

# Welcome to CSDU



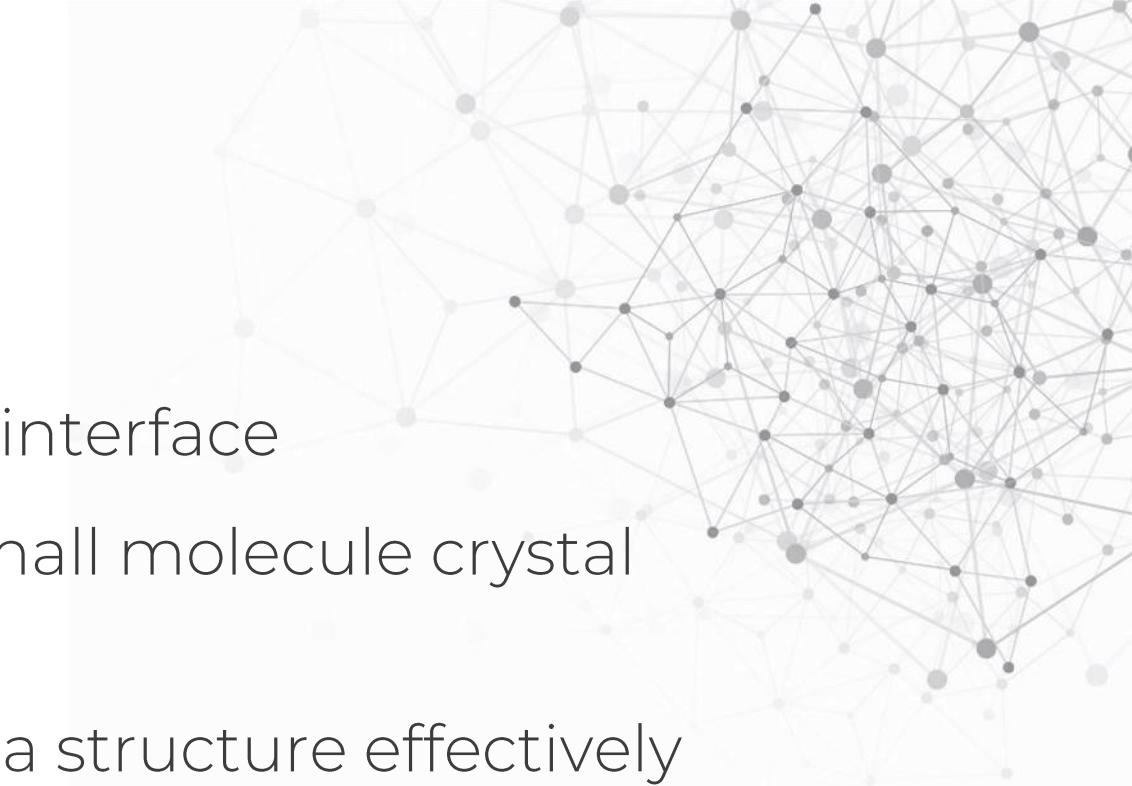
# Visualisation 101



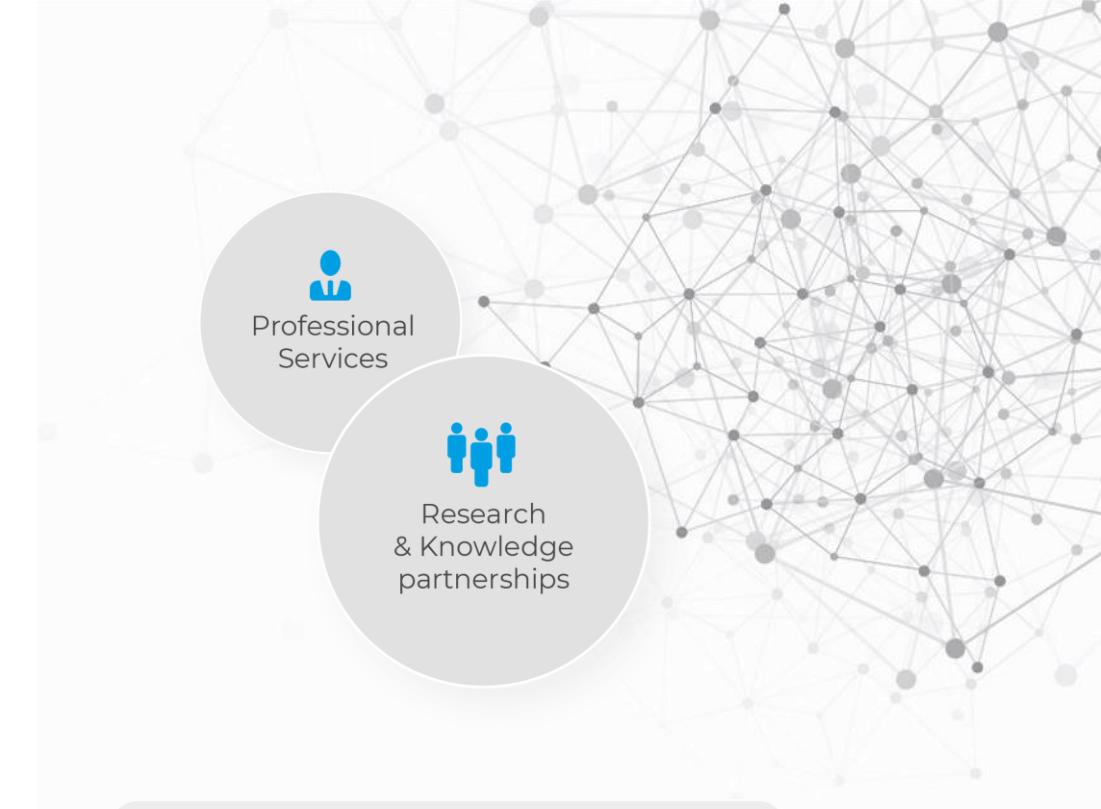
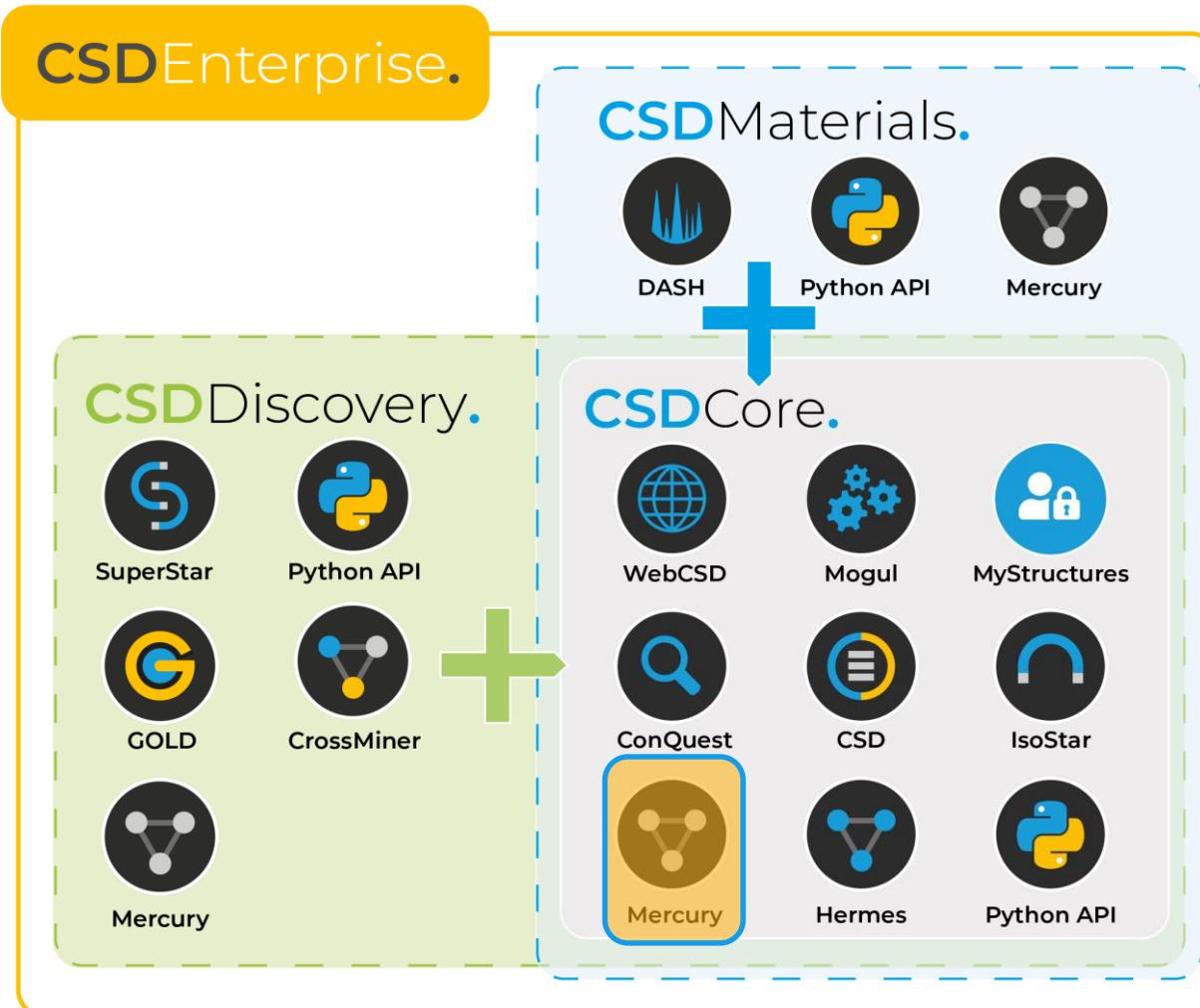
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# Learning outcomes

- 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



# The CSD Portfolio



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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



# The basics of navigating Mercury



# Mercury Overview



AABHTZ (P-1) - Mercury

File Edit Selection Display Calculate CSD-Community CSD-Core CSD-Materials CSD-Discovery CSD Python API Help

Picking Mode: Pick Atoms Clear Measurements Show Labels for All atoms with Atom Label

Style: Ball and Stick Colour: by Element or Suppression Manage Styles... Work Atom selections:

Animate... Default view: b a b c a\* b\* c\* x- x+ y- y+ z- z+ x-90 x+90 y-90 y+90 z-90 z+90 ← → ↓ ↑ zoom- zoom+ Select by SMARTS: [c]

Structure Navigator

**AABHTZ**

Crystal Structures	Spacegroup
AABHTZ	P-1
AACANI10	P21/c
AACANI11	P21/c
AACFAZ	Pbcn
AACFAZ10	Pbcn
AACMAL	P21/c
AACMHX10	Pbca
AACRHA	Pncm
AACRHC	P-1
AACRUB	Cc
AACRUB01	C2/c
AADAMC	P21/c
AADMKY	P-1
AADMKY10	P-1
AADRIB	P21
AAGAGG10	P212121
AAGGAG10	P21

Display Options

Display

Packing  
 Asymmetric Unit  
 Auto centre

Short Contact < (sum of vdW radii)  
 H-Bond Default definition

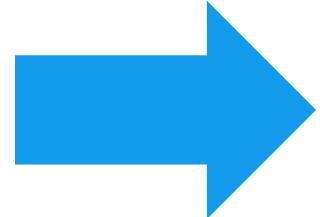
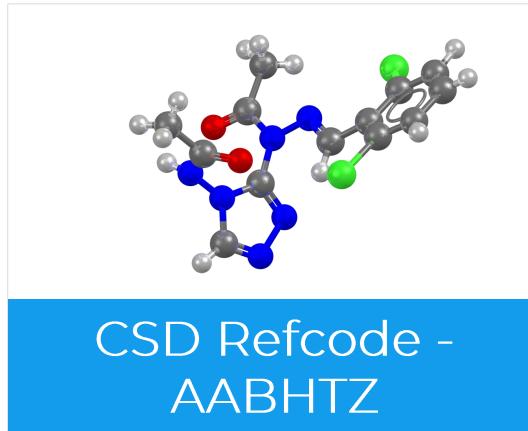
Options

