

Visualisation 101 Try

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# Try – it's your turn!

In the second part of the Visualisation 101 module, "Try", you will review the concepts and features presented in the first part, "Watch", and try them out yourself. If at any time you want to rewatch the videos, you can find them from the course webpage (https://www.ccdc.cam.ac.uk/Community/educationalresources/CSDU/visualisa tion-101/).

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, ensure that you have Mercury installed on your computer. You should be able to complete the exercises either with a registered copy of the CSD or with the <u>free version of Mercury</u>. For further information, please contact your site administrator or the CCDC (Contact Us).

### Objectives

Through these three exercises and bonus you will:

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

This workshop will take approximately **30 minutes** to be completed.

**Note:** The words in <u>Blue Italics</u> are reported in the Glossary at the end of this handout, where you can also find terminology from the Watch part of the module.



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# 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.

## 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 <u>Asymmetric Unit</u> 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 <u>Atomic Displacement Parameter Values</u>. 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 (A), 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.



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### **Polyhedral View**

Now we are going to generate a polyhedral view of the mer-Trichlorotris(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.



# 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 it 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 loction, but you may want to change the Output Directory location. Click **Browse...** to do this.



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- 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.

### POV-Ray Image ? $\times$ 5 Width (pixels) 1024 Height (pixels) 768 Material Properties Standard Mercury PNG File Format Background Custom Color Shiny Matt Generate Anim Metallic Iridescent Rotate around Width (pixels) Height (pixels) 768 1024 Material Properties Standard Mercury File Format PNG Transparent Custom Color Background 6 Preview Render Close 7 The same image in Shiny, Iridescent and Metallic materials

# 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.
- This will display the metal-organic salt compound, nona-aqua-curium(iii) tris(trifluoromethanesulfonate) which crystallises in the space group P6<sub>3</sub>/m. Tick and untick the <u>Asymmetric Unit</u> box to see what atoms are generated by symmetry (Step 3 in Example 1 Generating a Simple Molecular View).
- 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.



# 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 setting 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.



## Conclusions

After this workshop you will:

- Be comfortable with the Mercury interface and 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 make more effective fitting your structures and visualisation necessities.

## Next steps

Now that you have completed the Try part of the Visualisation 101 CSDU module, you can head to the final part: the quiz! Go back to the module webpage (https://www.ccdc.cam.ac.uk/Community/educationalresources/CSDU/visualisa tion-101/) and follow the instructions to complete the final quiz.





## 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 atrifluoromethyl group, -CF<sub>3</sub>, 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



Asymmetric unit for CCXAPT.



Suppressed atoms of PIYDEI are in pink.

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.

