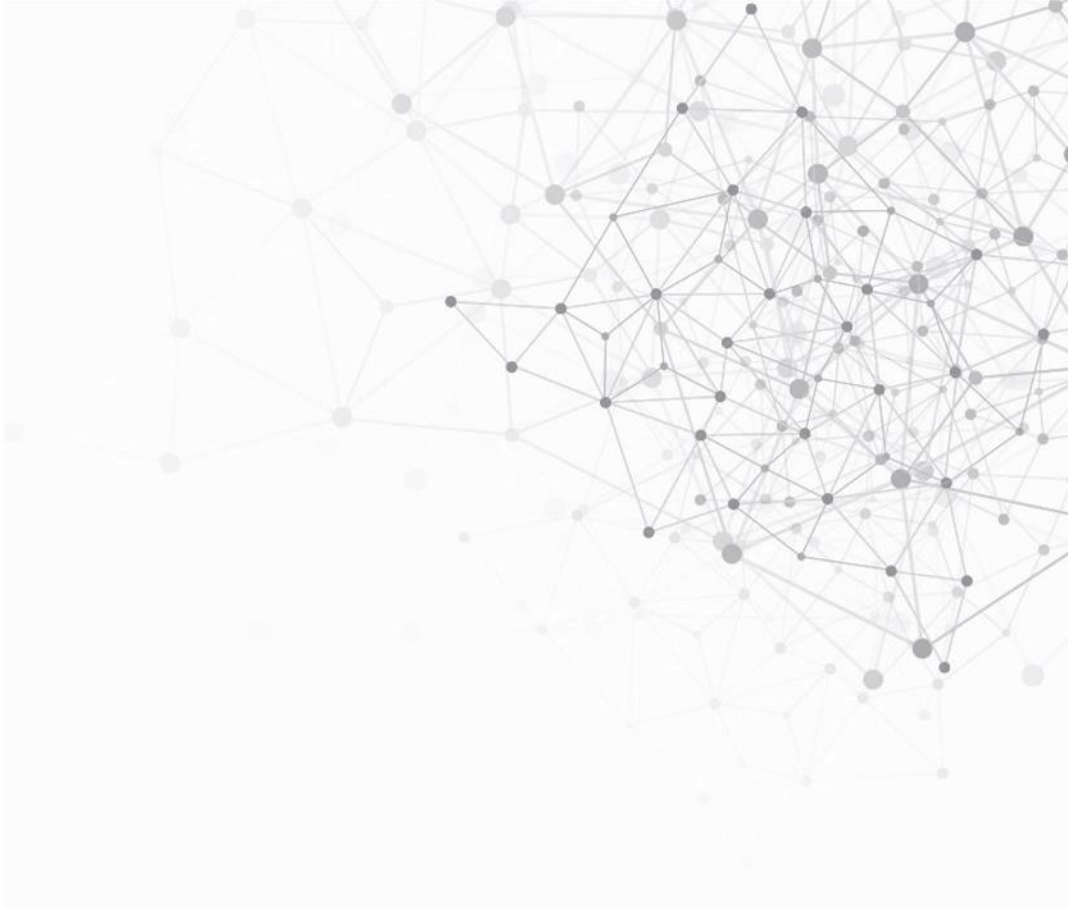
Welcome to CSDU

Visualisation 101



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Learning outcomes

- Familiarise yourself with the Mercury interface
- Learn the basic options to visualise small molecule crystal structures
- Learn how to visualise the packing of a structure effectively
- Learn how to create high resolution publication ready images of your structures

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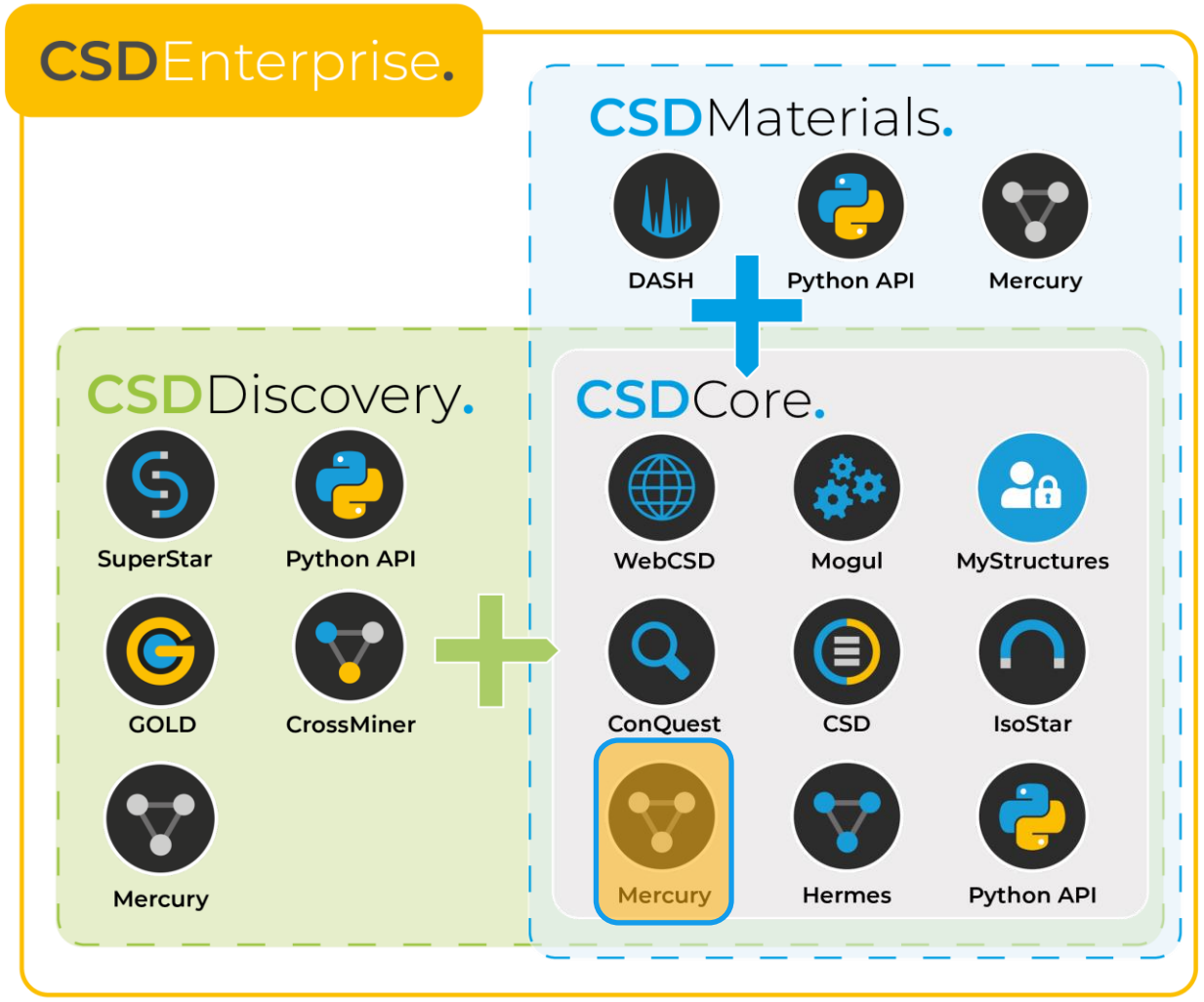
The CSD Portfolio



Professional Services

Research & Knowledge partnerships

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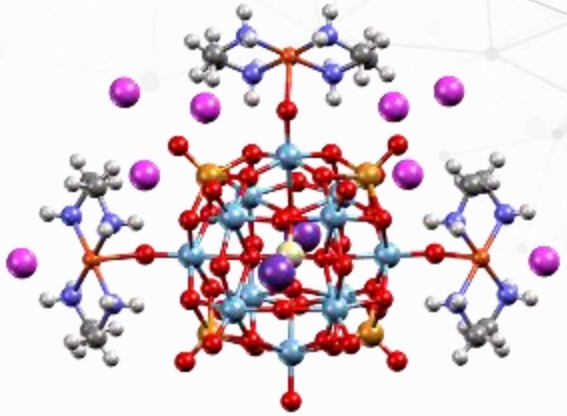
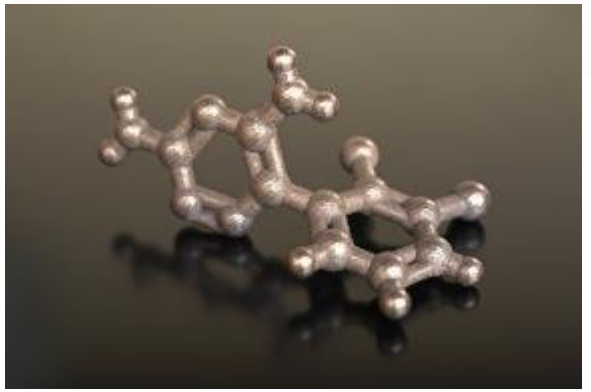
Mercury – Structure visualisation

With Mercury you can:

- Explore over 1 million crystal structures, molecular conformations, crystallographic planes and simulated morphologies
- Generate high quality structural images for effective scientific communication
- Output model files for 3D printing
- Analyse geometries, interactions and the packing inside structures





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The basics of navigating Mercury

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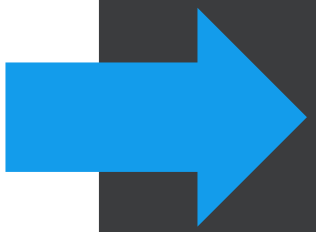
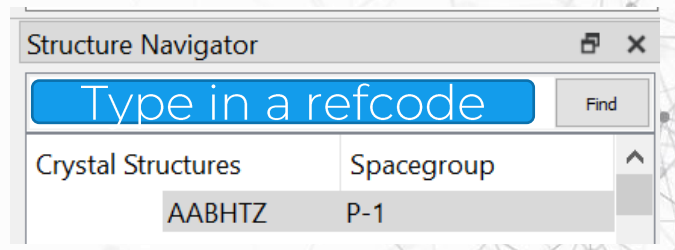
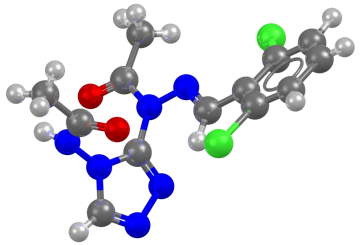
Mercury Overview



CSD Refcodes reminder





CSD Refcode - AABHTZ

What is AABHTZ?

- A CSD Refcode
- A database reference code
- Containing 6-8 characters
- Used to identify entries in the CSD

Refcode families

- The same substances are assigned the *same* 6 letter code plus an additional 2 numbers
  - Polymorphs
  - New determinations or re-refinements of the same substance
  - Determinations at different temperatures/pressures
- Stereoisomers or different solvates, co-crystals, etc are assigned *different* refcode families

- Some more recognisable refcodes: KITTEN, BATMAN, BADBOY, GAUTAM, GLYCIN

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The basics

- Left mouse button and move – allows you to rotate structure
- Middle Mouse button and move – allows you to move structure
- Right mouse button and move – allows you to zoom in and out of structure

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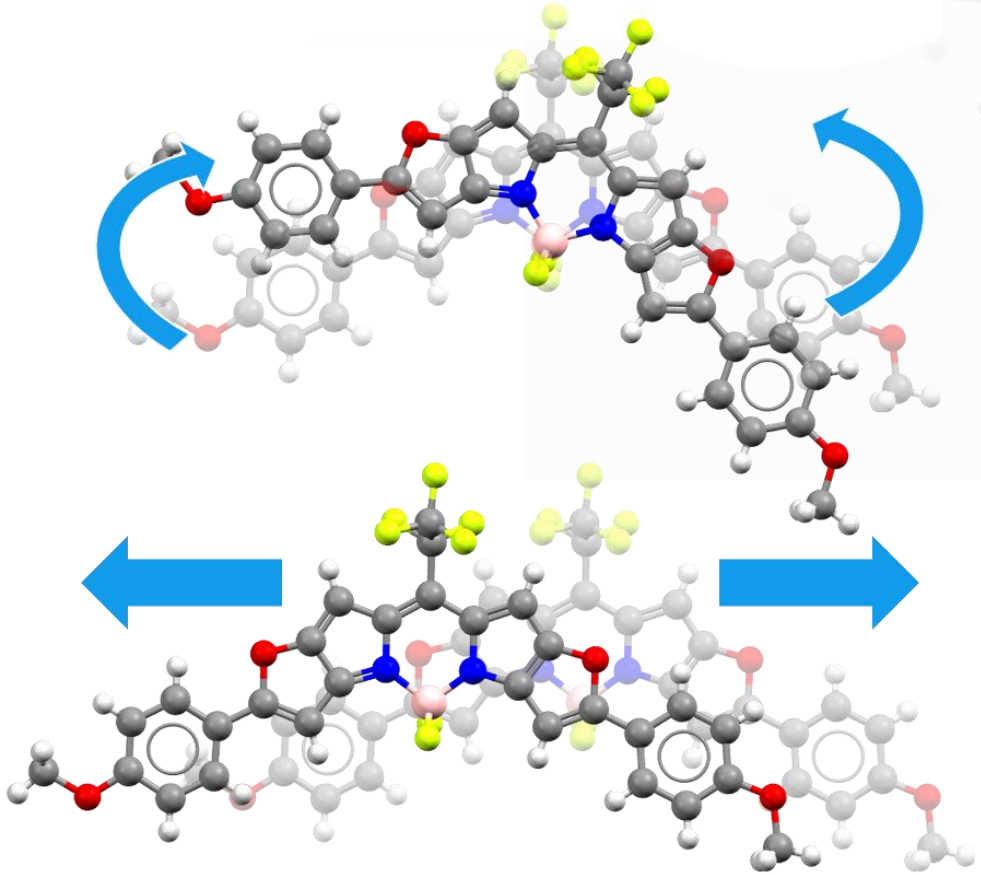
The basics

