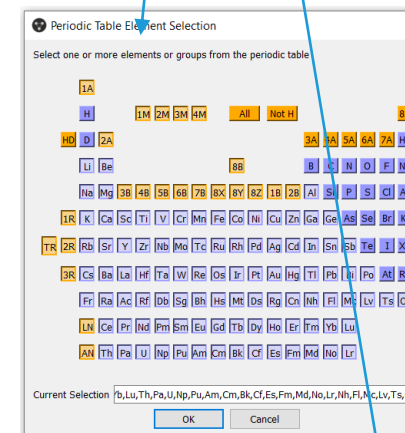
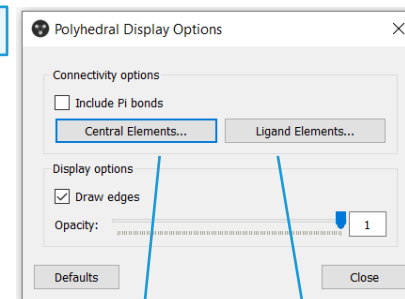
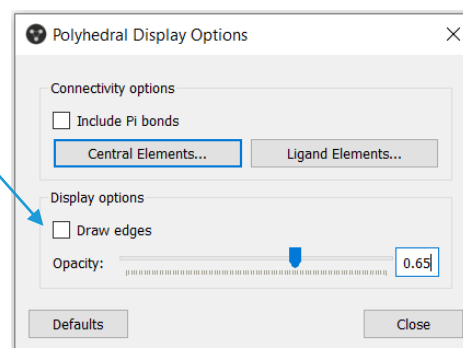
7



8



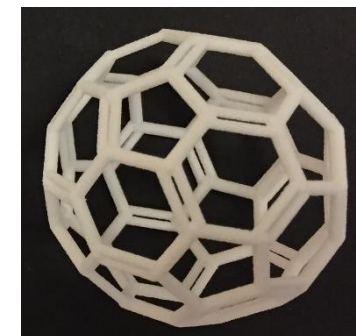
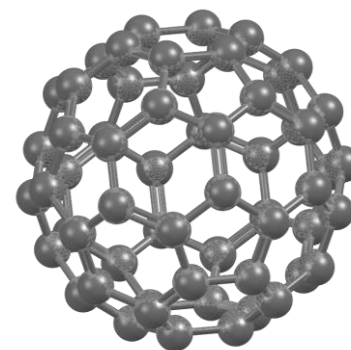
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Example 2. Generating High-Res Images

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 exercise will show you how to generate high-resolution graphics files from Mercury.