Show hydrogens  
 Show cell axes  
 Label atoms

Depth cue  
 Z-Clipping  
 Stereo

Press the left mouse button and move the mouse to rotate the structure

# CSD Refcodes reminder



Structure Navigator

Type in a refcode  Find

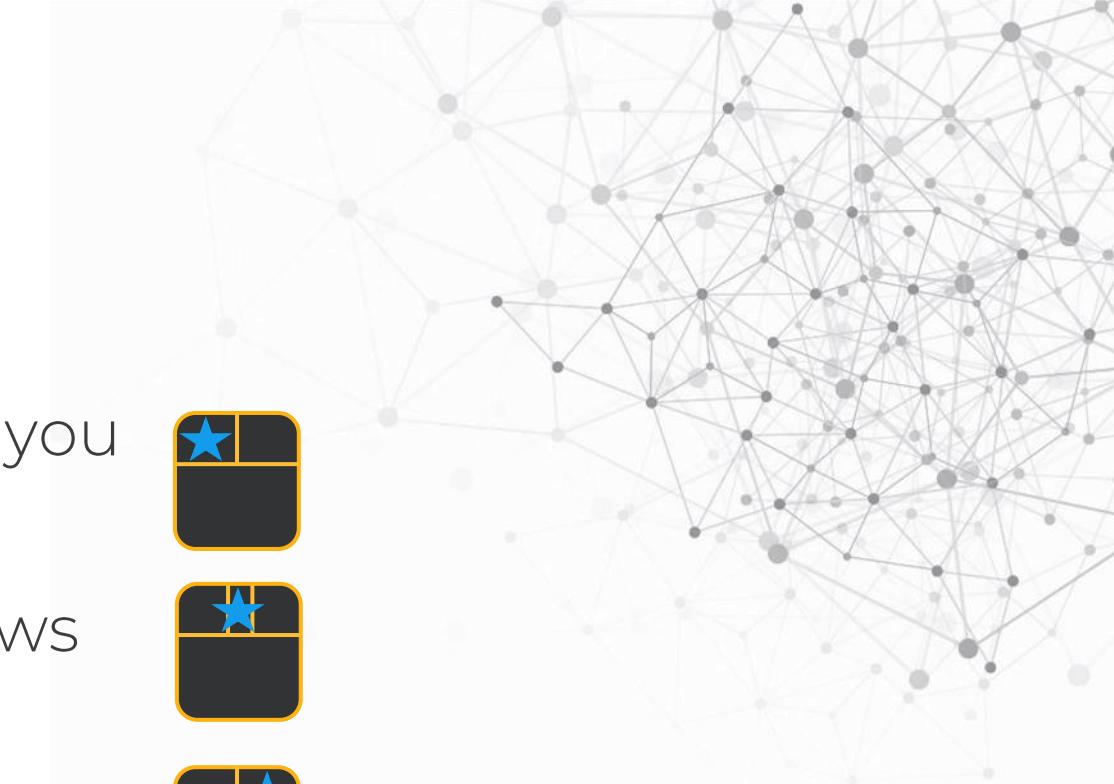
Crystal Structures	Spacegroup
AABHTZ	P-1

## 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

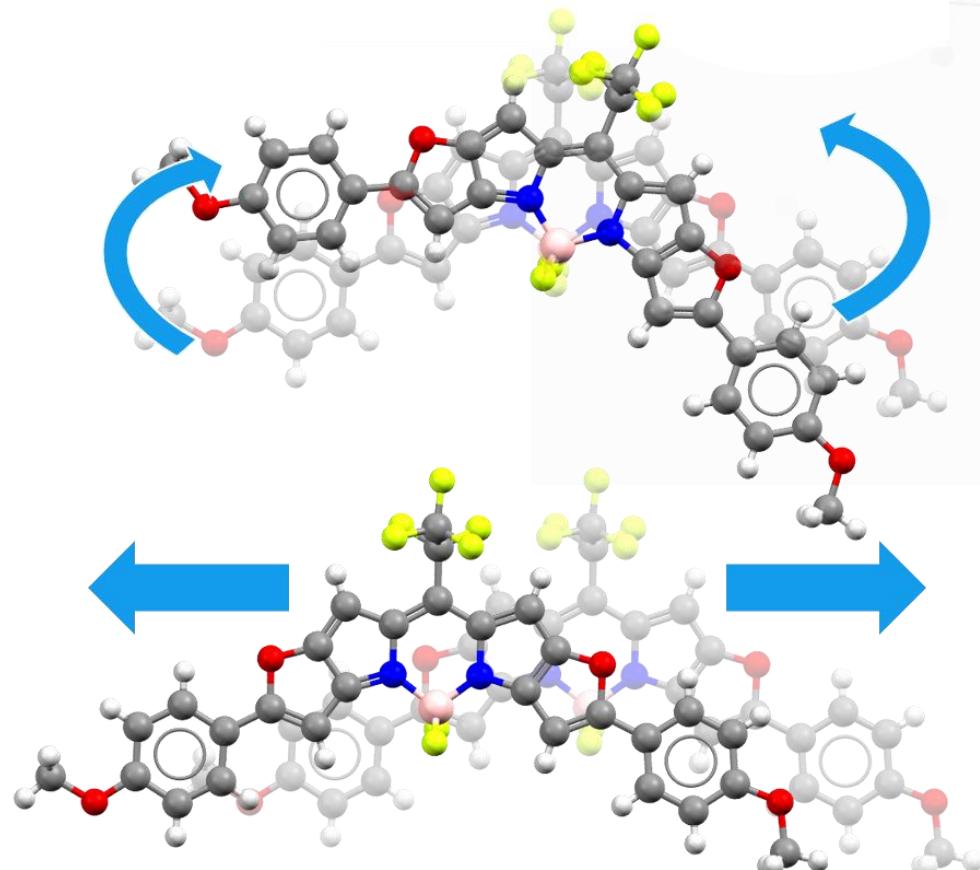
# The basics

- 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



# The basics

With the keyboard:

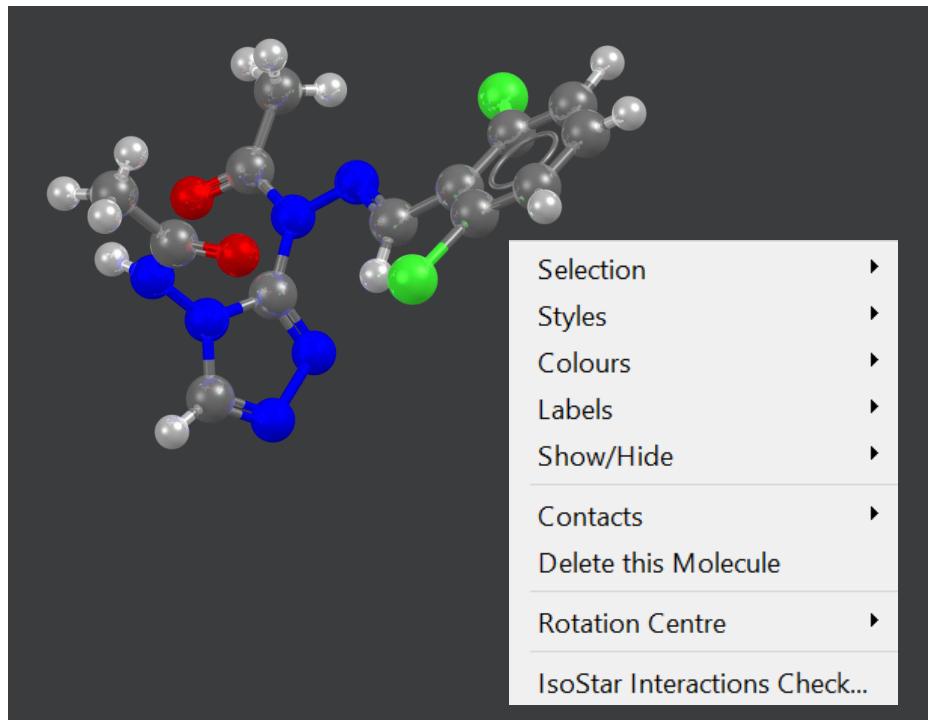


CSD Refcode: GIMXUY

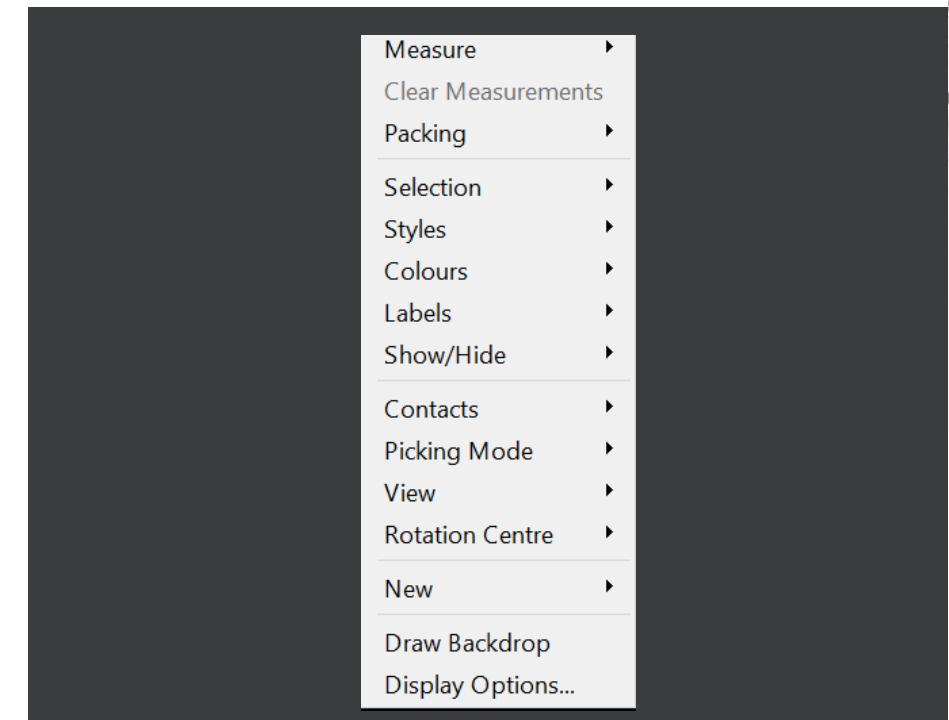
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# Right mouse click

Near a molecule



Away from a molecule



Picking Mode: Pick Atom

Styles

Labels

Colours

Show/Hide

More Information

Symmetry Elements...

Voids...

Display Options...

Manage Styles...

View along

Dial box...

Splash screen

Toolbars

Measurements

 Show Labels for All atoms with Atom Label

Manage Styles... Work Atom selections:

b\*

c\*

x-

x+

y-

y+

z-

z+

x-90

x+90

y-90

y+90

z-90

z+90

&lt;

&gt;

↓

↑

zoom-

&gt;&gt; Select by SMARTS: &gt;&gt;

Display Options

Graph Sets

Intermolecular Potentials

Searches

Post Search Options

Structure Navigator

Picking Toolbar

Labels

Display

Style Manager Toolbar

Atom Selection Toolbar

Select by SMARTS

Animation Toolbar

Crystal Orientation Operations

Alignment and Orientation Operations

Structure Navigator

Type in a refcode

Find

Crystal Structures	Spacegroup
AABHTZ	P-1
AACANI10	P21/c
AACANI11	P21/c
AACFAZ	Pbcn
AACFAZ10	Pbcn
AACMAL	P21/c
AACMHX10	Pbca
AACRHA	Pncm
AACRHC	P-1
AACRUB	Cc
AACRUB01	C2/c
AADAMC	P21/c
AADMPPY	P-1
AADMPPY10	P-1
AADRIB	P21
AAGAGG10	P212121
AAGGAG10	P21
AALCFE	P21/c
AALPRO	P21/c
AAMAND	P212121
AAMTCO	P-1
AAMTCO10	P-1
AAMTXP	P21/n
AANHOX	Pna21
AANHOX01	Pna21
AANOPM	P21
AAPUNI	P21/a

&lt;&lt; &gt;&gt;

Tree View

 Multiple Structures

Structures...

Display Options

Display

&lt; (sum of vdW radii)

Default definition

Contacts...

