# Mercury Tips & Tricks from attendees at the Virtual Workshop of 30/04/2024

Thank you all for sharing your tips and tricks on using Mercury!

We have collected all of them and divided by topic. Similar tips have been merged.

## **BFDH Morphology**

- Accessed from: CSD-Particle Morphology > BFDH
- Tip: Using BFDH morphology t compare the experimental indexing.

>	CSD-Particle	CSD-Discovery		CSD Python API				P
	Morphology 🕨 🕨		BFDH					
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## Symmetry Functionality

- Colour molecules by symmetry equivalence.
- Tip: When colouring molecules according to symmetry equivalence (eg for Z'=2) DO

,	Style: Ball and Stick	Colour:	by Element	$\sim$
		Default view	by Element	
	Animate		by Symmetry equivalence	
			by Atomic displacement	
			by Symmetry operation	
			by Gasteiger charge	
			by Partial charge	
			by Element or Suppression	

NOT use red and green since they will both appear to be the same to a colour blind reader. Black and orange are two good contrasting colours.

• Extra Tip: To change the default colours for symmetry equivalence, go to Display > Colours > Symmetry Equivalence colours



### **Calculate Menu**

• Tips: Calculate planes – see how to on the slides!

#### PXRD

- Accessed from: Click on the Powder button below the 3D visualiser in Mercury.
- Tip: Calculating PXRD from cif files and customising the output pattern
- Tip: Preparing theoretical PXRD patters which can be read in Excel or diffrac.eva



### Other uses of Mercury

• I like to use Mercury to analyze my DFT structures.

#### Input molecules and files

- Tip: You could use the SMILES to Molecule feature (accessed from the File menu) to specify the stereochemistry of the initial structure to use in Conformer Generator.
- Tip: You can drag any file that Mercury can read either into an open Mercury window or onto the Mercury icon on your desktop and it will open it.





#### **Create animations**

• Tip: Tick Generate Animation Frames in the POV-Ray window to create frames for an animation showing the structure rotating. Use a gif creator software to collate the frames into a gif / movie.

😵 POV-Ray Imag	e				×		
Width (pixels)	1200	] Height (pixels)	1200				
Material Properties	Metallic $\checkmark$	File Format	PNG	$\sim$			
Background	Transparent v	Custom Color	-				
Generate Animation Frames							
Rotate around $\bigcirc x  \textcircled{o}  y  \bigcirc  z  Number \ of \ Frames \ 45$							
			Preview	Render	Close		
Droviow							