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

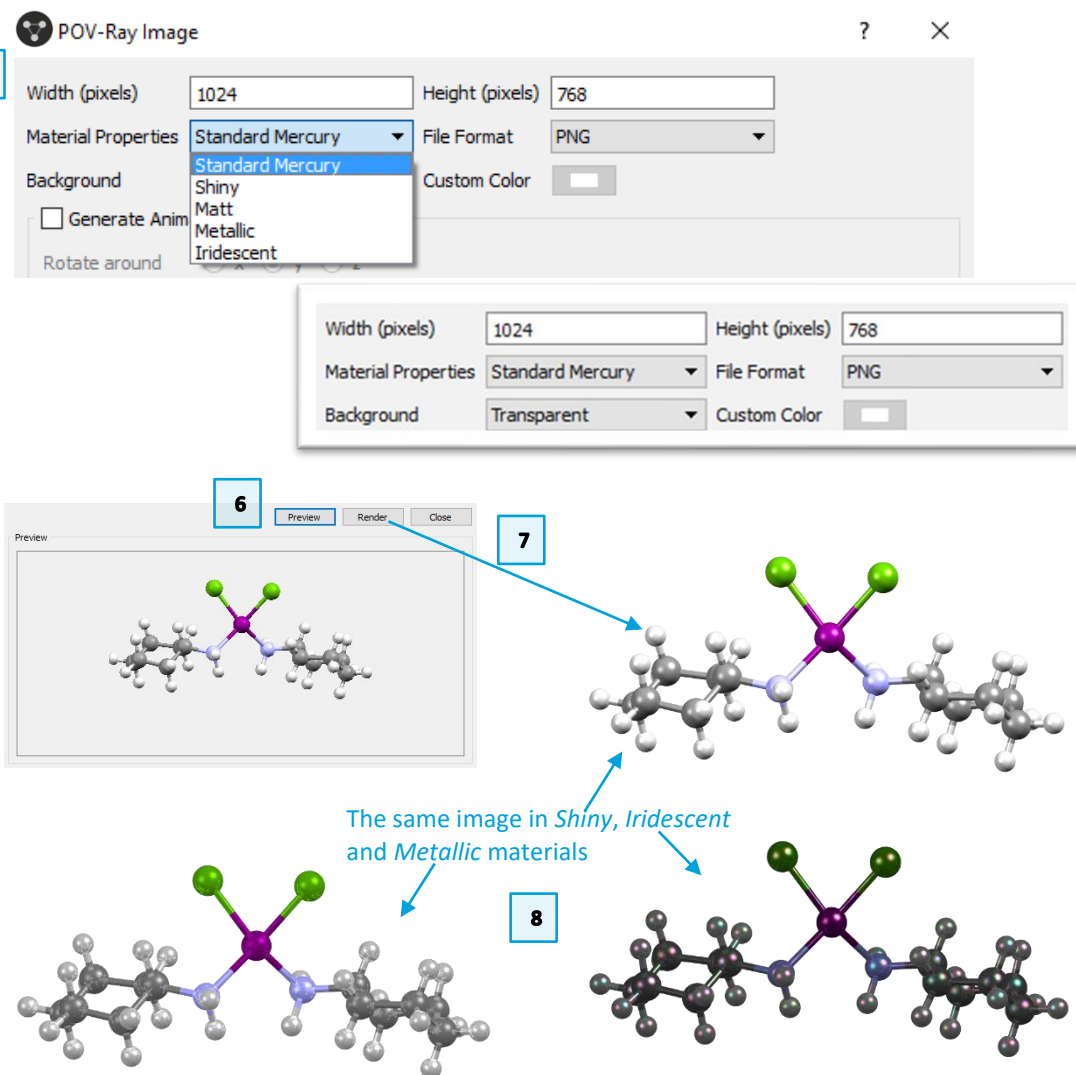
High-resolution images

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 sequence of images shows the workflow: 1. Opening Mercury. 2. Searching for 'CCXAPT' in the Structure Navigator. 3. Viewing the resulting cisplatin derivative structure in the main window. 4. Accessing the 'POV-Ray Image...' option from the File menu to open the rendering dialog.