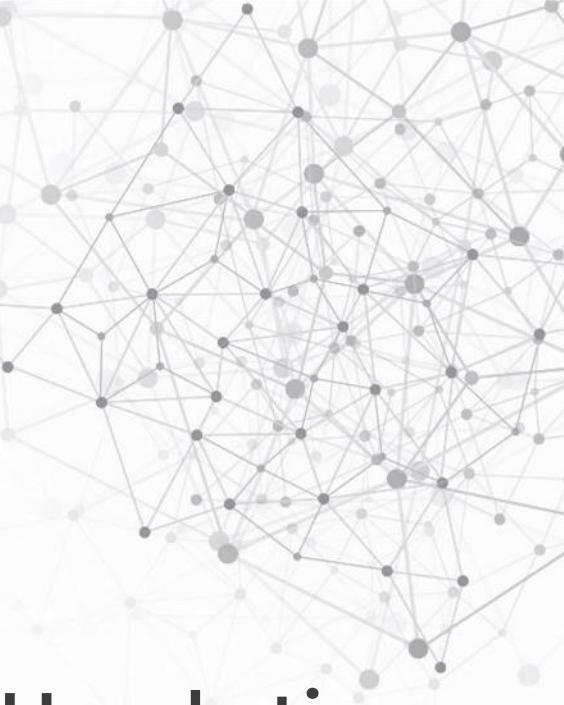
More Info

Powder...

Options

 Show hydrogens Depth cue Show cell axes Z-Clipping Label atoms Stereo

Reset



## Handy tips:

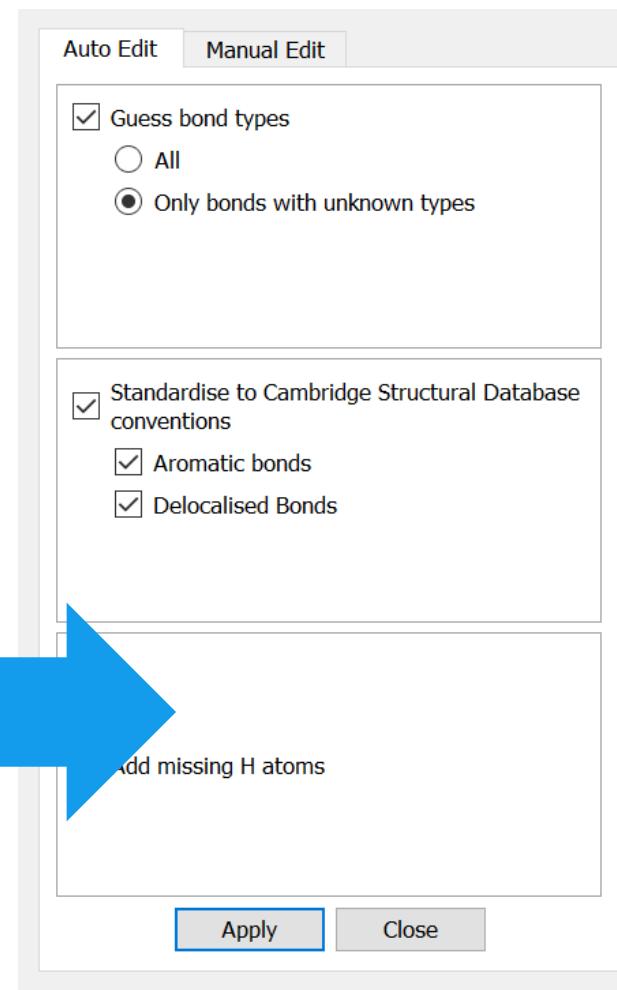
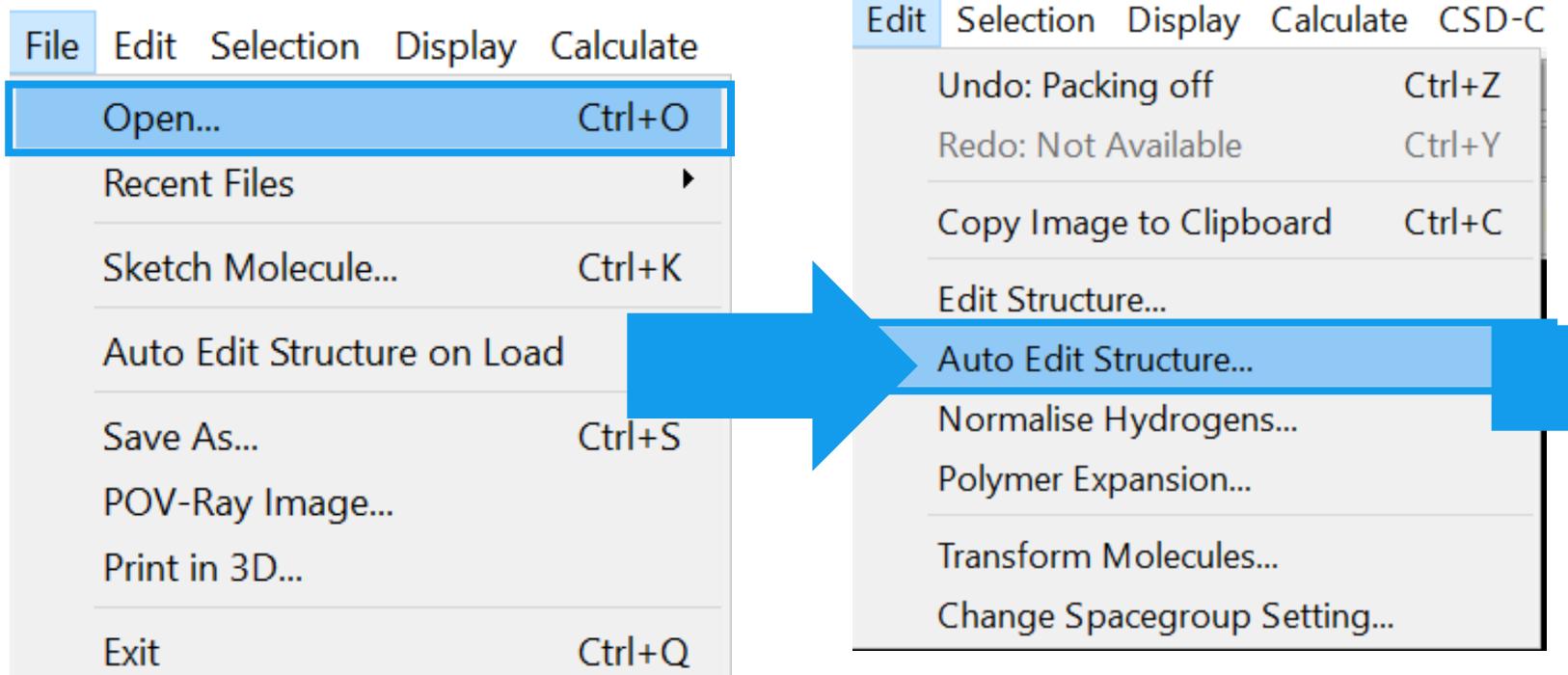
- Recovering Toolbars
- Resetting view

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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

AABHTZ (P-1) - Mercury



# Styles and colours options



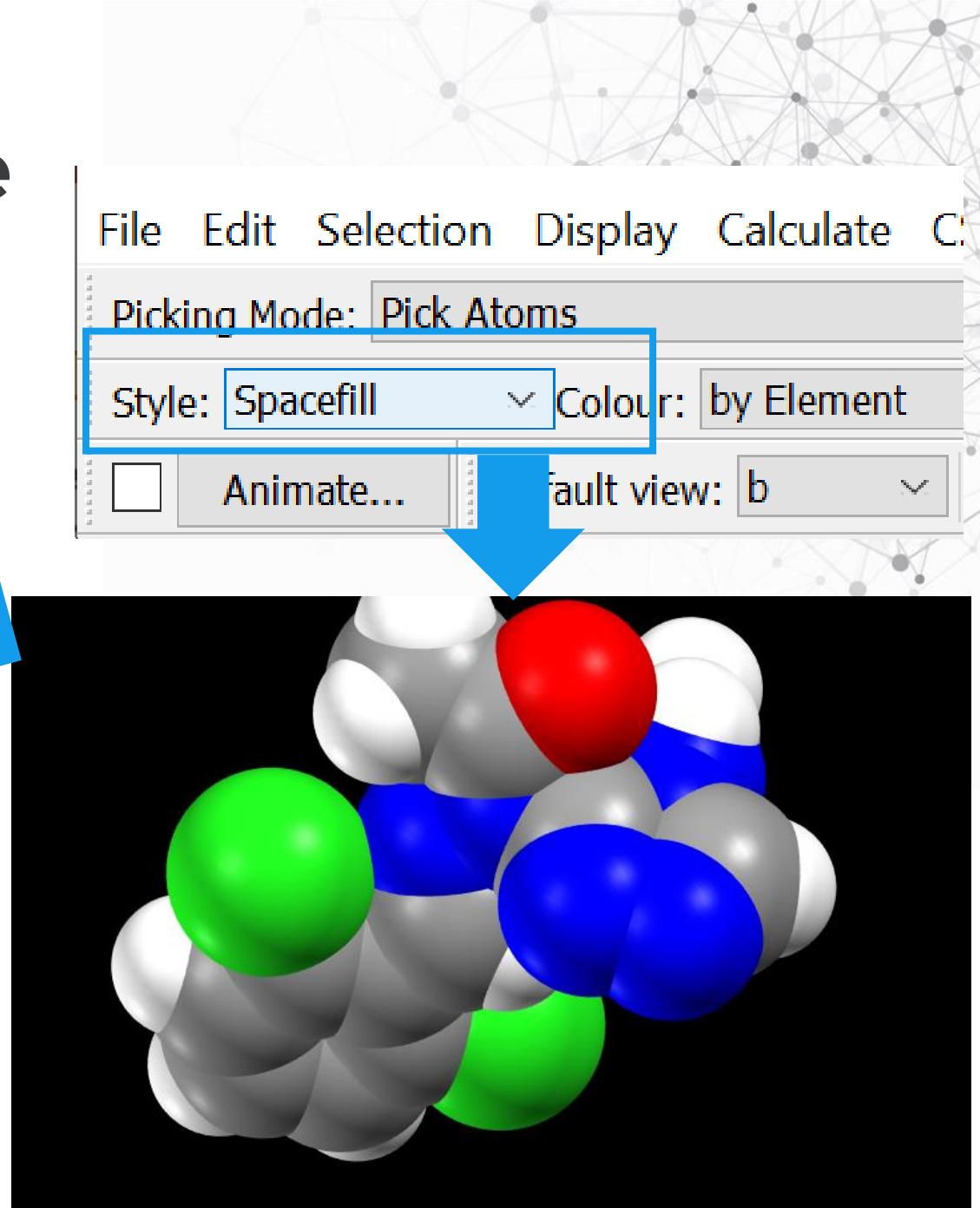
# Changing display - Style

Display Calculate CSD-Community CSD-System CSD-M

- Styles ▾
- Labels ▾
- Colours ▾
- Show/Hide ▾
- More Information ▾
- Symmetry Elements...
- Voids...
- Display Options...
- Manage Styles...
- View along ▾
- Dial box...
- Splash screen ▾
- Toolbars ▾