With the keyboard:



CSD Refcode: GIMXUY

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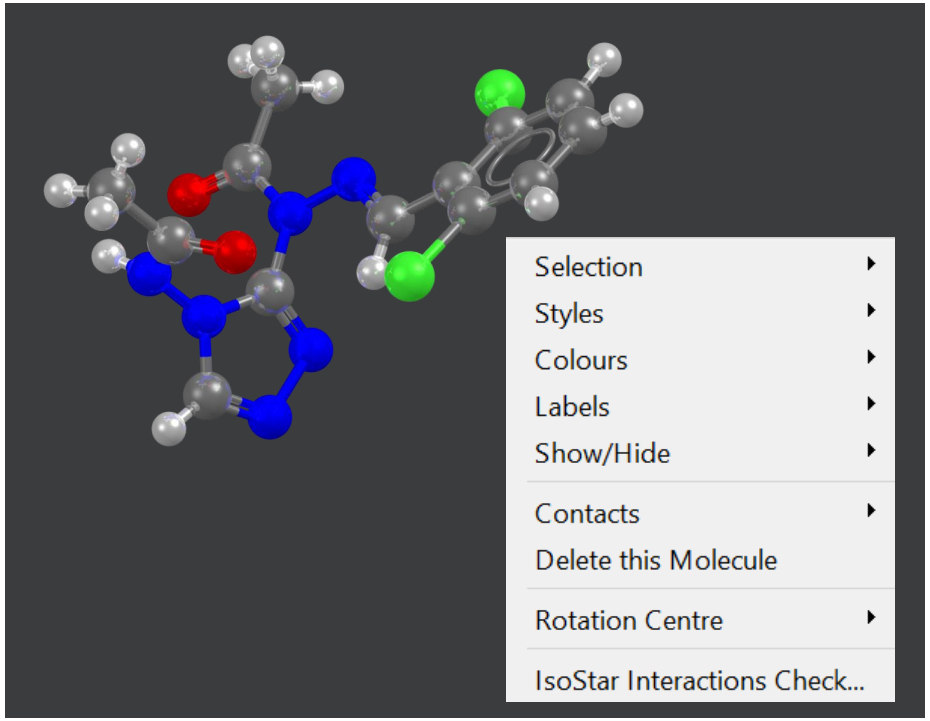
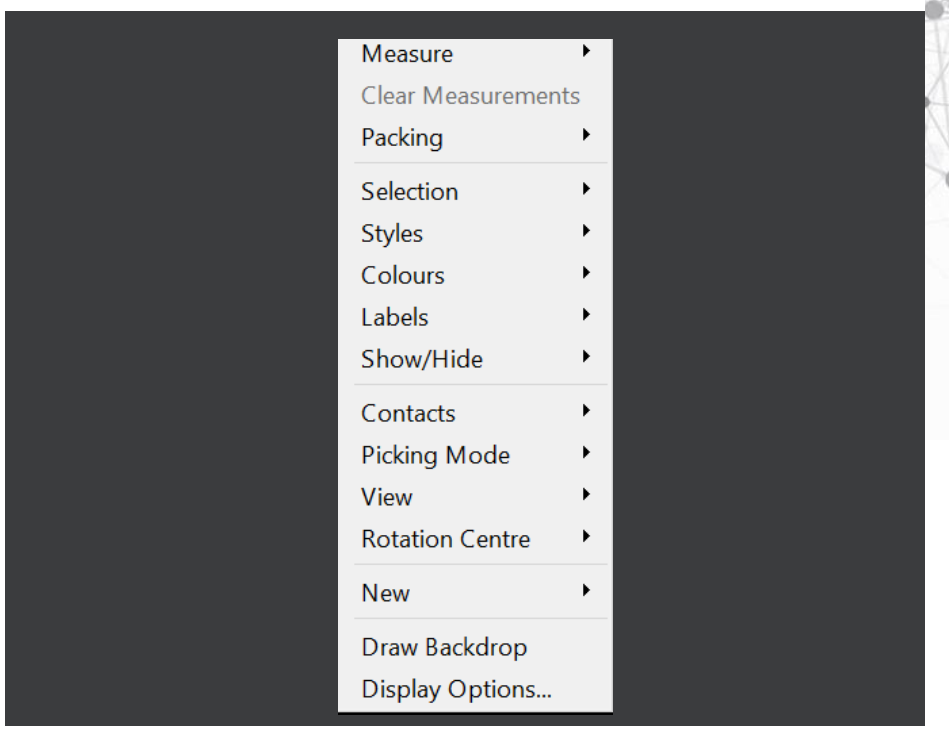
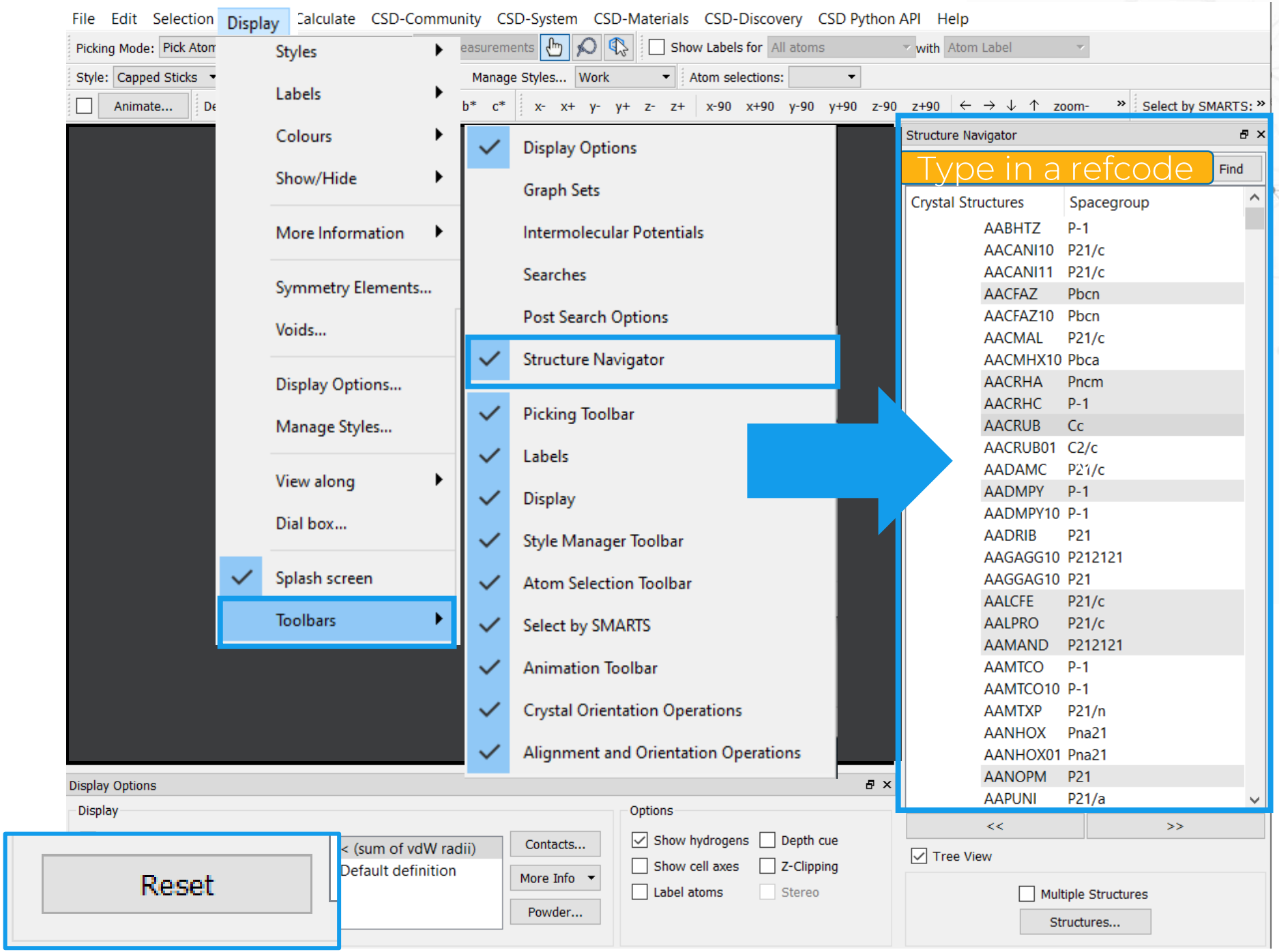
Right mouse click

Near a molecule



Away from a molecule





Handy tips:

- Recovering Toolbars
- Resetting view

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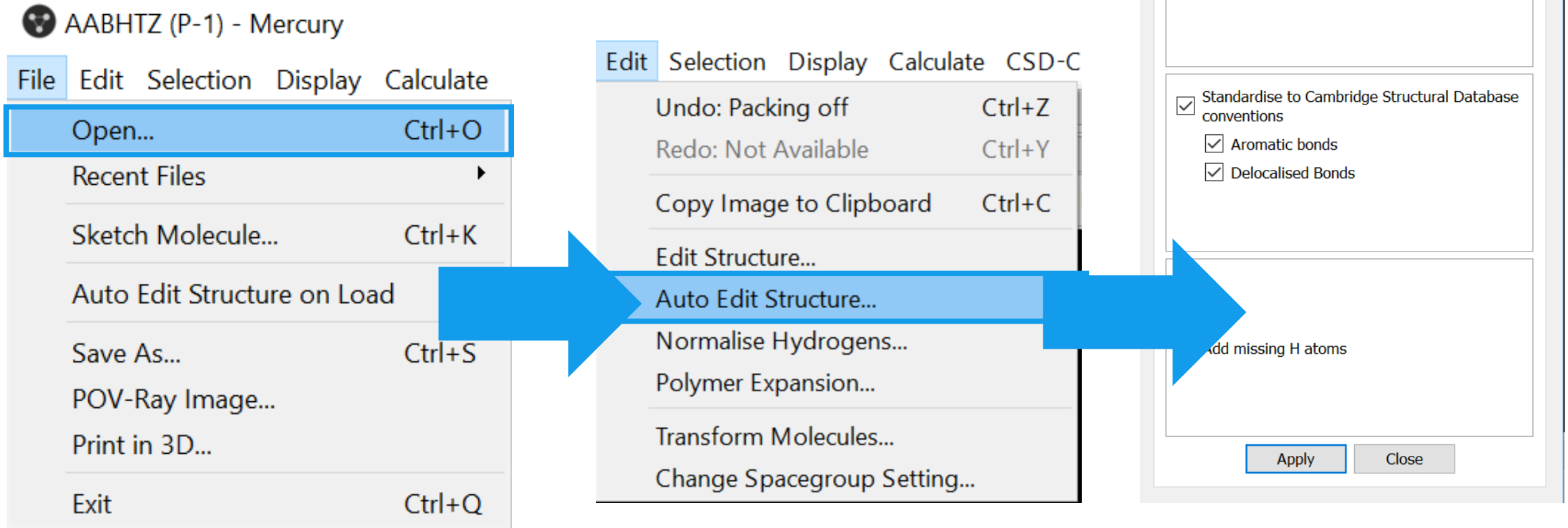
Using your own file

- File > Open – to open one of your own files for example a CIF
- Edit > Auto Edit Structure to assign bond types
- File > Auto Edit Structure on Load to automate