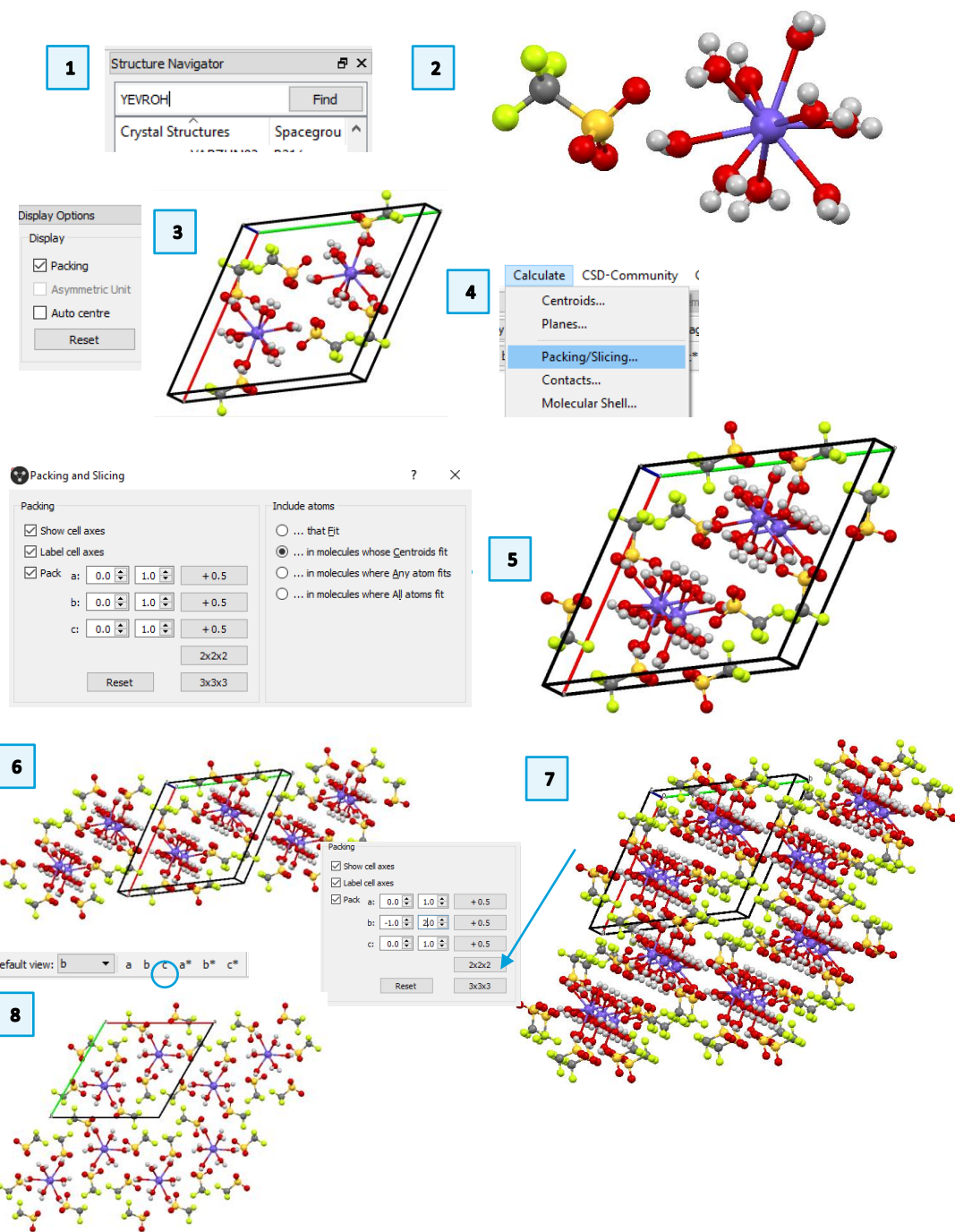
5. Change the *Material Properties* to the desired setting by clicking in the dropdown box and clicking the appropriate type. Select *Transparent* from the *Background* dropdown menu. Leave all other default values the same.
6. For complicated or large images, or on slow computers, POV-Ray may take a 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.
8. Using different *Material Properties* creates different image styles. Try different materials to see the effects.



Example 3. 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 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.



Conclusions

After this workshop you will:

- Be comfortable with the Mercury interface and with exploring options and functions in Mercury.
- Know how to change between different visualisation options, select styles and colours to display your structure of interest effectively.
- Know how to create publication-ready high-quality images, selecting resolution, material, and background.
- Know how to calculate and display the packing of a crystal structure, and the asymmetric unit.
- Bonus: be able to create your own style (or styles), with settings defined by you to fit your requirements for structure visualisation.