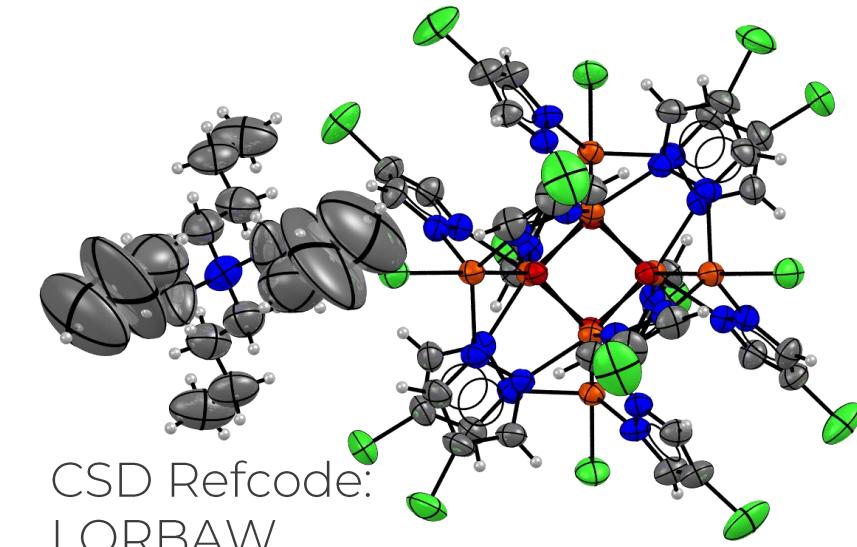
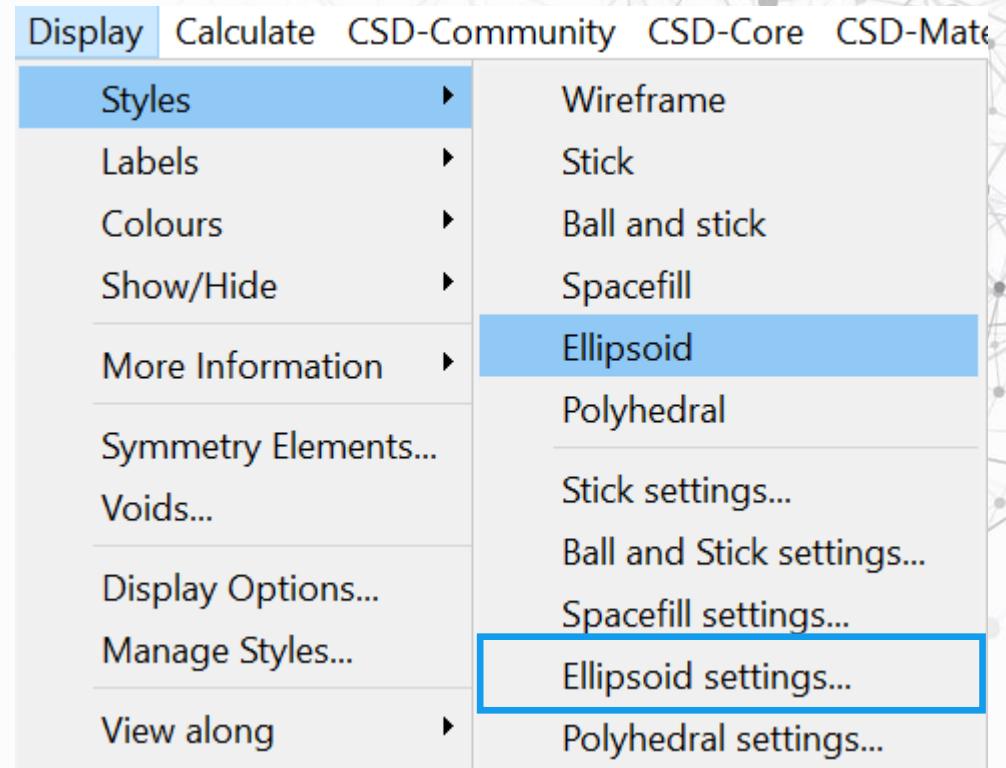
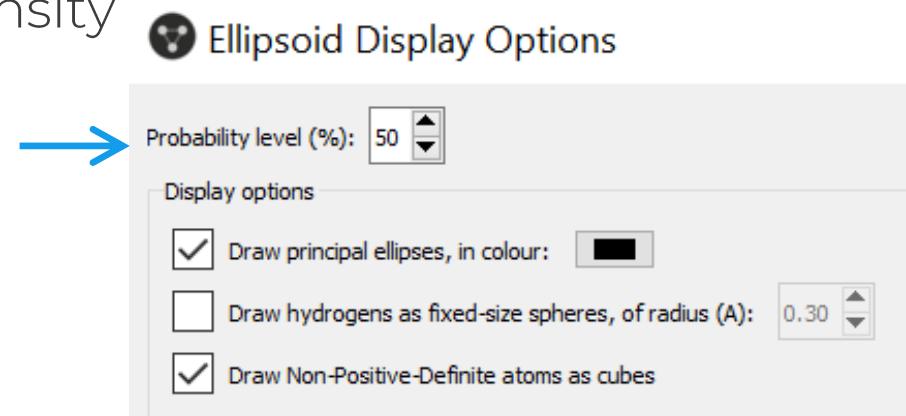
Wireframe  
Stick  
Ball and stick  
**Spacefill**  
Ellipsoid  
Polyhedral

Stick settings...  
Ball and Stick settings...  
Spacefill settings...  
Ellipsoid settings...  
Polyhedral settings...  
Contact settings...  
Measurement settings...  
Selected atoms



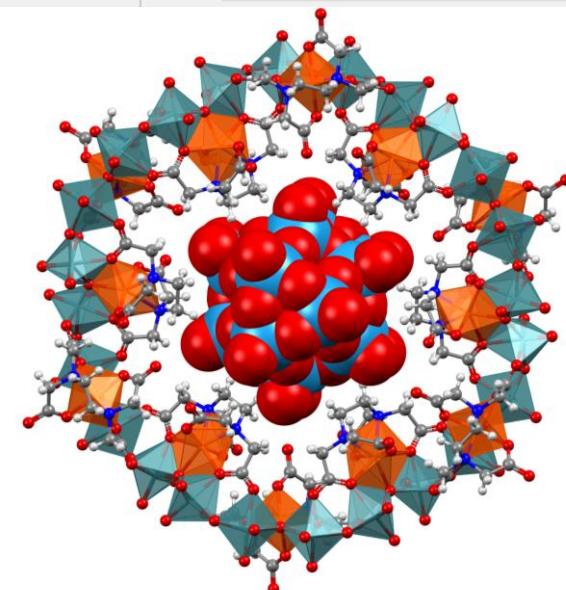
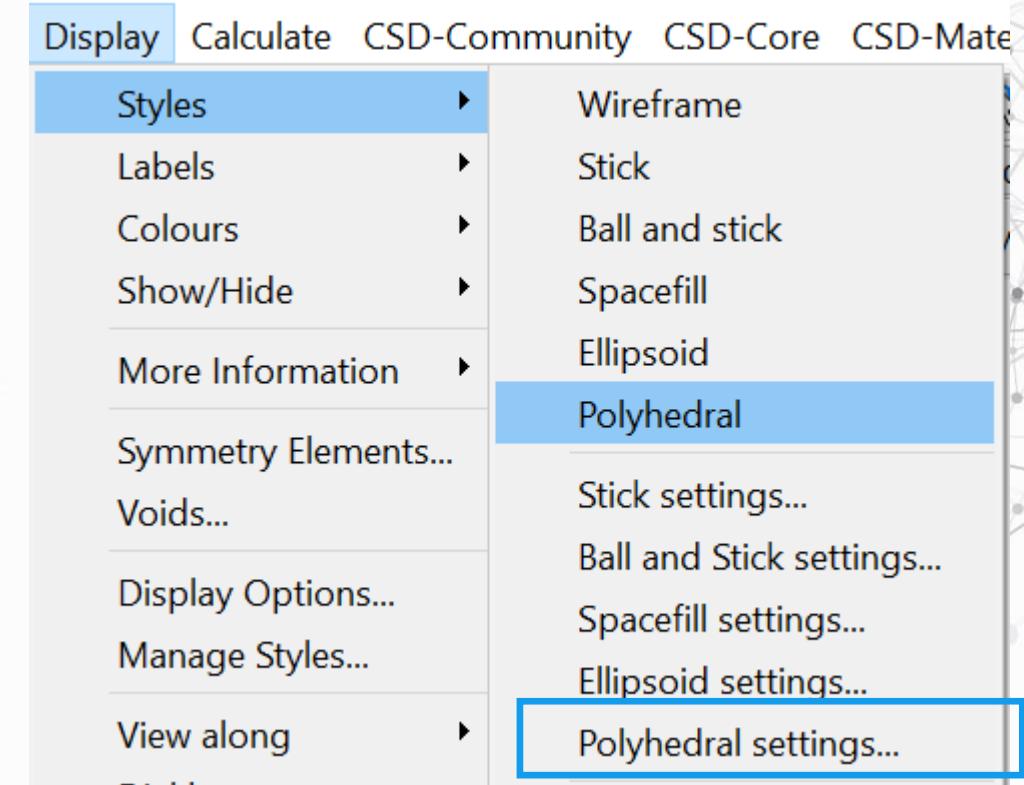
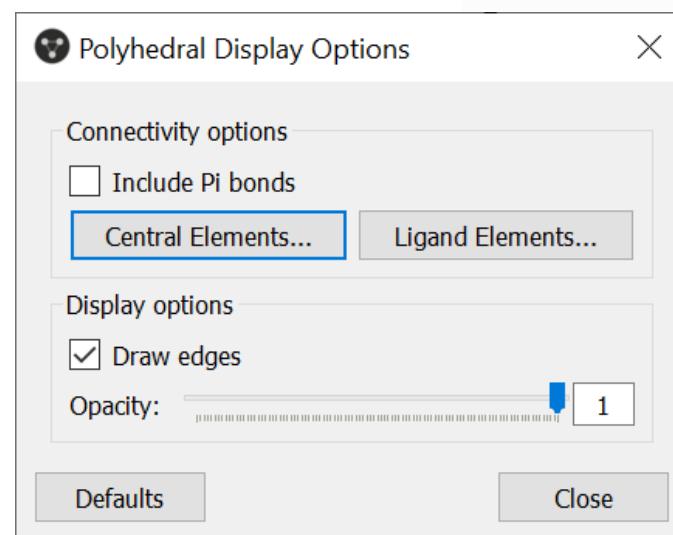
# Thermal ellipsoids

- 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

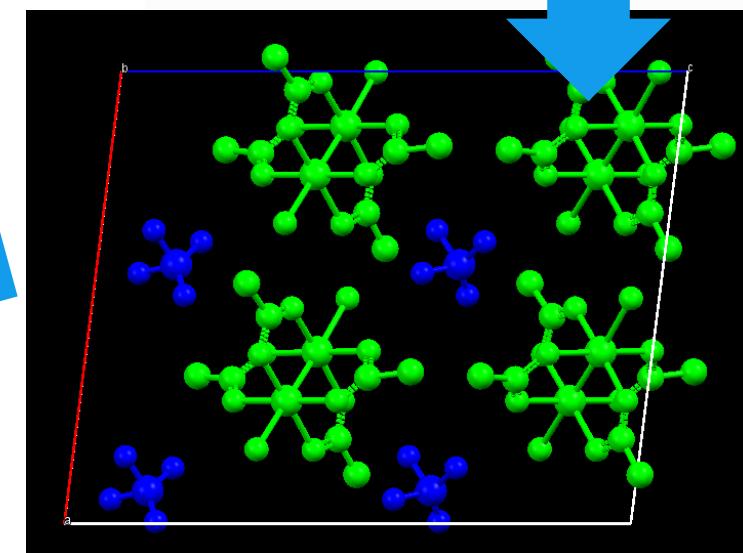
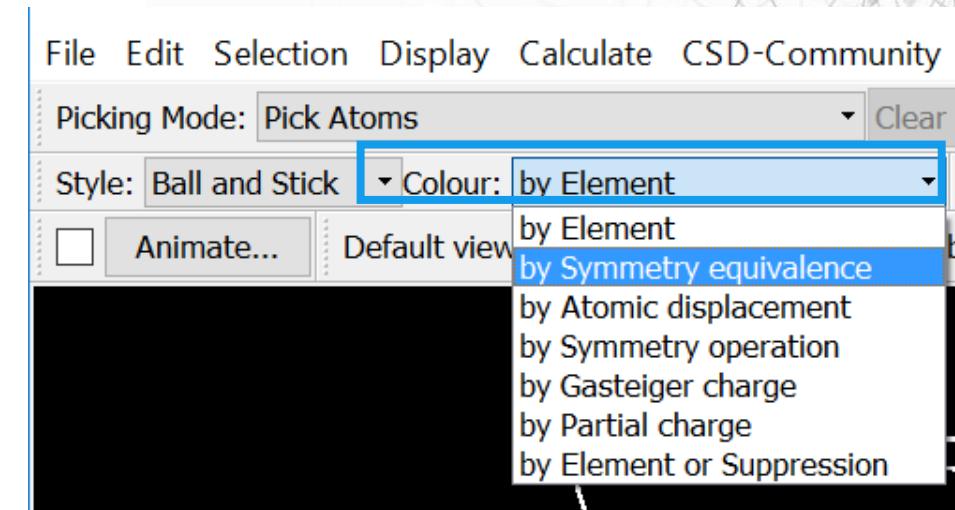
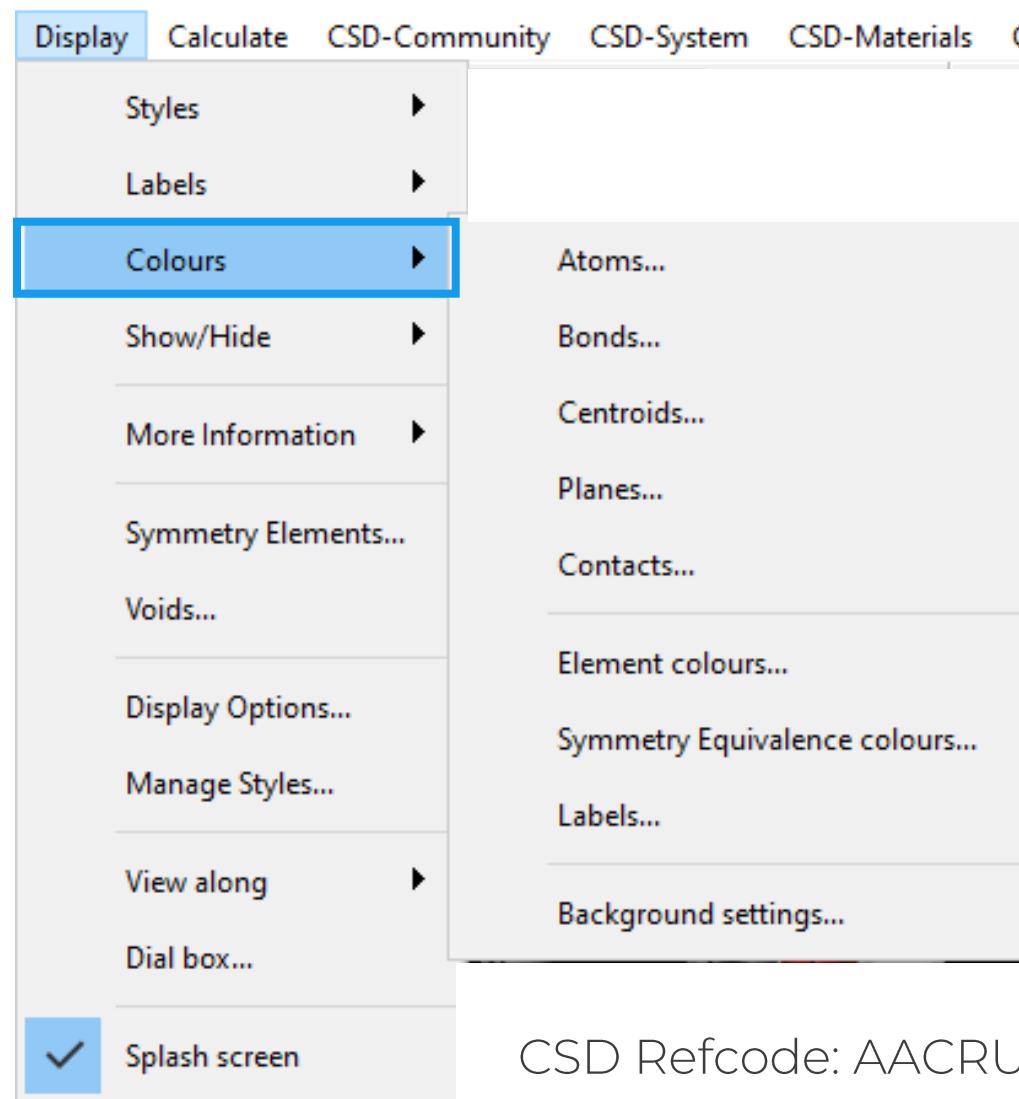