Styles and colours options

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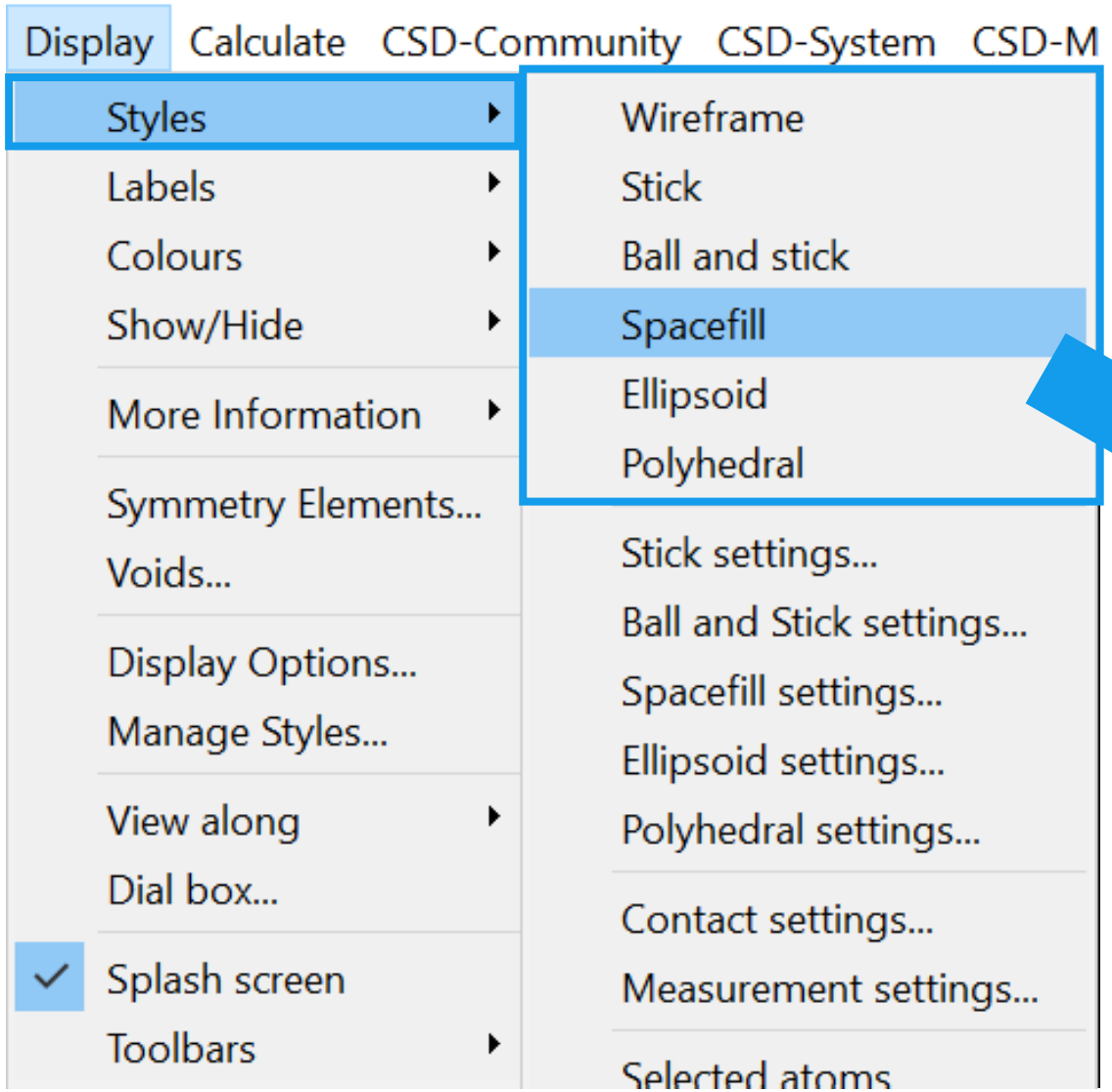
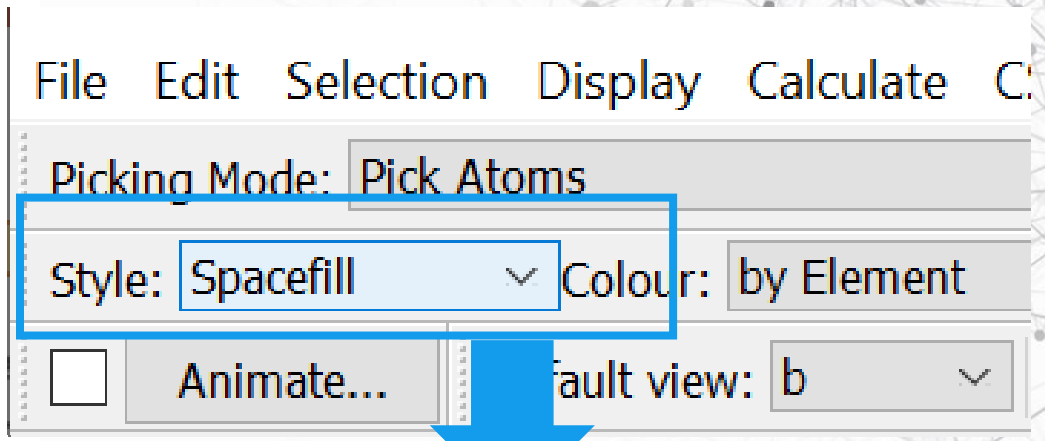
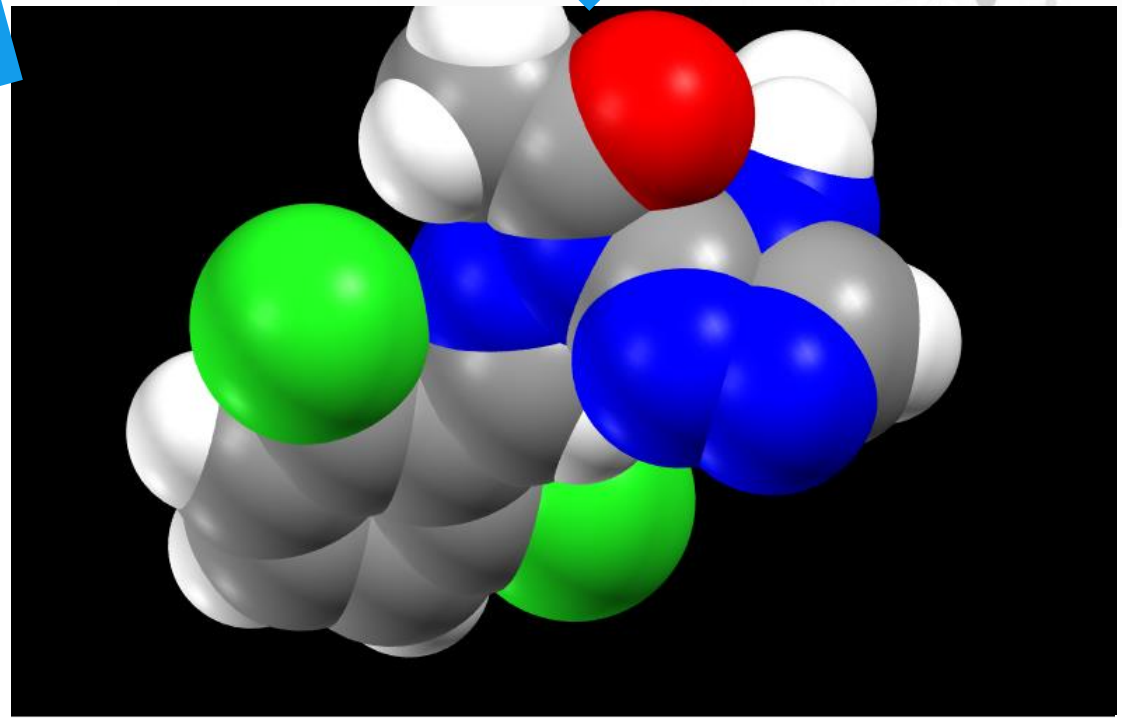
Changing display - Style

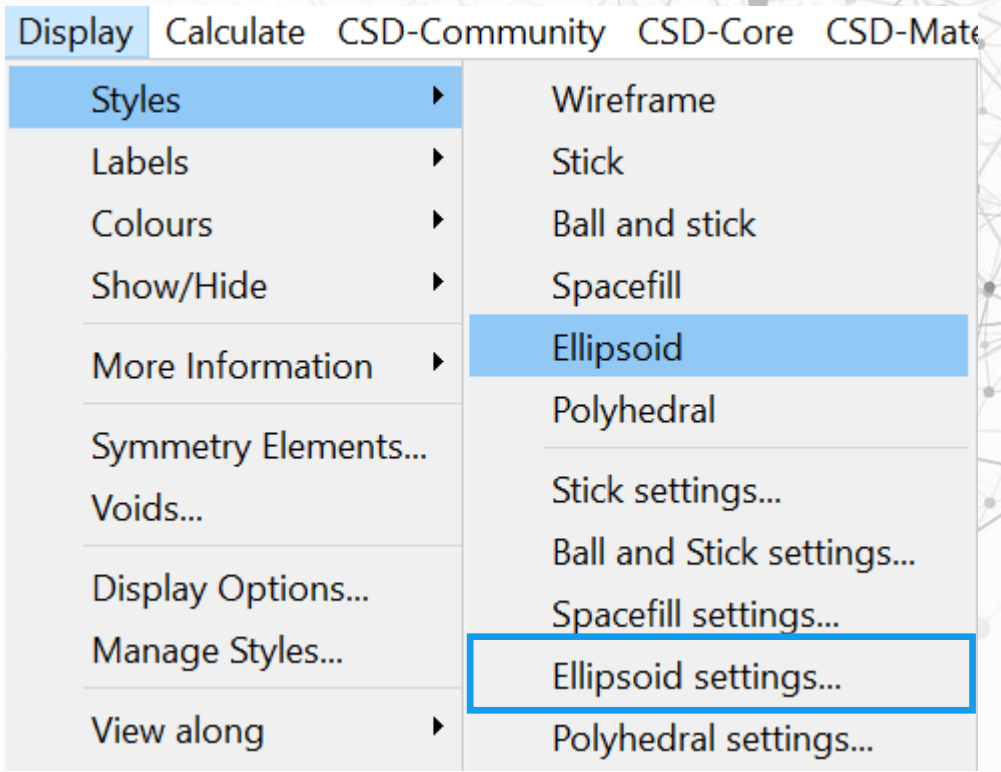


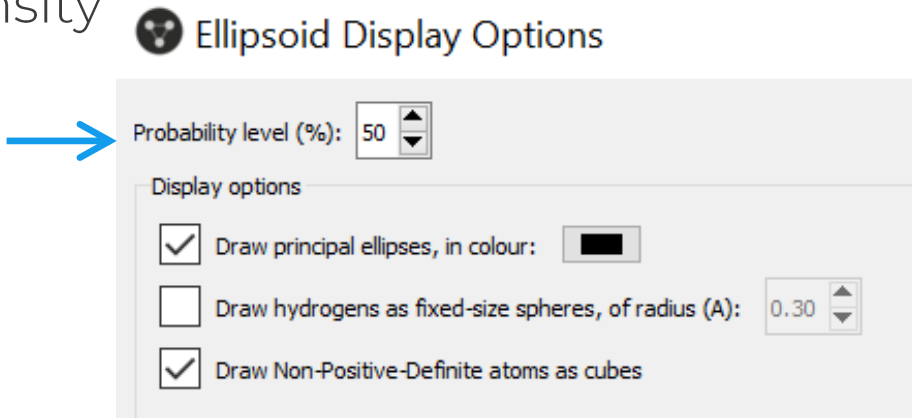


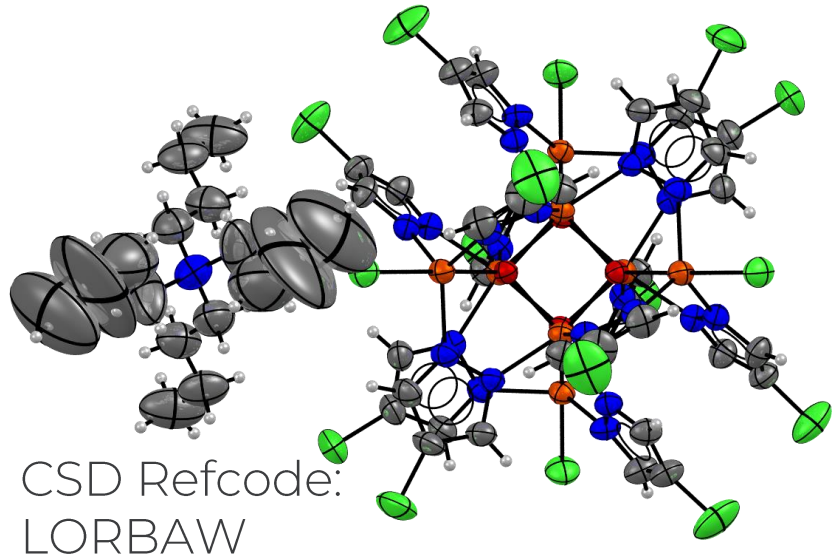


Thermal ellipsoids

- Anisotropic Displacement Parameters
- Only available for CSD structures with ADPs
- Indicate thermal vibrations of atoms
- Size of ellipsoid is scaled
  - Usually to probability of finding 50% of electron density