Next steps

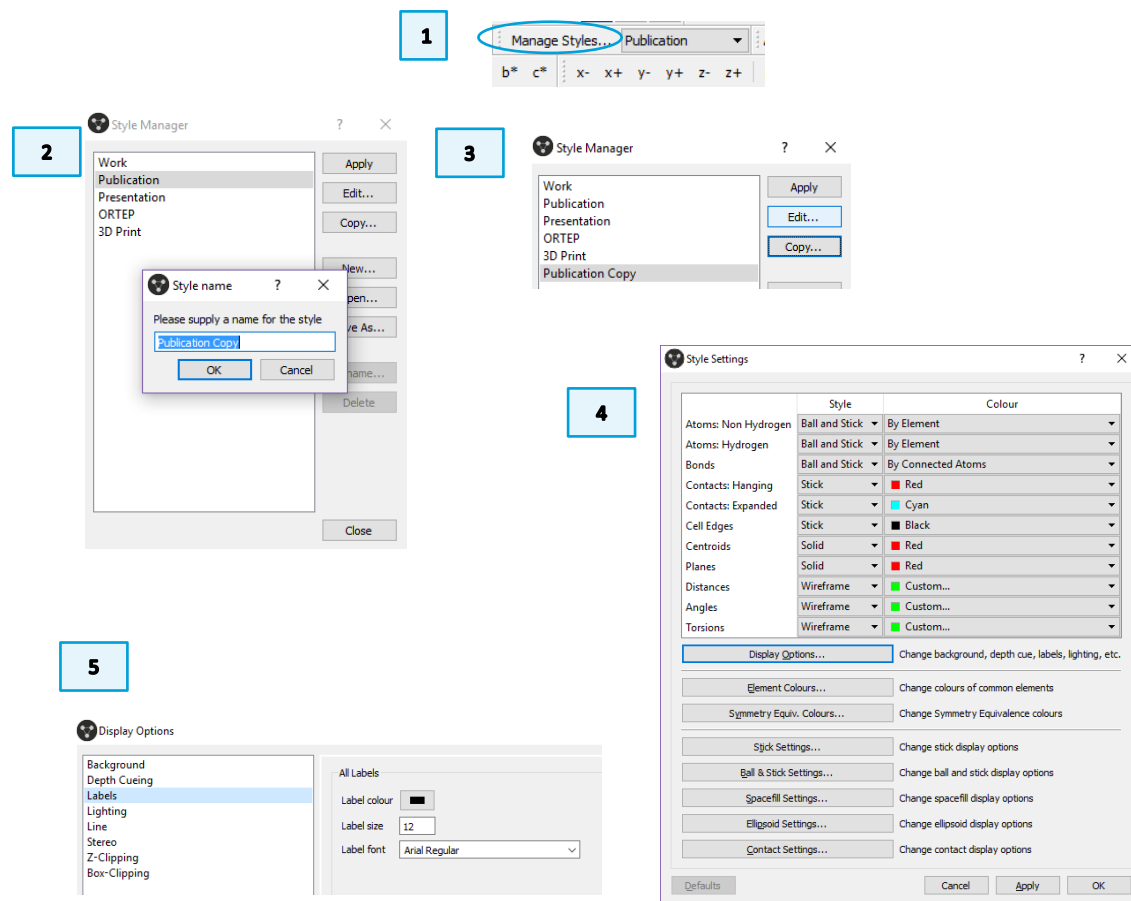
If you finished early these exercises, head to the bonus exercise to learn how to create your own style: this will appear in the Style Manager dropdown menu next to the pre-defined ones. Or ask the tutors for more challenges!

After this workshop, you can find more exercises in the “Structure Visualisation” self-guided workshop available in the [CSD-System workshops area](#) on our website. In this area, you can also find entry level self-guided workshop to guide you in the exploration of other software available with your license.

Bonus Exercise. Create your own Style Type

To create images that are perfect for your presentations, manuscripts, and publications, you might find out that you need to change visualisation settings and that you need to do it quite frequently. In Mercury, you can save these settings by creating your own style type. The following exercise will show you how.

1. 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.
2. 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**.
3. 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.
4. **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.)
5. 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.
6. You should now be able to create a structure view with your preferred styles.



Dictionary

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).