# Polyhedral display

- 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



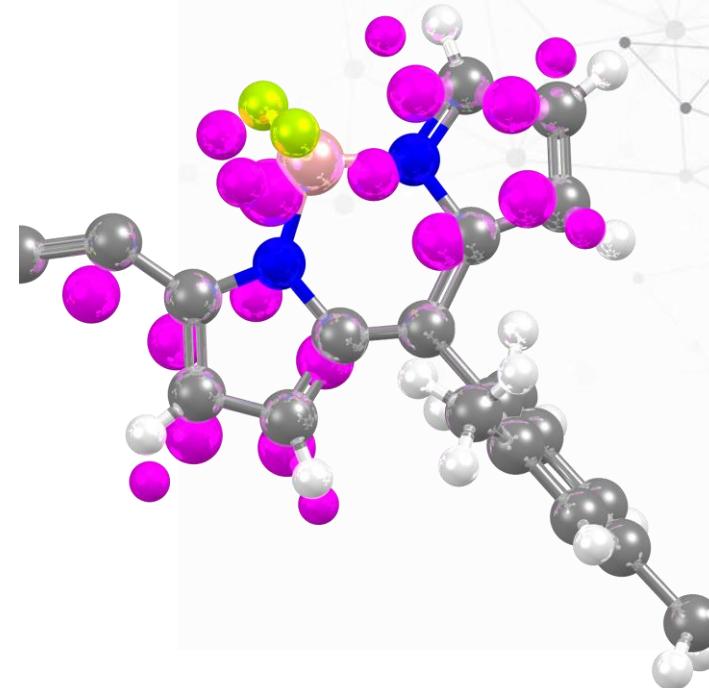
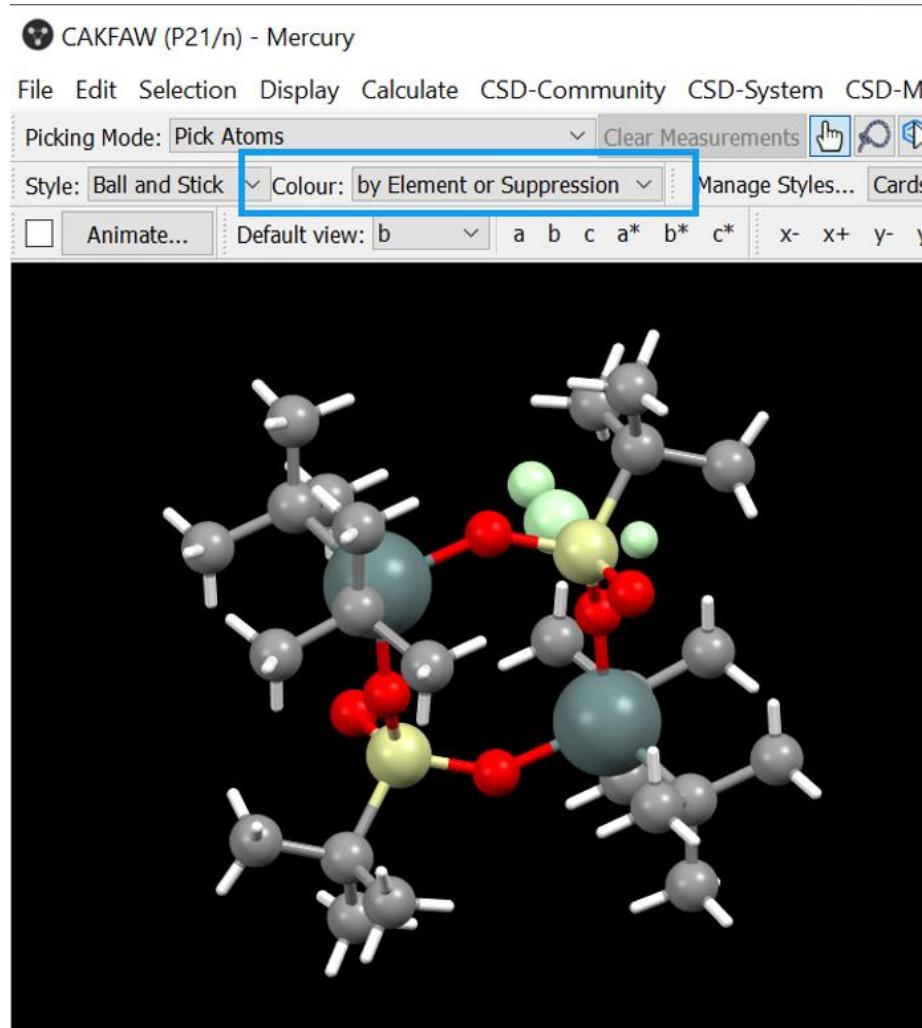
# Changing display - Colours



CSD Refcode: AACRUB

CCDC

# Changing display - Colours

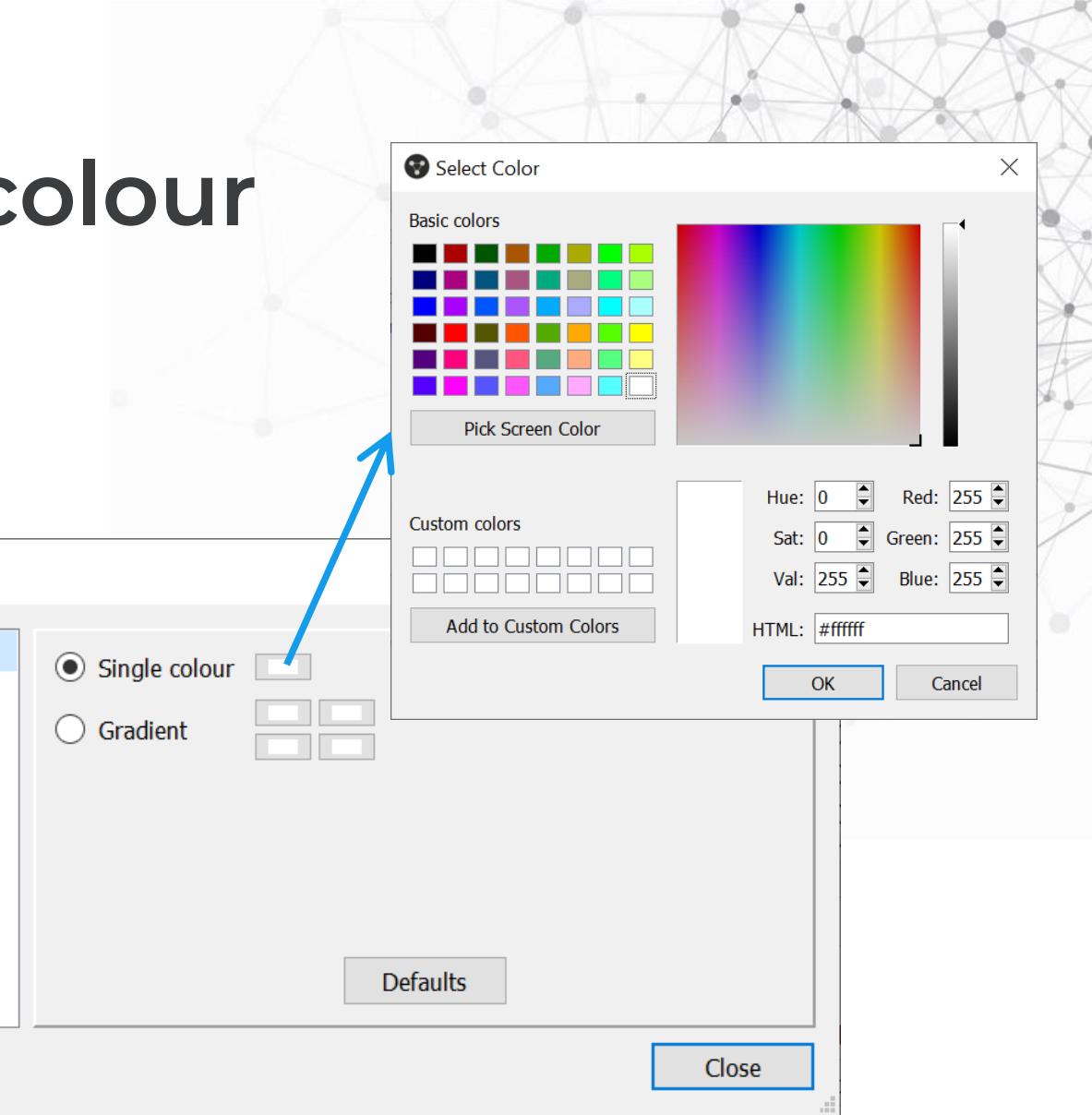
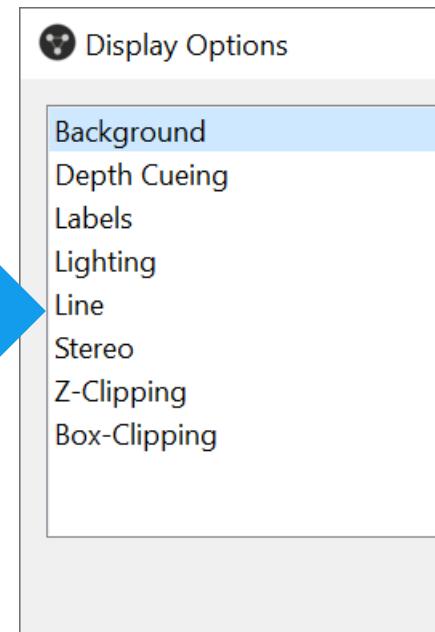
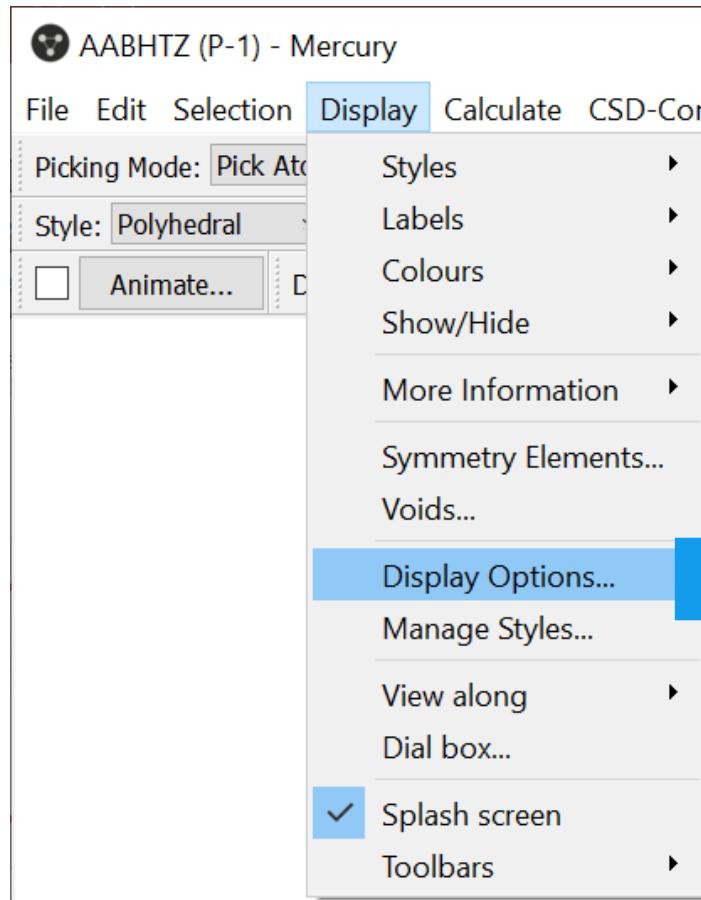