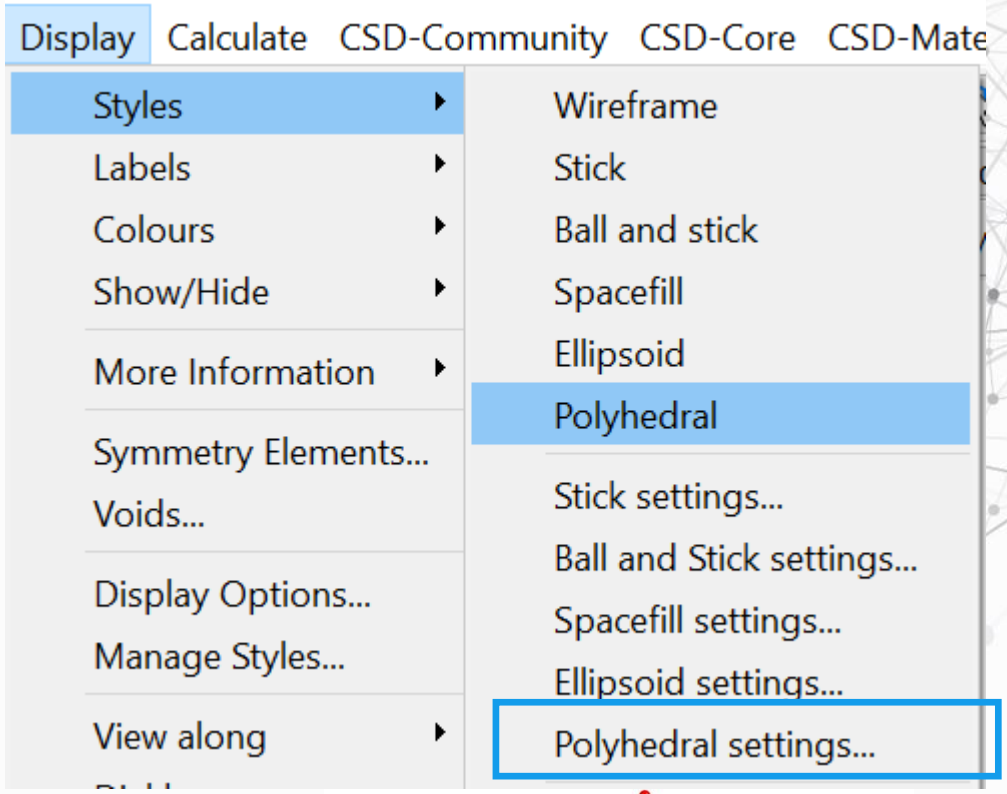


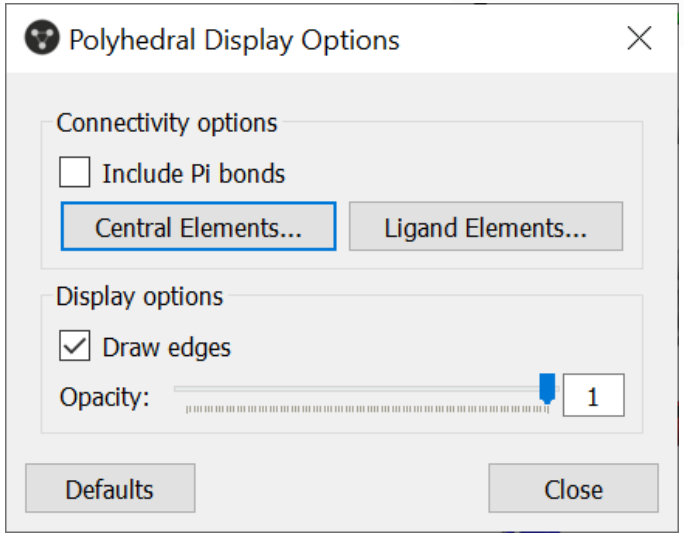


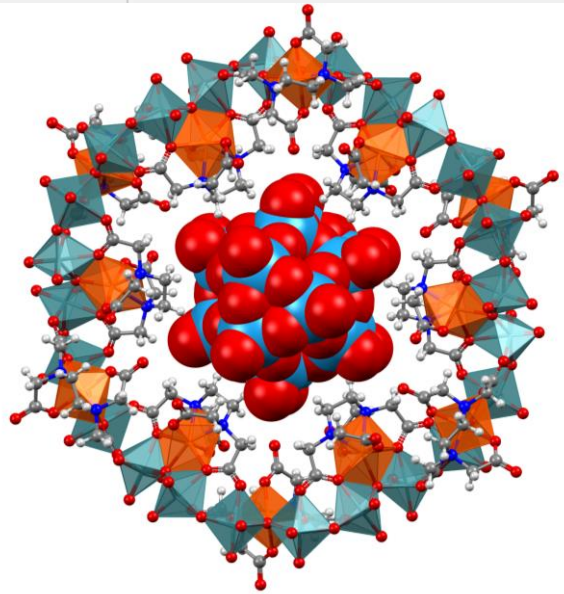
CSD Refcode: LORBAW

Polyhedral display

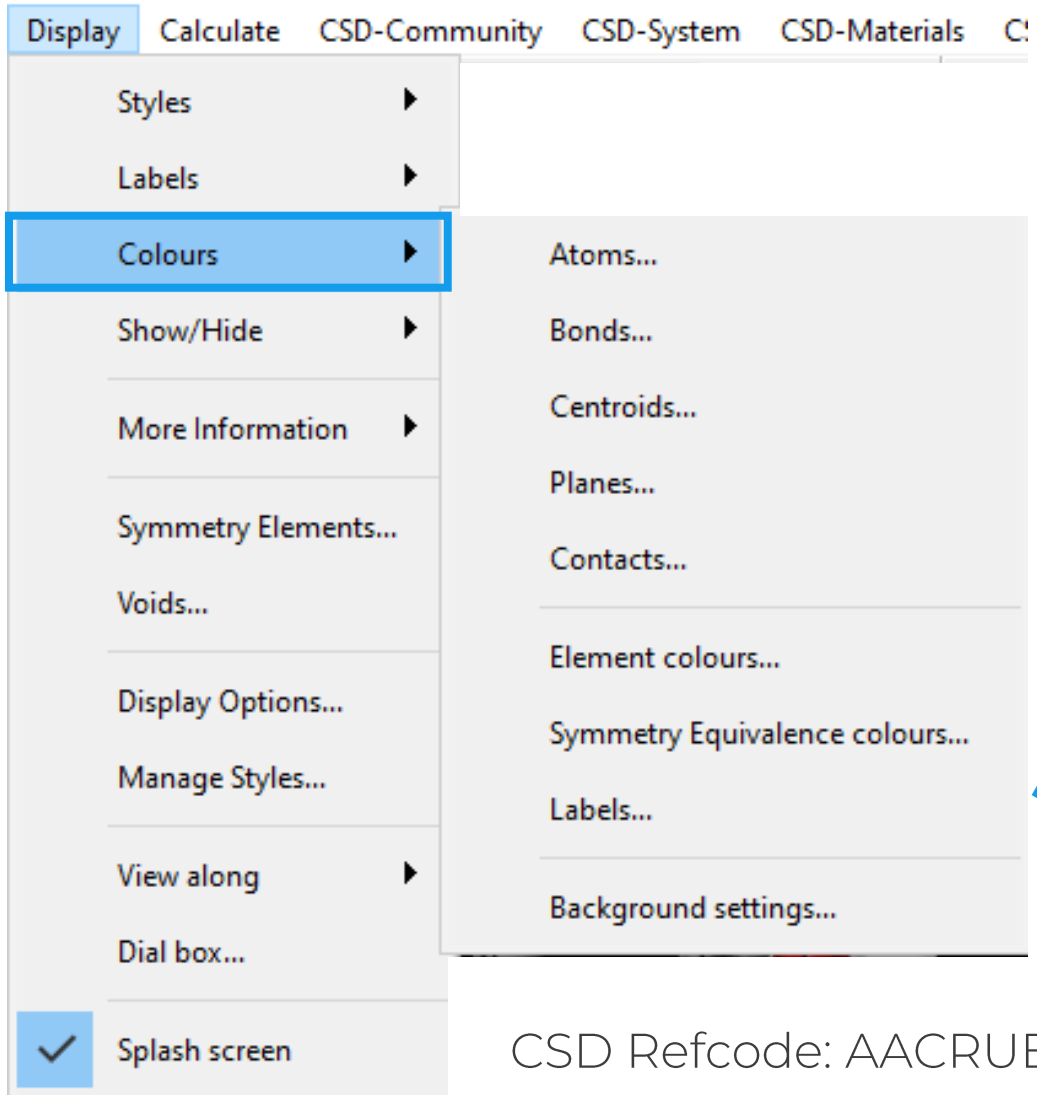
- Visualise metal-organic structures using polyhedral representations for the metal-organic coordination centres.
  - Central Elements - atoms around which polyhedra are centred
  - Ligand Elements - neighbouring atoms which create the corners of the polyhedron

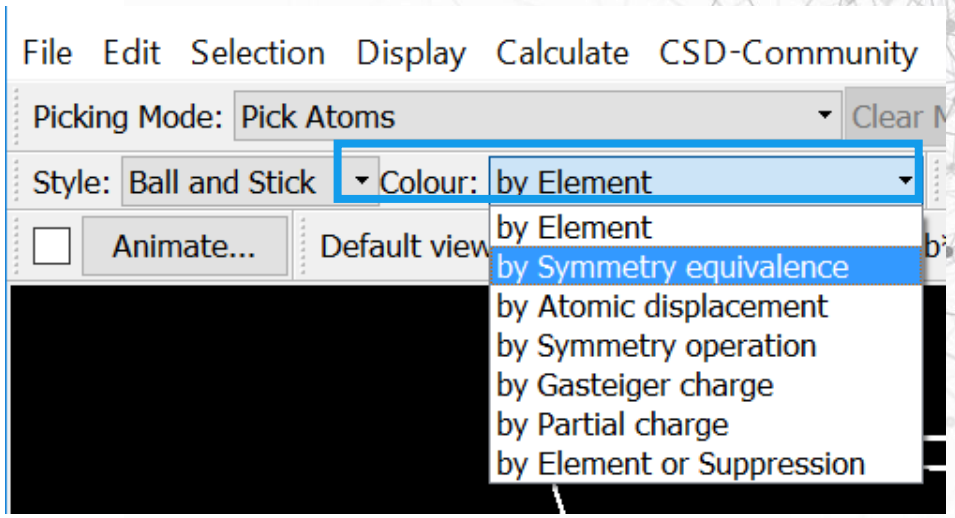


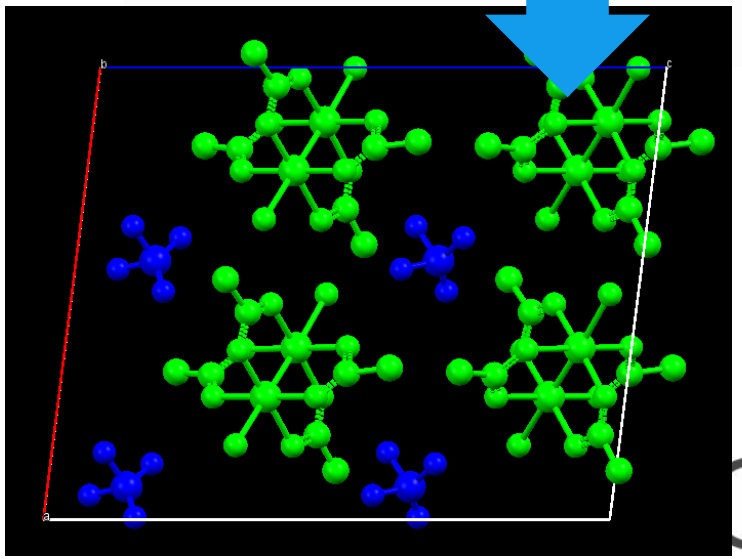




Changing display - Colours

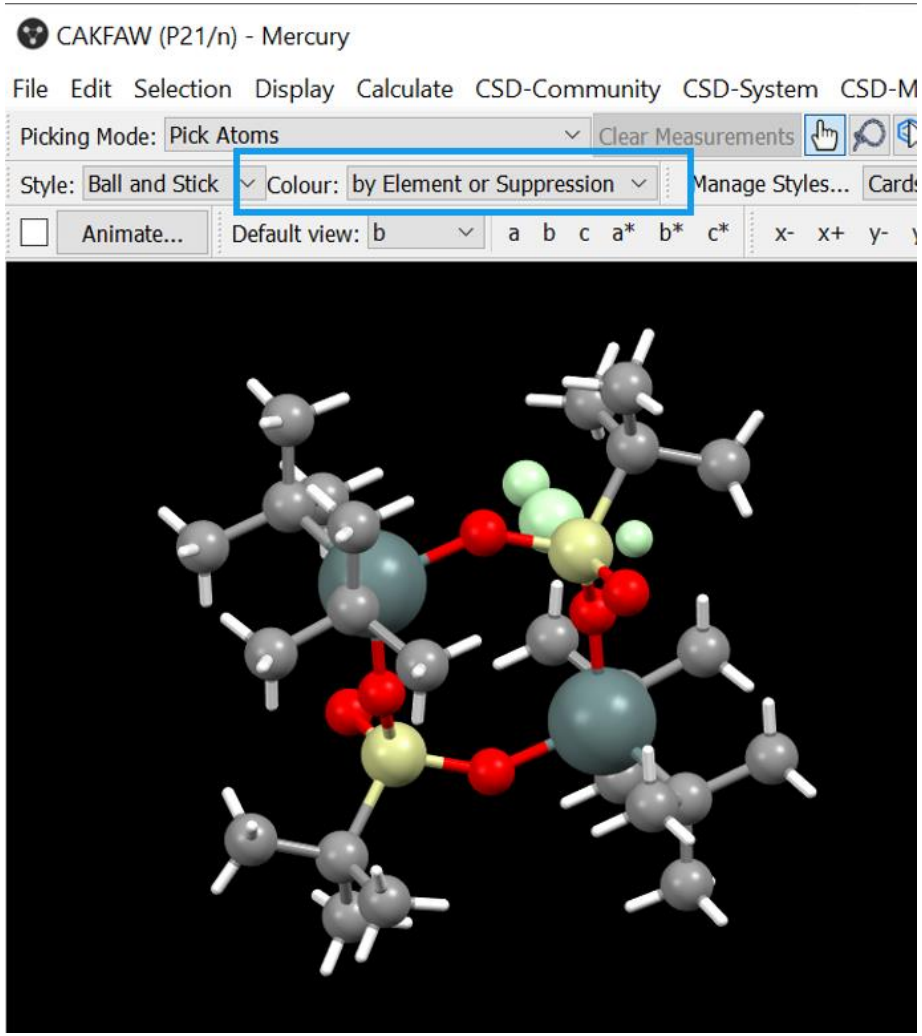


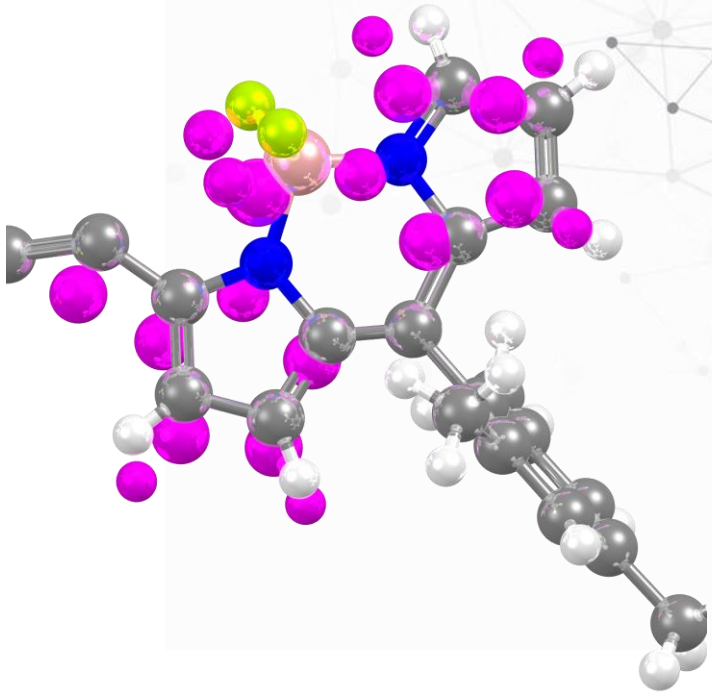




CSD Refcode: AACRUB

Changing display - Colours





Disordered structures report two sets of atomic coordinates: major and minor sites. In most cases the atoms of the minor site will be suppressed.