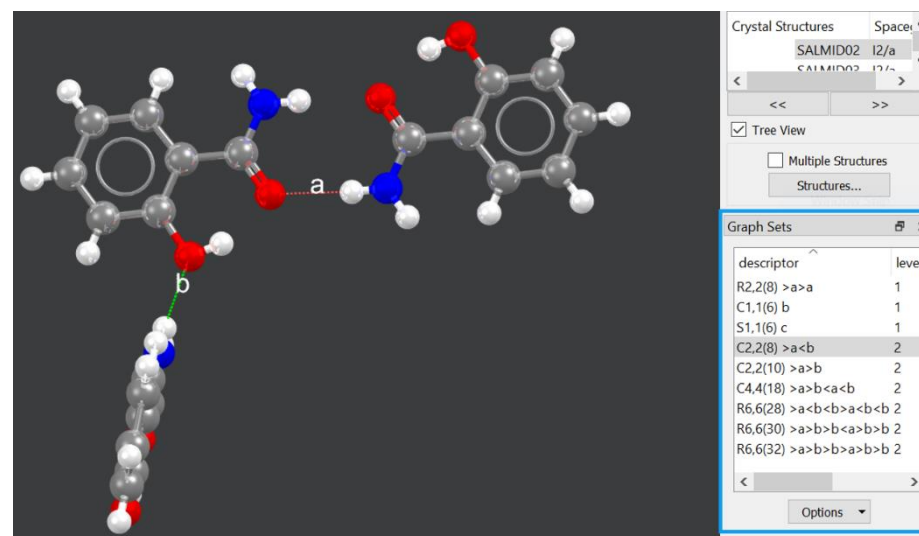
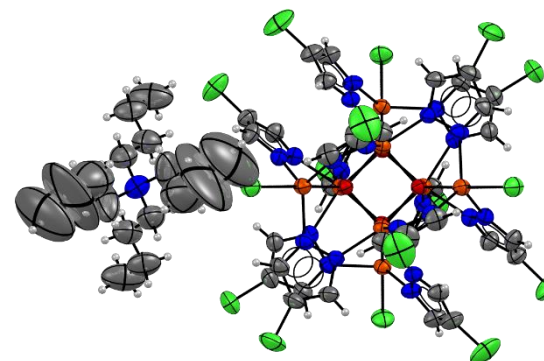
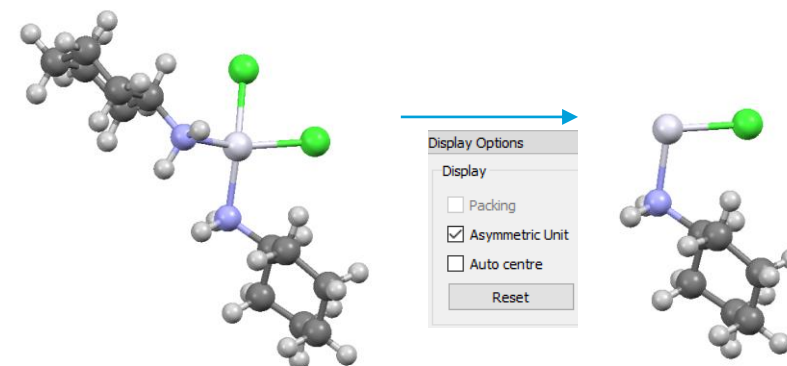
Graph Sets

Graph set analysis of hydrogen-bonding describes the pattern of the hydrogen-bond chains or motif and includes the numbers of hydrogen-bond donors and acceptors.

A graph-set descriptor is written as $G^a_d(n)$, in which **G** represents the type of pattern, **a** is the number of hydrogen bond acceptors involved in that pattern, **d** is the number of donors and **n** the number of atoms in the pattern. The pattern type, G, can be one of four different options: C for an infinite chain, S for an intramolecular hydrogen bonding pattern, R for an intermolecular ring and D for a discrete, finite hydrogen-bonding pattern.

Relevant bibliographic references:

- M. C. Etter, Acc. Chem. Res., 23, 120, 1990
- J. Bernstein, R. E. Davis, L. Shimon and N.-L. Chang, Angew. Chem. Int. Ed., 34, 1555, 1995
- W. D. S. Motherwell, G. P. Shields and F. H. Allen, Acta. Cryst. B56, 466, 2000



Suppressed Atoms

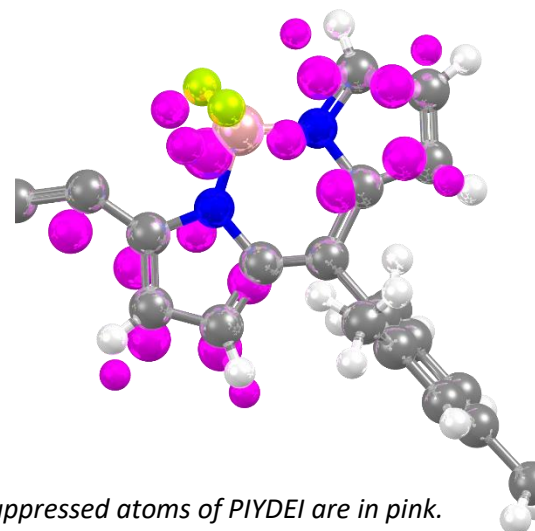
In Cambridge Structural Database (CSD) structures one or more atoms may be suppressed. A common example is when the author reports two sets of atomic coordinates, for major and minor sites, in a disordered structure. In most cases the atoms of the minor site will be suppressed.

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 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.



Suppressed atoms of PIYDEI are in pink.