Disordered structures report two sets of atomic coordinates: major and minor sites. In most cases the atoms of the minor site will be suppressed.

CSD Refcodes: CAKFAW and PIYDEI

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# Changing background colour



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# More advanced display options

Display   Calculate   CSD-Comm

- Styles
- Labels
- Colours
- Show/Hide
- More Information
- Symmetry Elements...
- Voids...
- Display Options...**
- Manage Styles...
- View along
- Dial box...

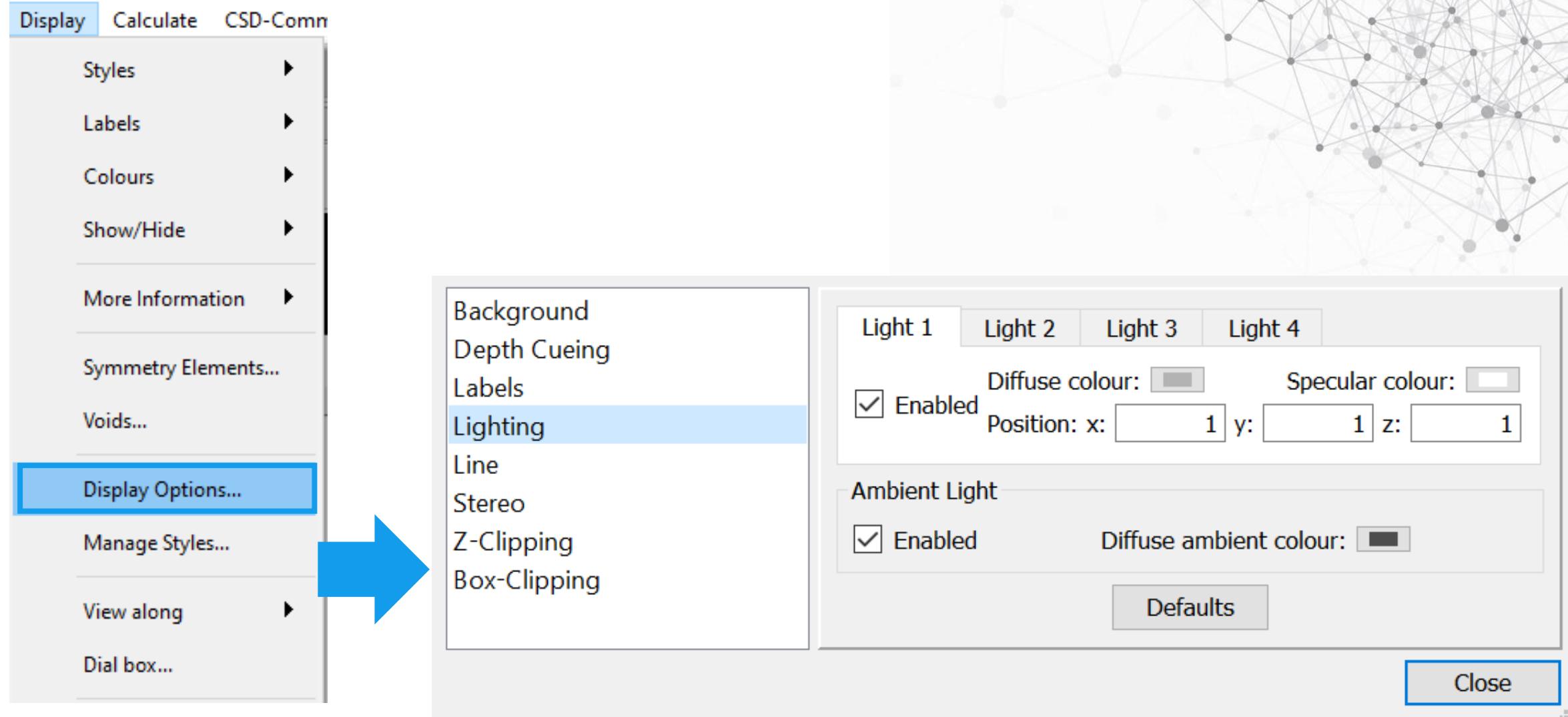
Background  
Depth Cueing  
Labels  
**Lighting**  
Line  
Stereo  
Z-Clipping  
Box-Clipping

**Light 1**   **Light 2**   **Light 3**   **Light 4**

Enabled   Diffuse colour:    Specular colour:   
Position: x:  y:  z:

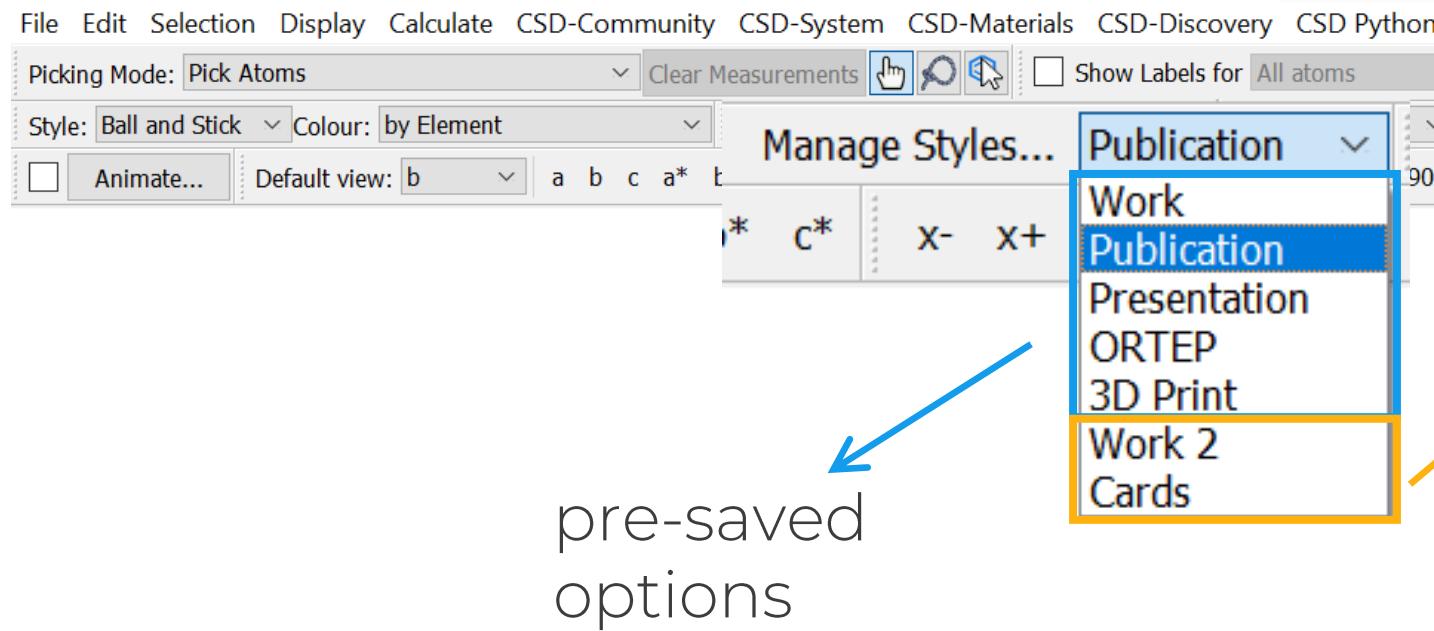
Ambient Light  
 Enabled   Diffuse ambient colour:

Defaults   Close



# Manage styles

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



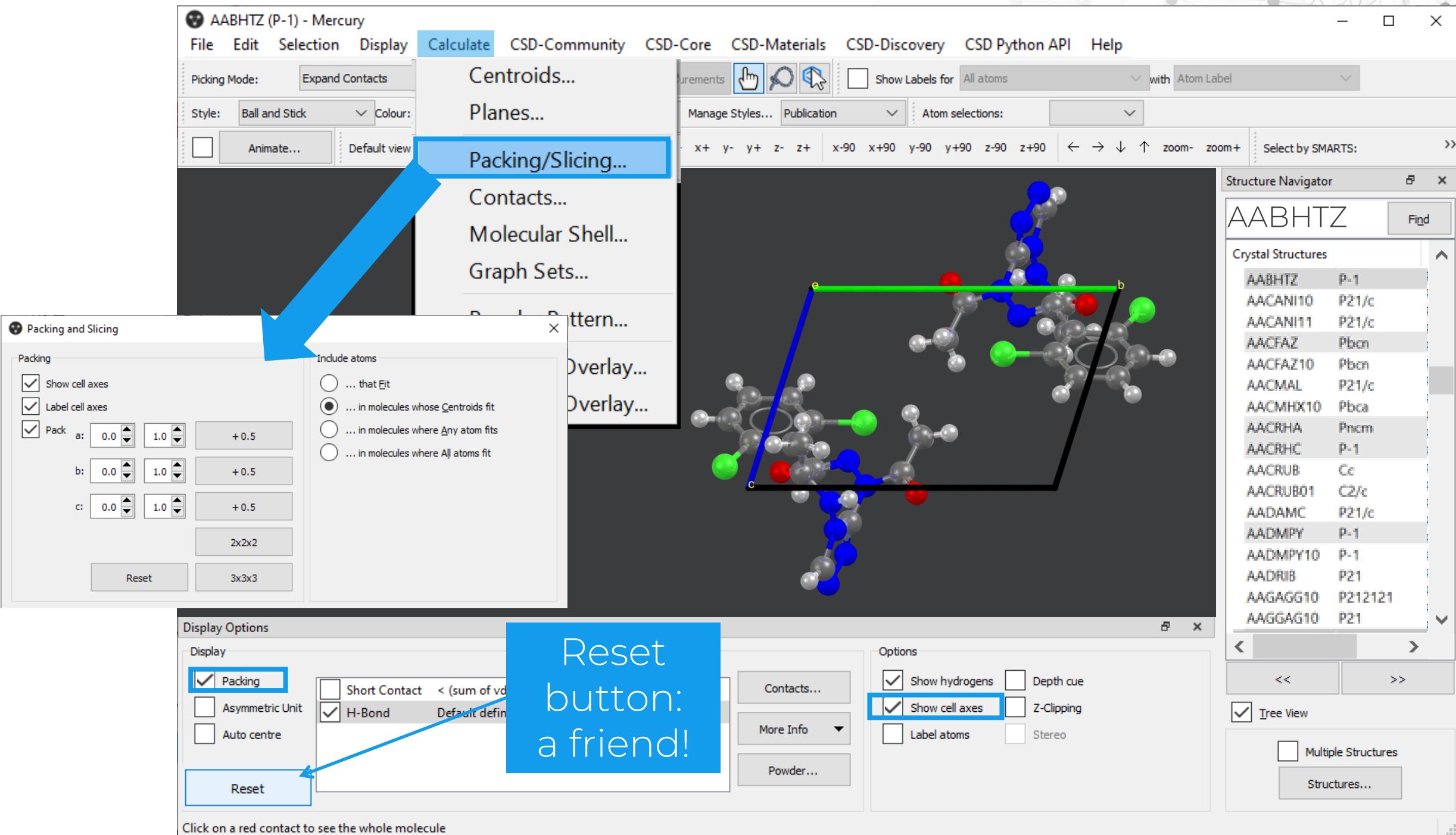
pre-saved  
options

personalised  
options

# Display packing



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# Other display options

Display Options

Display

Packing    Short ... < (sum of vdW radii)    Asymmetric Unit    H-Bon... Default definition    Auto centre    Contacts...    More Info    Powder...    Reset