CSD Refcodes: CAKFAW and PIYDEI

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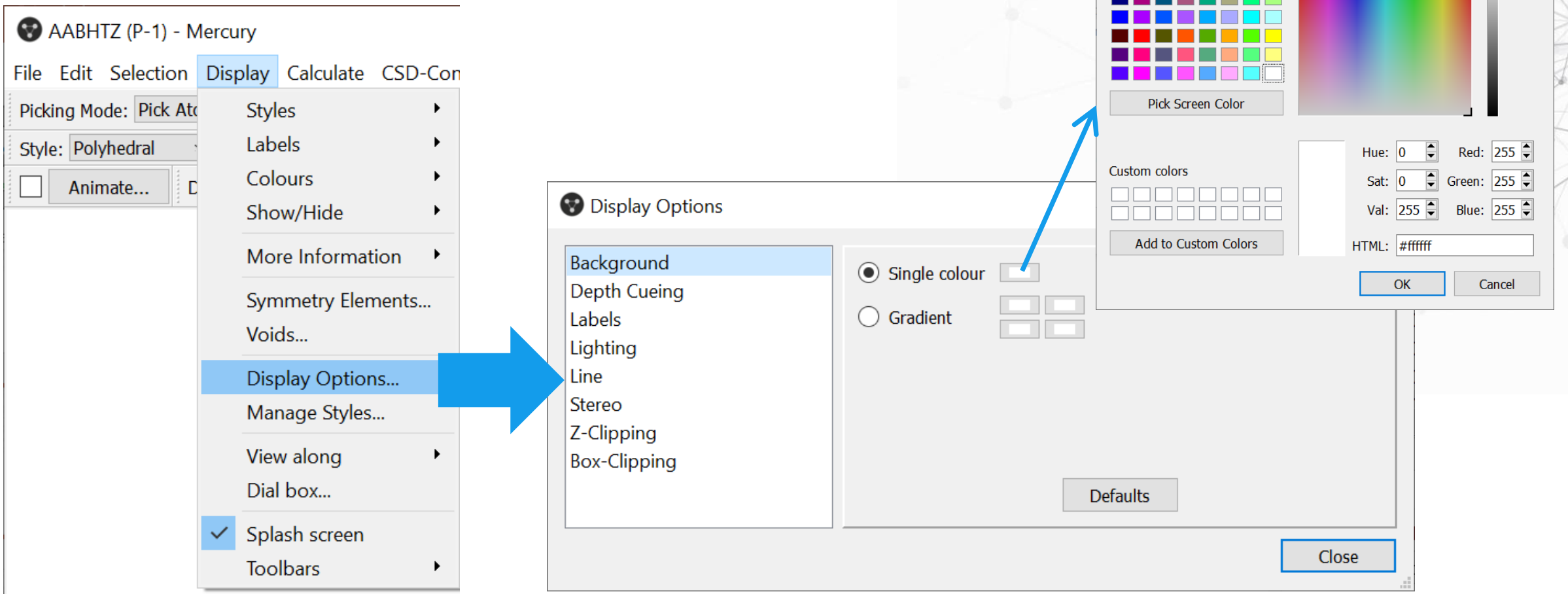
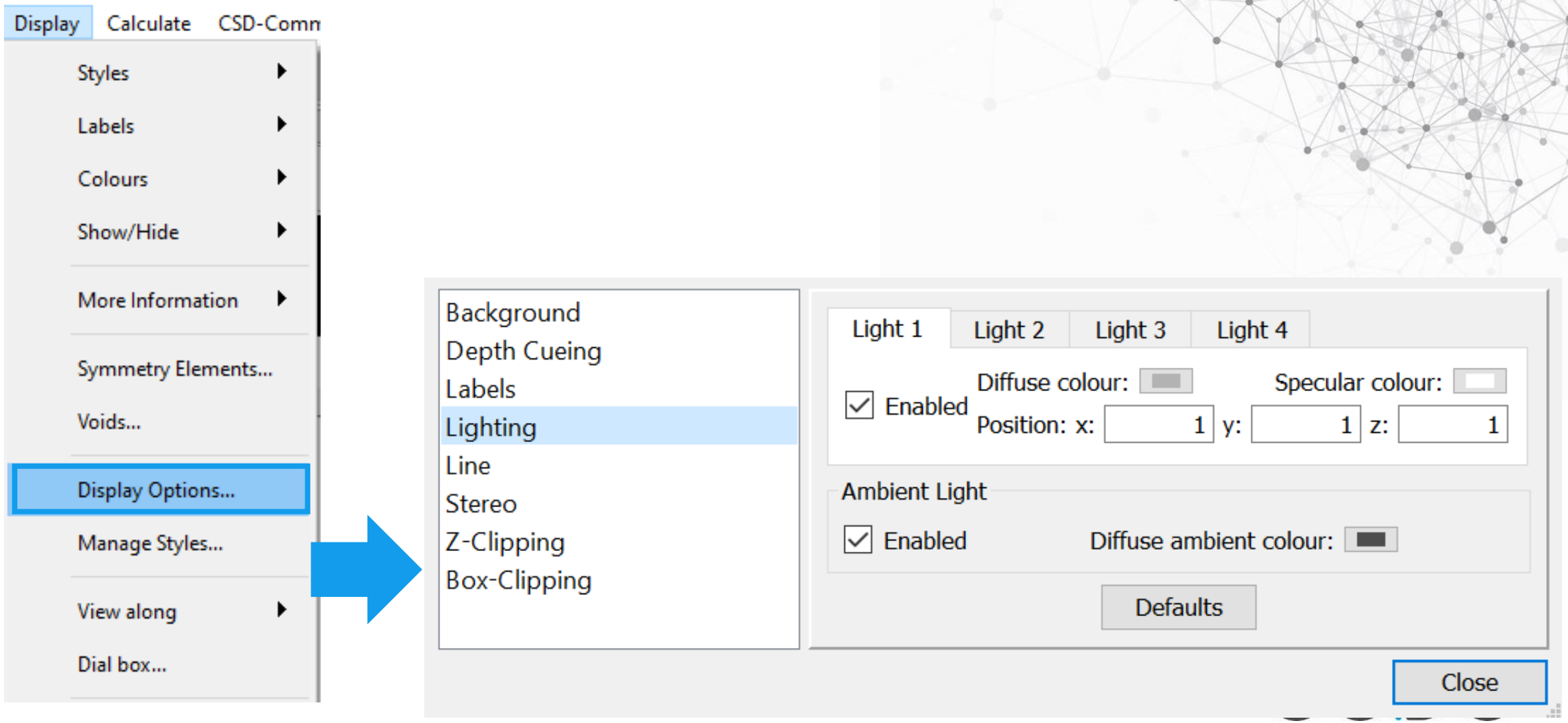
Changing background colour

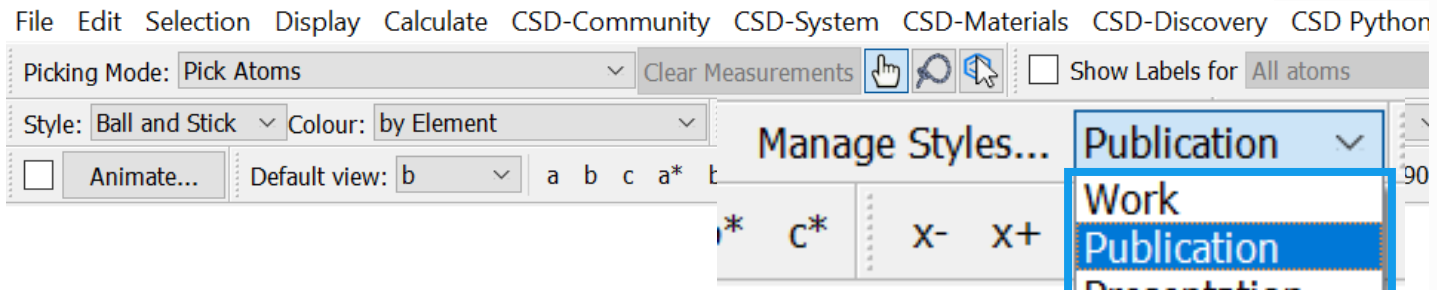


More advanced display options



Manage styles

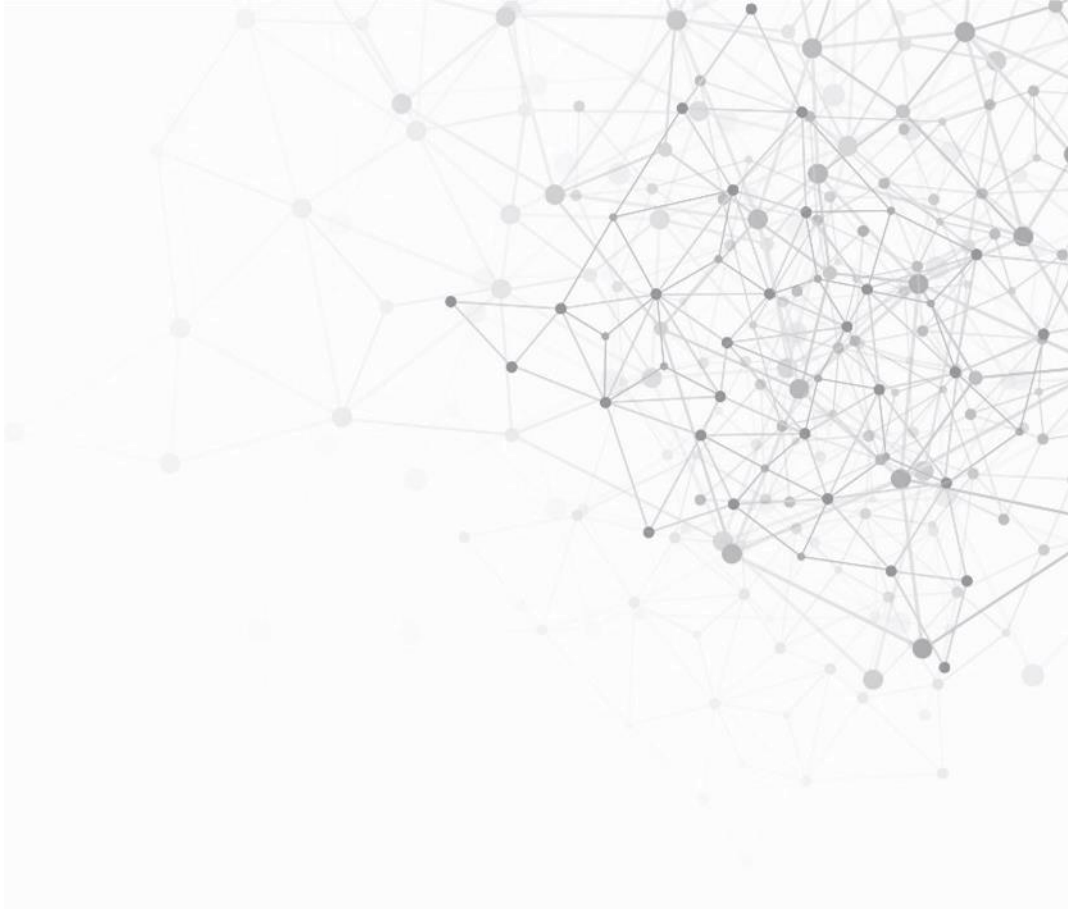
- Pre-saved combinations of settings (styles, styles options, colours, background colour, …)