Structure Information...    Chemical Diagram...    Atom List...    Bond List...    Contacts List...    Centroids List...    Planes List...    Symmetry Operators...    Distances List...    Torsions List...    All Angles List...    All Torsions List...    Contacts    Centroids    Planes    Symmetry    Distances    Torsions    All Angles    All Torsions

Options

Show hydrogens    Depth cue  
 Show cell axes    Z-Clipping  
 Label atoms    Stereo

Formula: C<sub>13</sub>H<sub>12</sub>Cl<sub>2</sub>N<sub>6</sub>O<sub>2</sub>

Compound Name: 4-Acetoamido-3-(1-acetyl-2-robenzylidene)hydrazine)-1,2-

Synonym:

Space Group: P -1

Cell Lengths: a 11.372(9) b 10.272(5) c 7.35

Cell Angles: α 108.75(6) β 71.07(4) γ 96.16

Cell Volume: 769.978

Z, Z': Z: 2 Z': 1

Current structure: AABHTZ

Click and drag left mouse button to zoom in.

Customise...   Reset zoom   Save...   Save image...

Intensity

Wavelength: 1.54056

2 theta: 29.952, -2040

h, k, l = 1, 1, 2

Close

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# 3D printing

File Edit Selection Display Calculate CSD-Community CSD-System CSD-Materials CSD-Discovery CSD Python API Help

Open... Ctrl+O

Recent Files

Sketch Molecule... Ctrl+K

Auto Edit Structure on Load

Save As... Ctrl+S

POV-Ray Image...

**Print in 3D...**

Exit Ctrl+Q

**3D Printing**

File Format VRML (colour)

Scale (mm/Å) 10.0 Output Size (mm):

Generate Support Framework

Plinth Thickness (Å) 0.8

Column Radius (Å) 0.4

Generate Close

Display C

Settings

Output Directory Documents/Education Browse...

The screenshot shows the CSD software interface. At the top is a menu bar with File, Edit, Selection, Display, Calculate, CSD-Community, CSD-System, CSD-Materials, CSD-Discovery, CSD Python API, and Help. Below the menu is a toolbar with various icons. A main window displays a 3D ball-and-stick model of a molecule. Overlaid on this is a '3D Printing' dialog box. The dialog box has fields for File Format (set to VRML (colour)), Scale (mm/Å) (set to 10.0), and Output Size (mm). It also contains checkboxes for 'Generate Support Framework', 'Plinth Thickness (Å)' (set to 0.8), and 'Column Radius (Å)' (set to 0.4). At the bottom of the dialog are 'Generate' and 'Close' buttons.

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



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

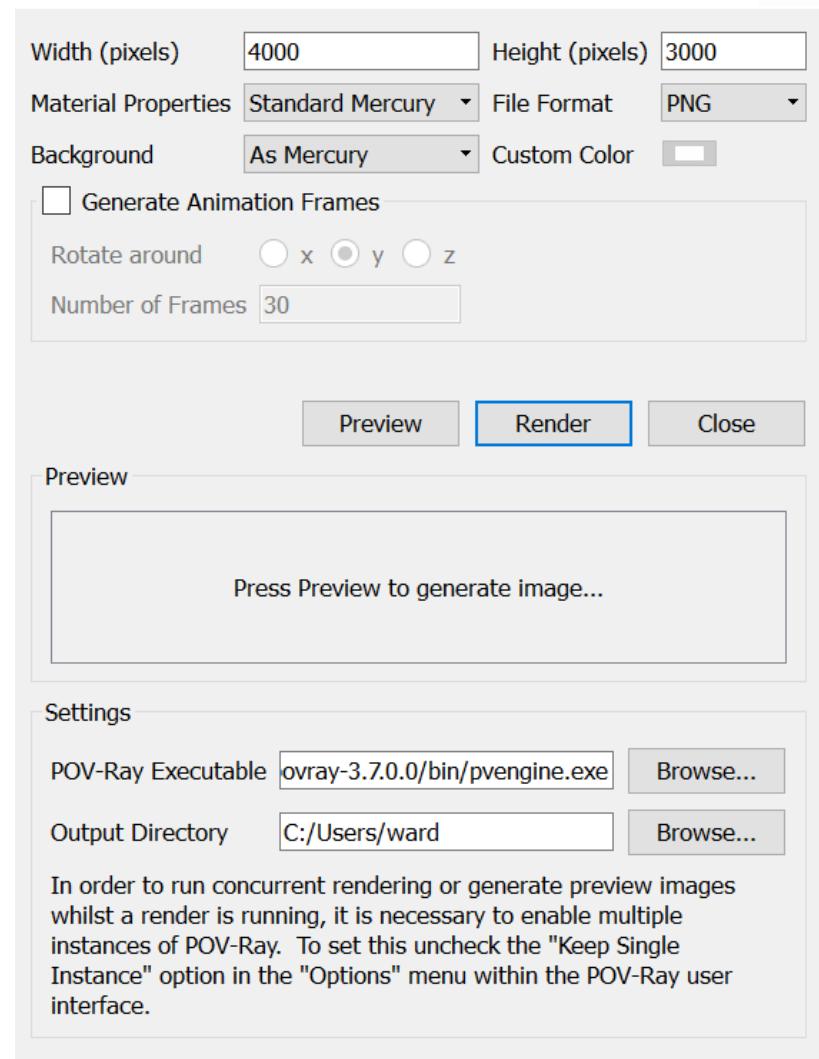
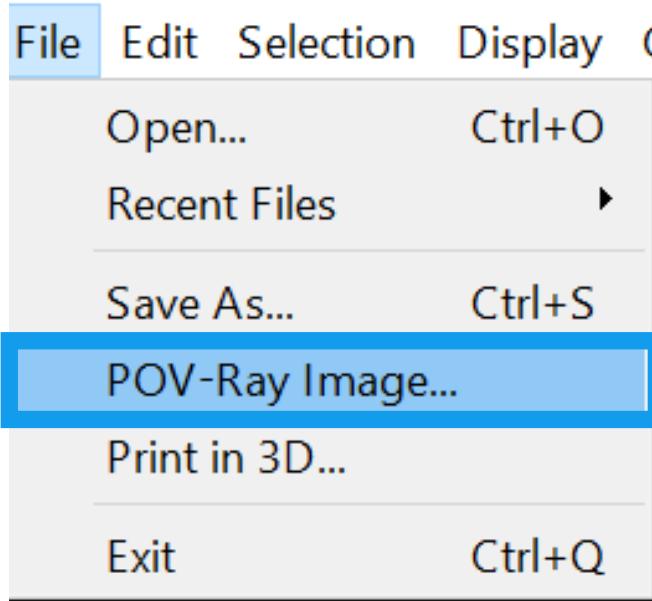
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# High-resolution images



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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

Width (pixels)  Height (pixels)

Material Properties  File Format

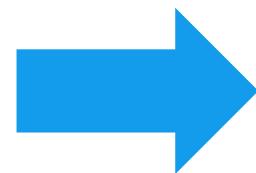
Background  Custom Color

Generate Animation Frames

Rotate around  x  y  z

Number of Frames

Preview  
Press Preview to generate image...



Width (pixels)  Height (pixels)