personalised options

pre-saved options

Display packing



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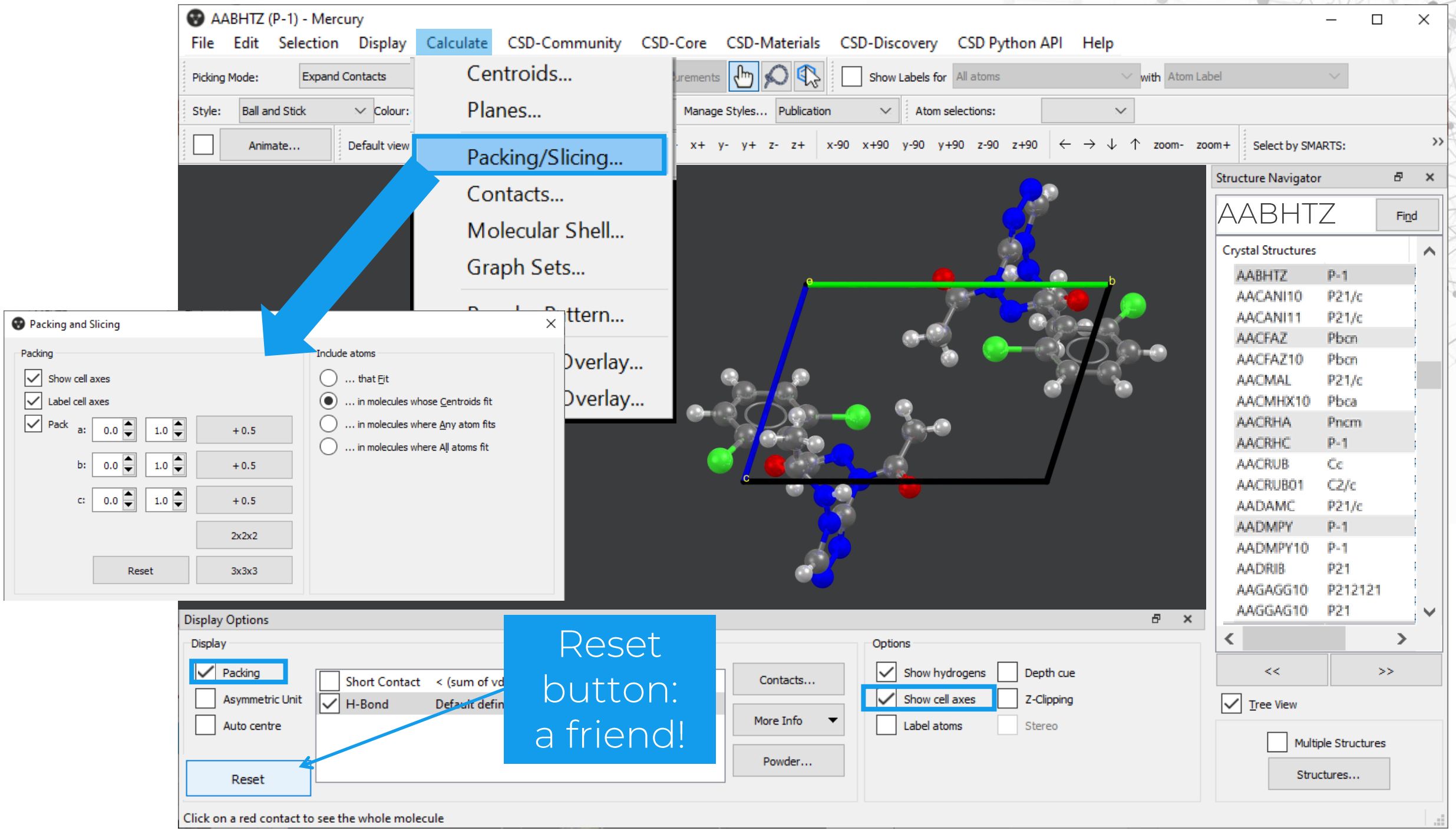
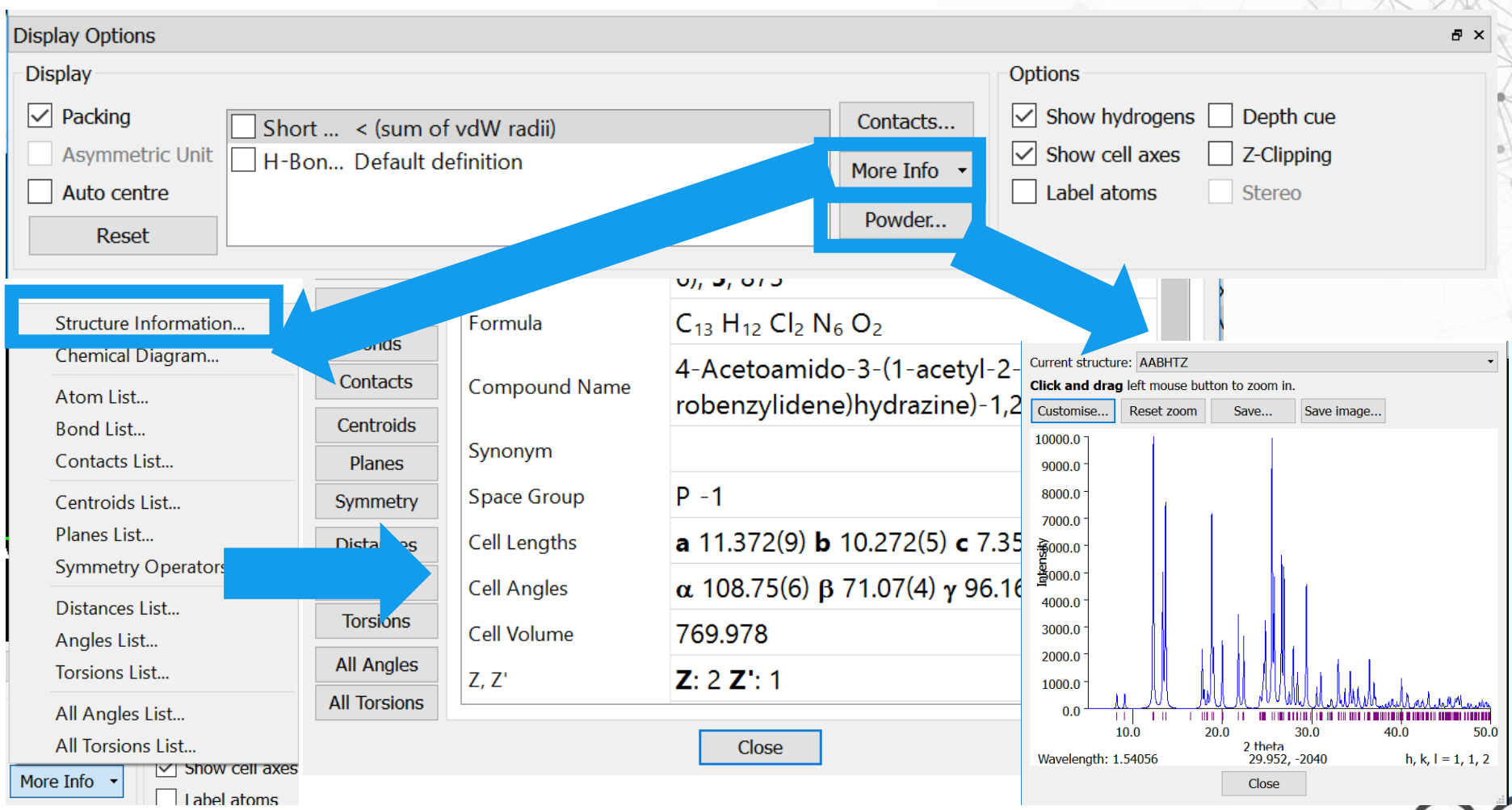
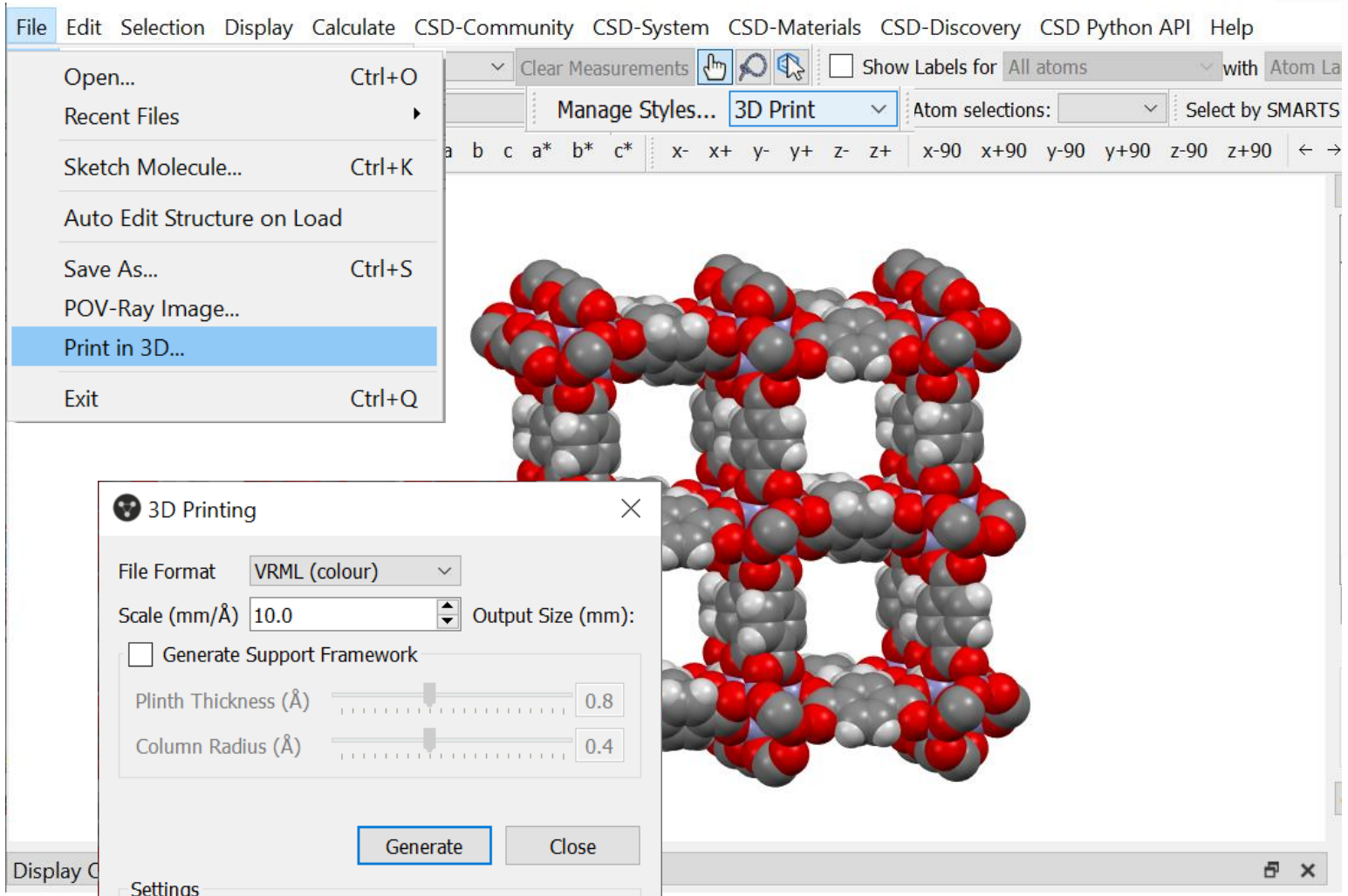

AABHTZ (P-1) - Mercury
File Edit Selection Display Calculate CSD-Community CSD-Core CSD-Materials CSD-Discovery CSD Python API Help
Centroids...
Planes...
Packing/Slicing...
Contacts...
Molecular Shell...
Graph Sets...
Overlay...
Overlay...
Packing and Slicing
Packing
Show cell axes
Label cell axes
Pack
Include atoms
... that Fit
... in molecules whose Centroids fit
... in molecules where Any atom fits
... in molecules where All atoms fit
+0.5
2x2x2
3x3x3
Reset
Structure Navigator
AABHTZ
Find
Crystal Structures
Display Options
Display
Packing
Asymmetric Unit
Auto centre
Short Contact
H-Bond
Contacts...
More Info
Powder...
Options
Show hydrogens
Depth cue
Show cell axes
Z-Clipping
Label atoms
Stereo
Tree View
Multiple Structures
Structures...
Reset button: a friend!
Click on a red contact to see the whole molecule

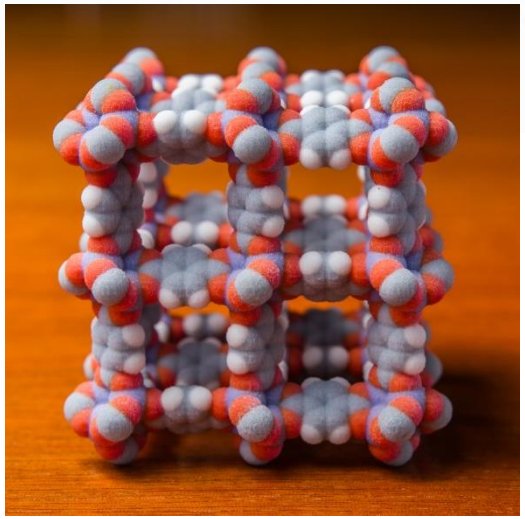
Other display options



3D printing



Simple interface to set up file production + 3D print style



P. A. Wood, A. A. Sarjeant, et al., *CrystEngComm*, 2017, **19**, 690-698

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High-resolution images

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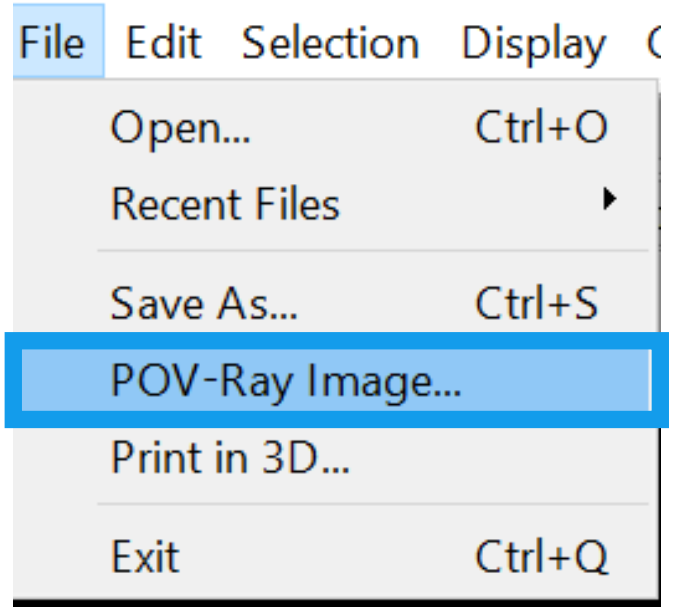
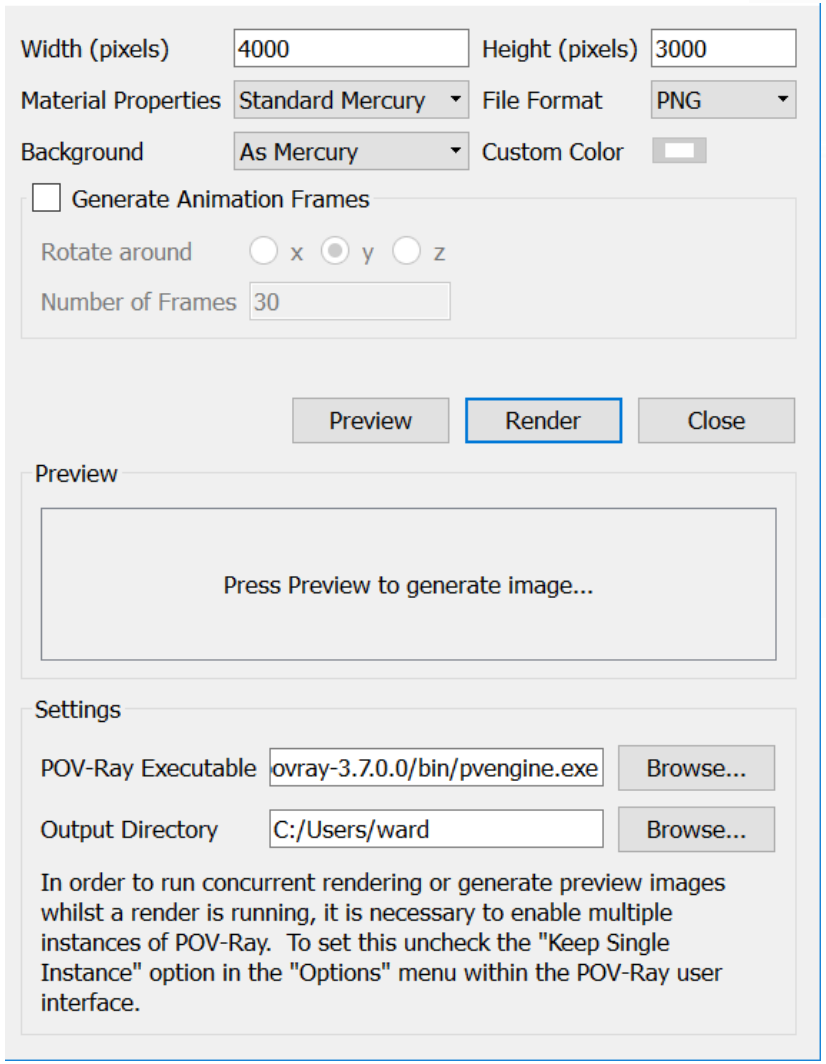
Generating high quality images





File > POV-Ray Image

Change Resolution

- Width = 4000
- Height = 3000

Change ‘Material Properties’ to ‘Metallic’

Set ‘Background’ to ‘Transparent’

Press ‘Preview’

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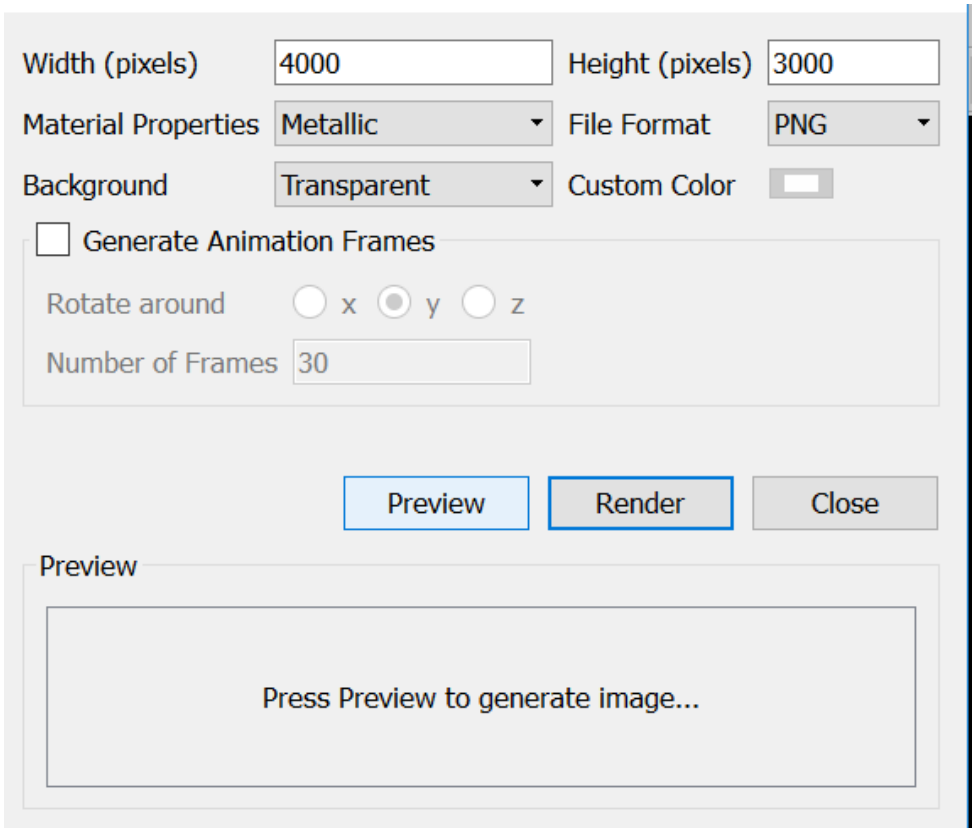
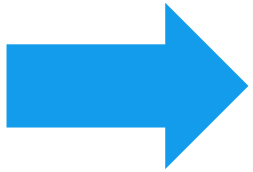
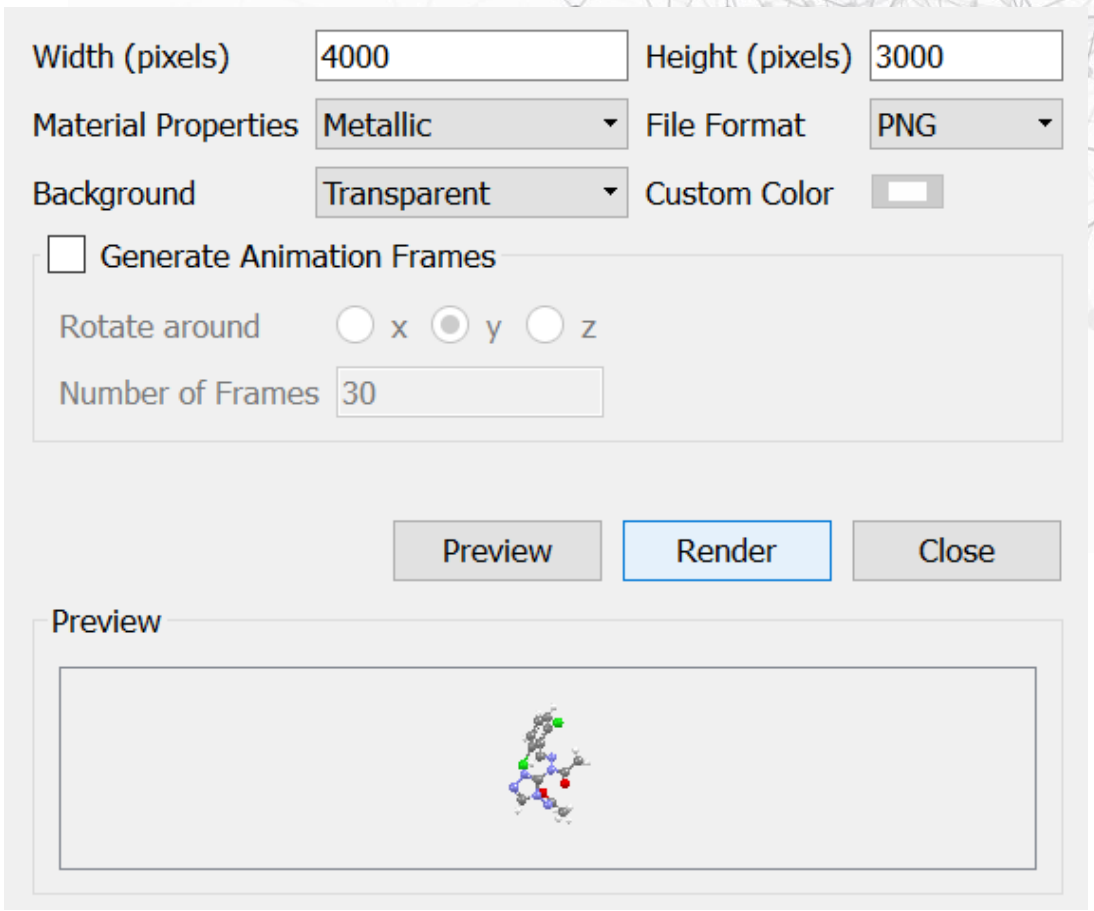
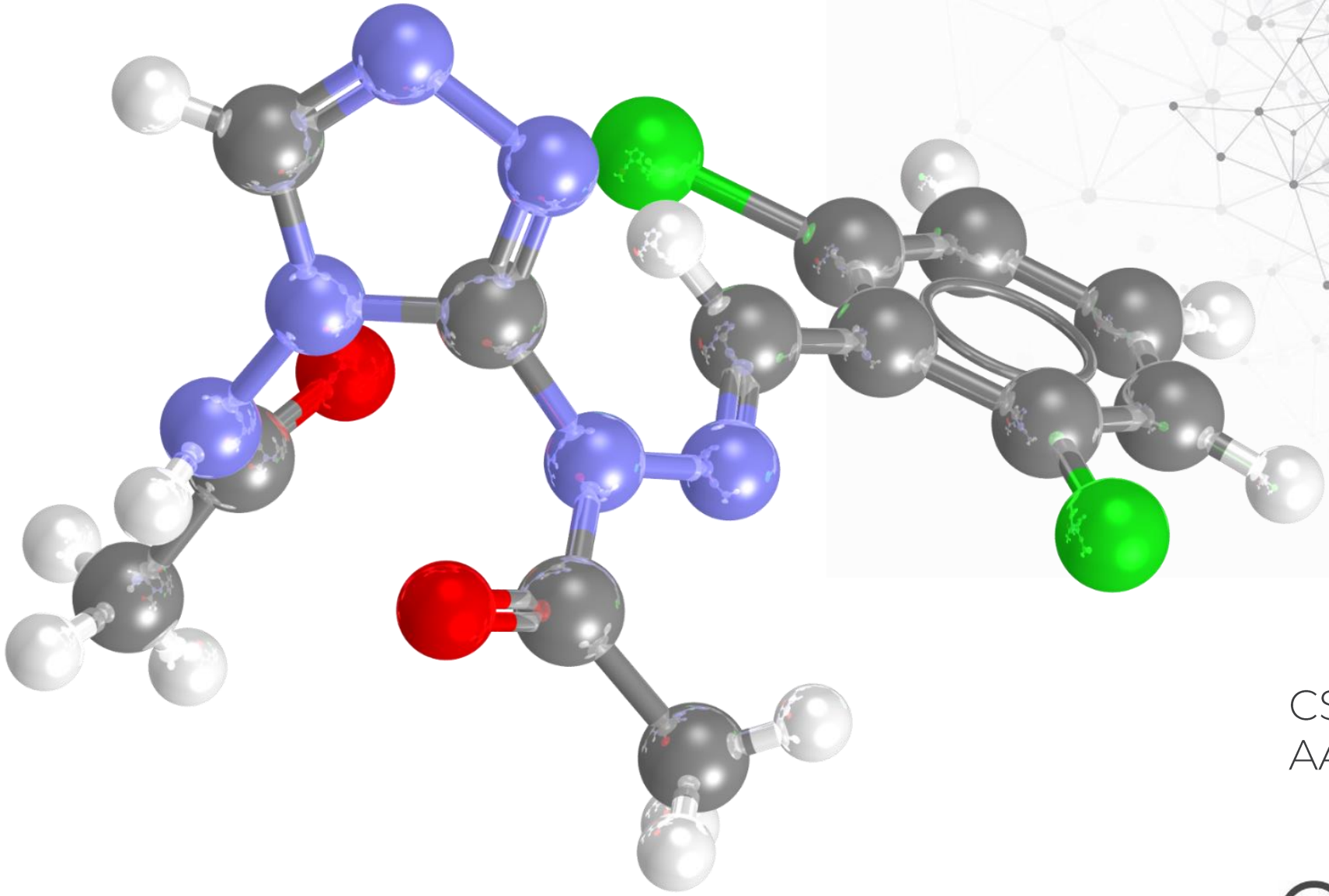
Previewing and rendering an image









CSD Refcode:
AABHTZ

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A few more tips & tricks

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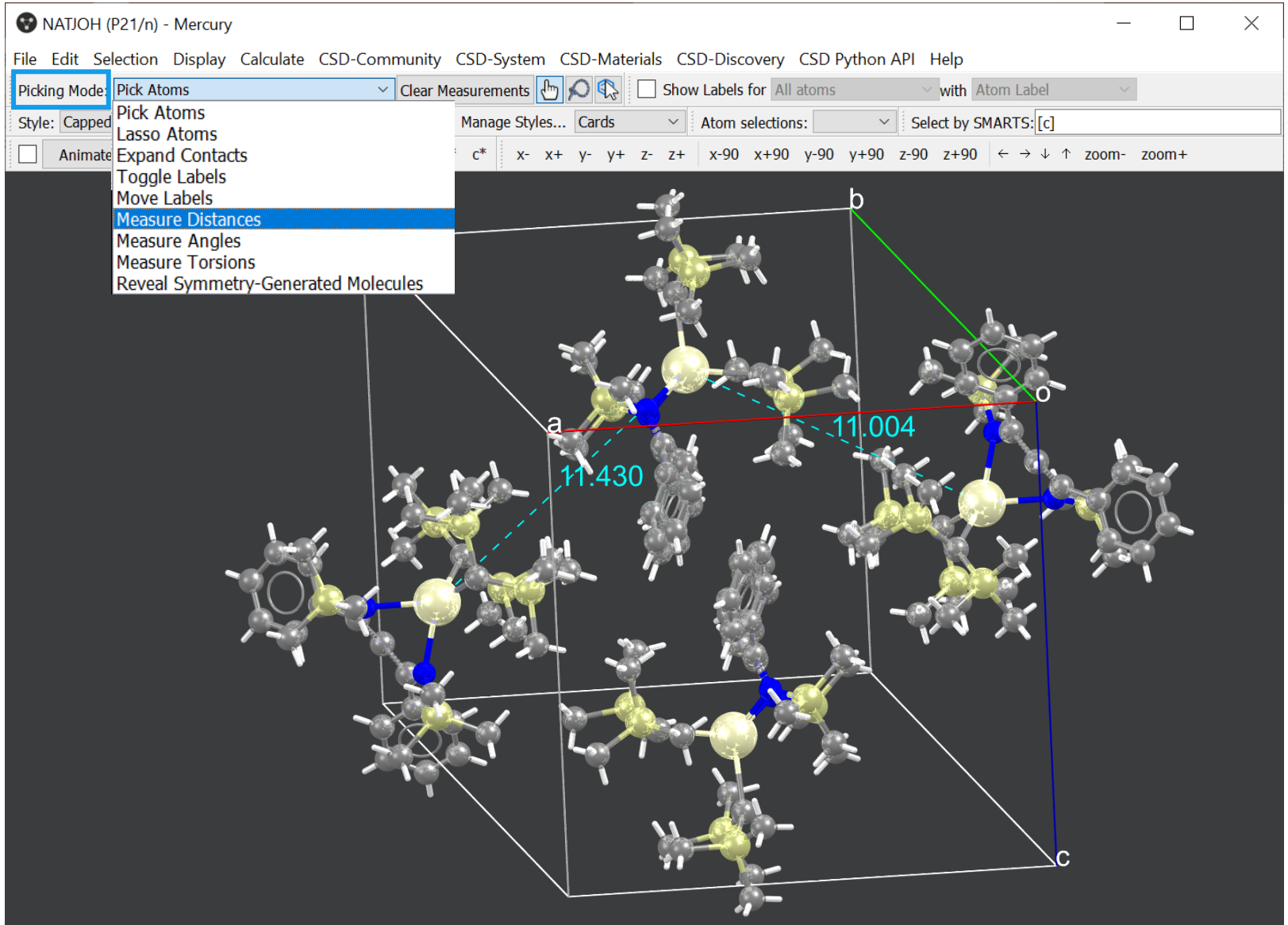
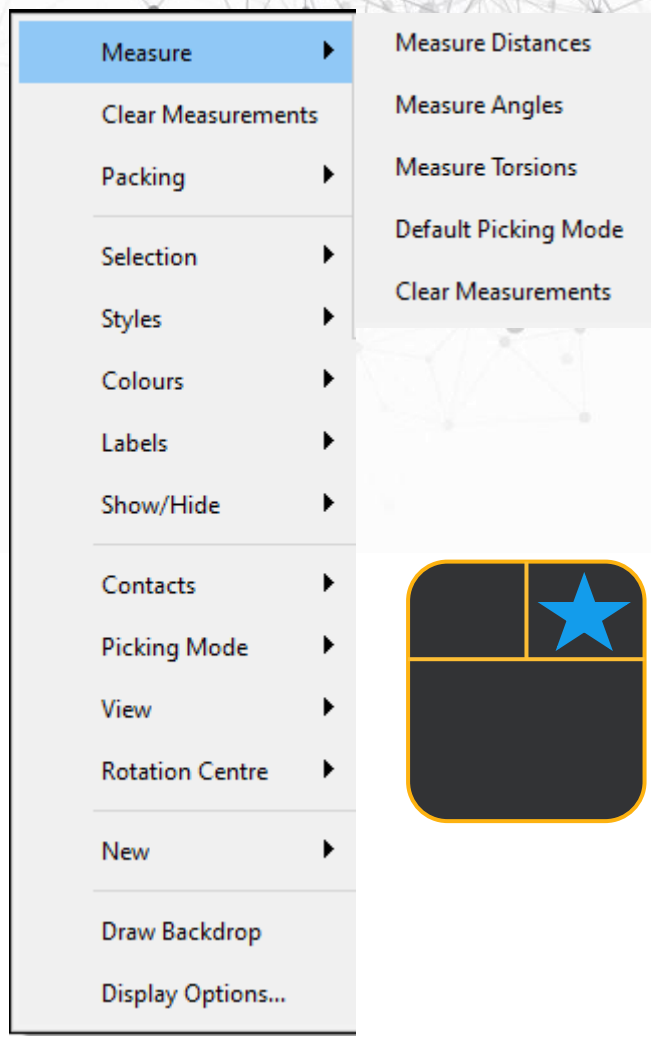
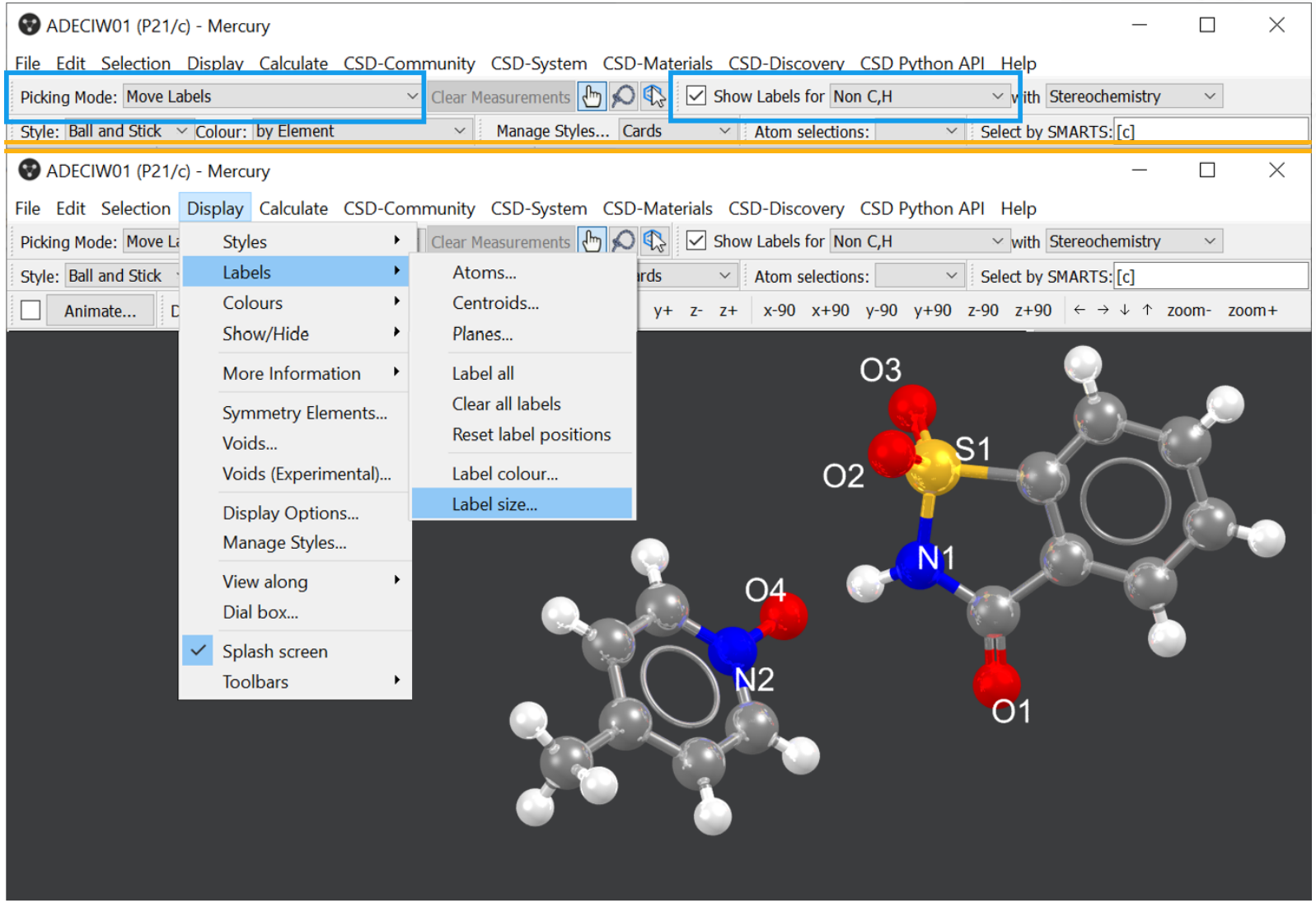
Measure distances

CSD Refcode:
NATJOH





Adding, moving and sizing labels



CSD Refcode: ADECIW01

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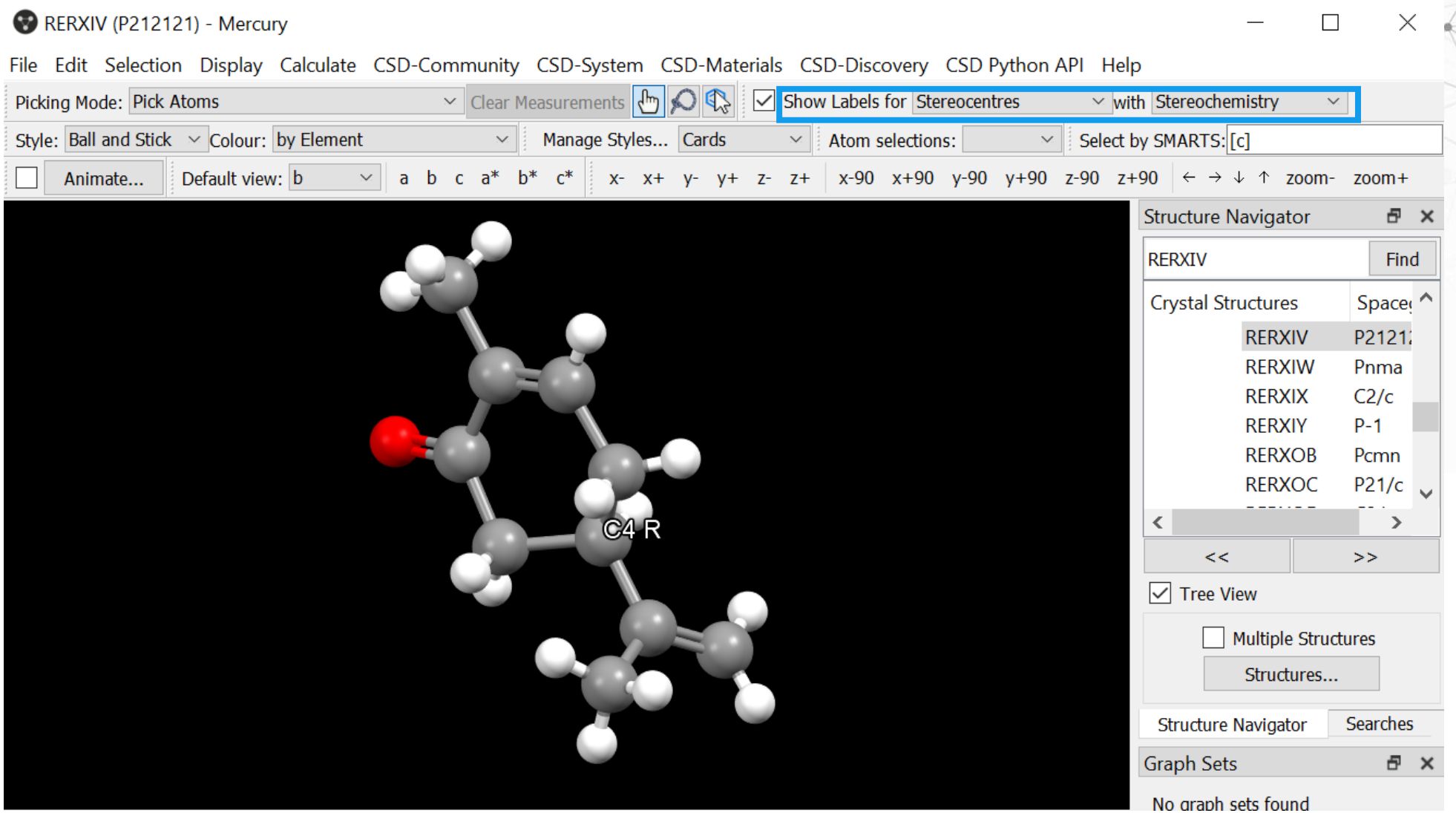
Labelling chiral molecules



CSD Refcode: RERXIV

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