Material Properties  File Format

Background  Custom Color

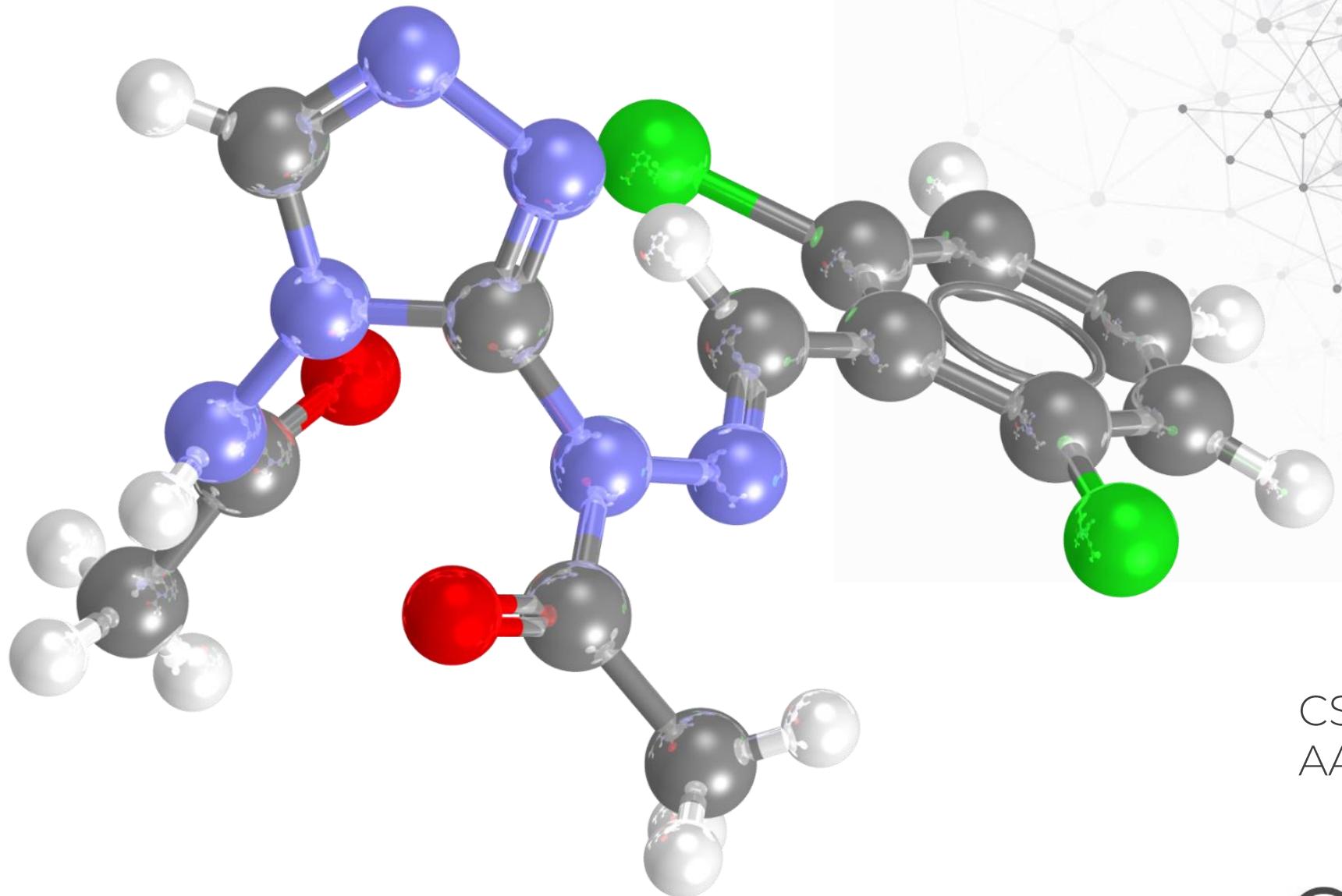
Generate Animation Frames

Rotate around  x  y  z

Number of Frames

Preview

CCDC



CSD Refcode:  
AABHTZ

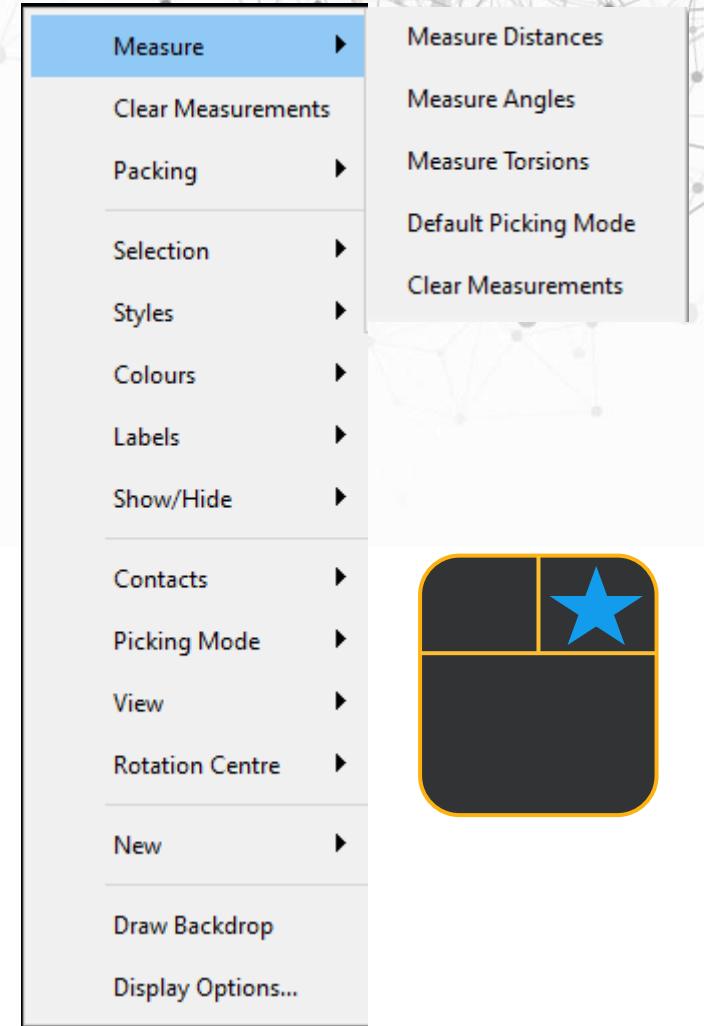
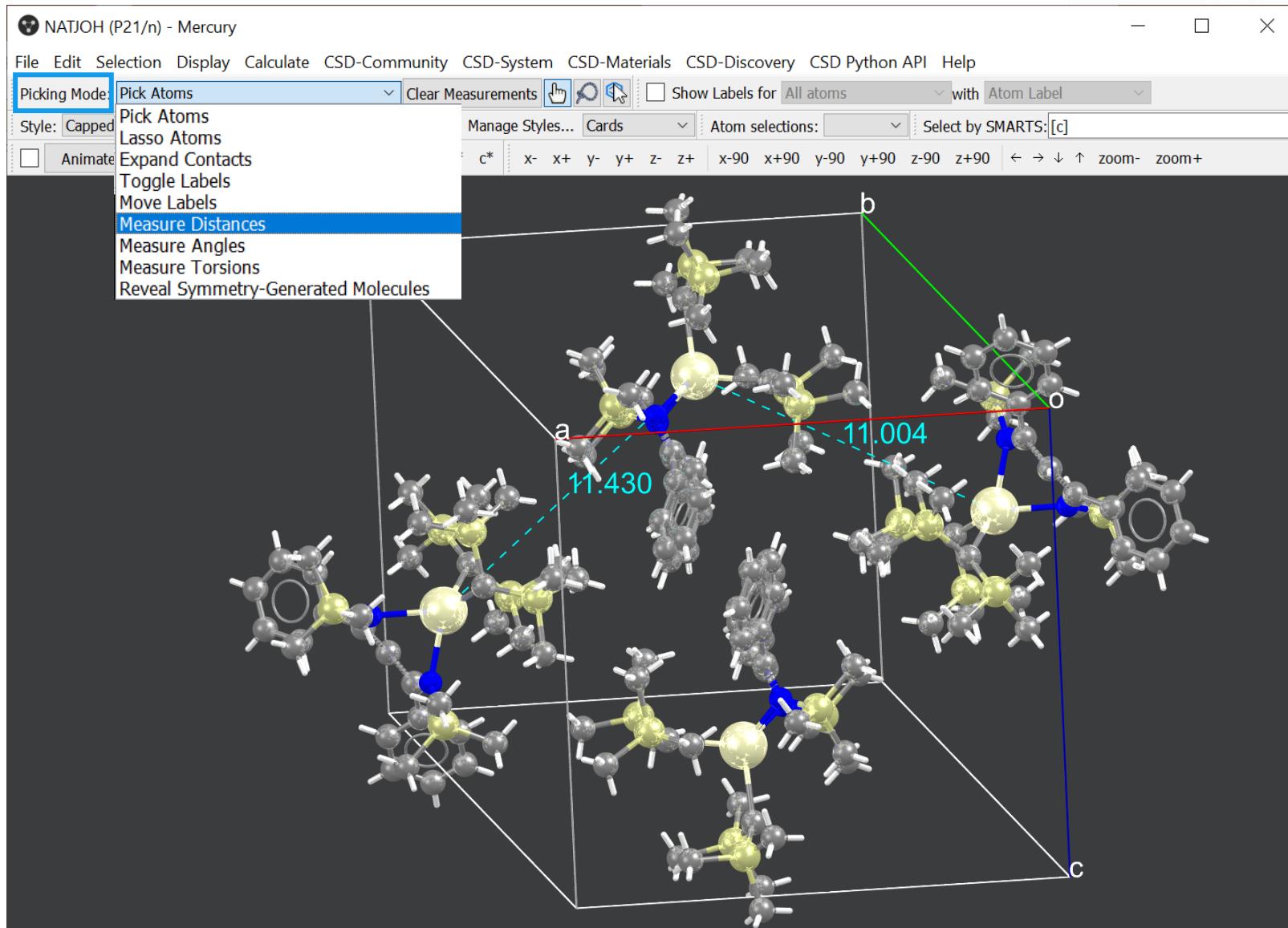
CCDC

# A few more tips & tricks

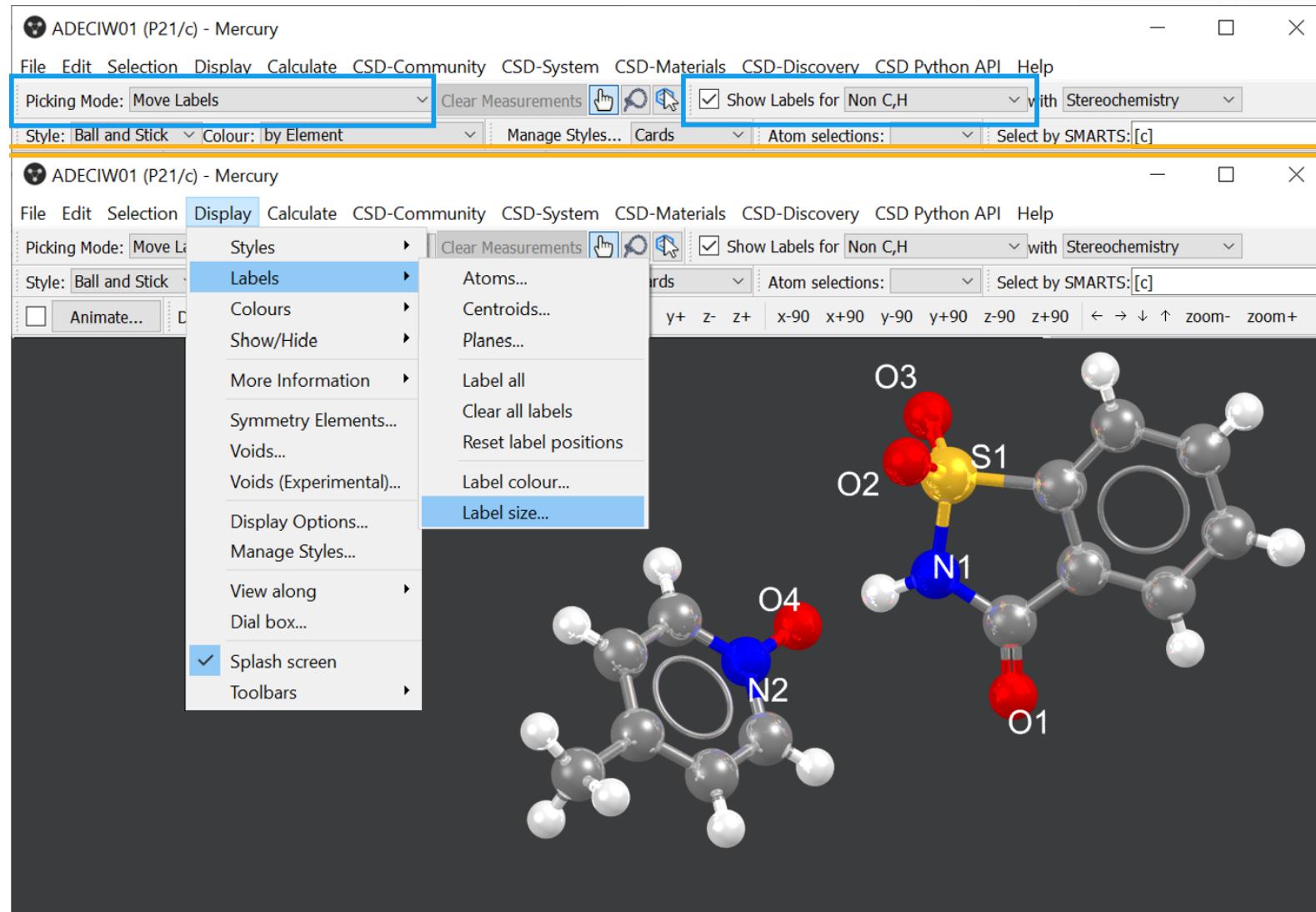


# Measure distances

CSD Refcode:  
NATJOH



# Adding, moving and sizing labels



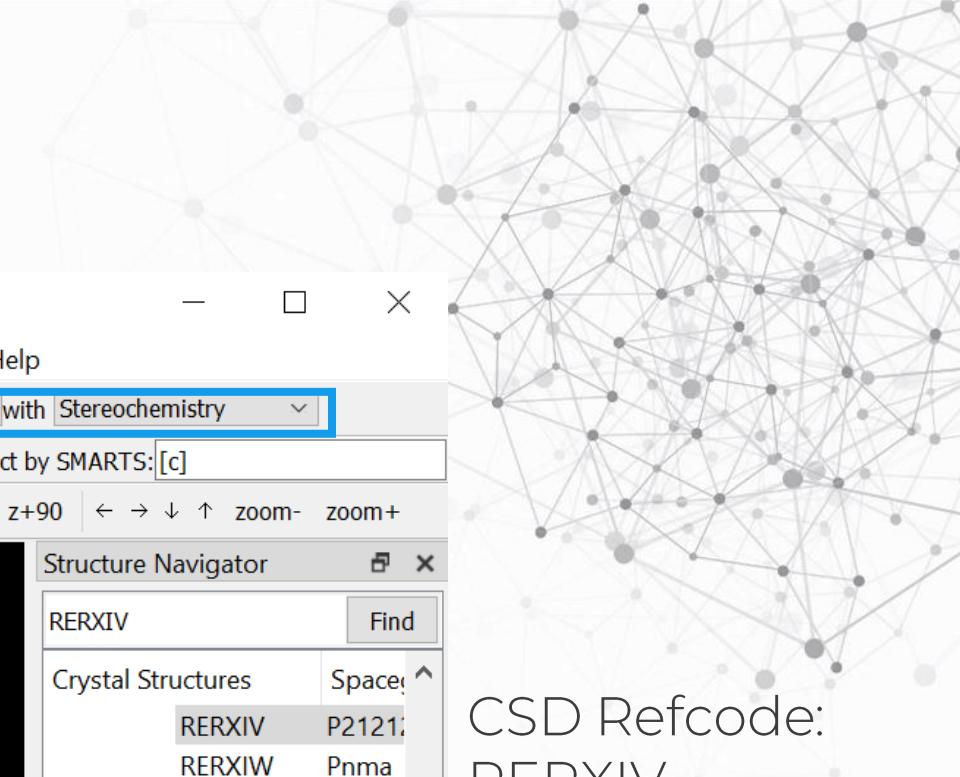
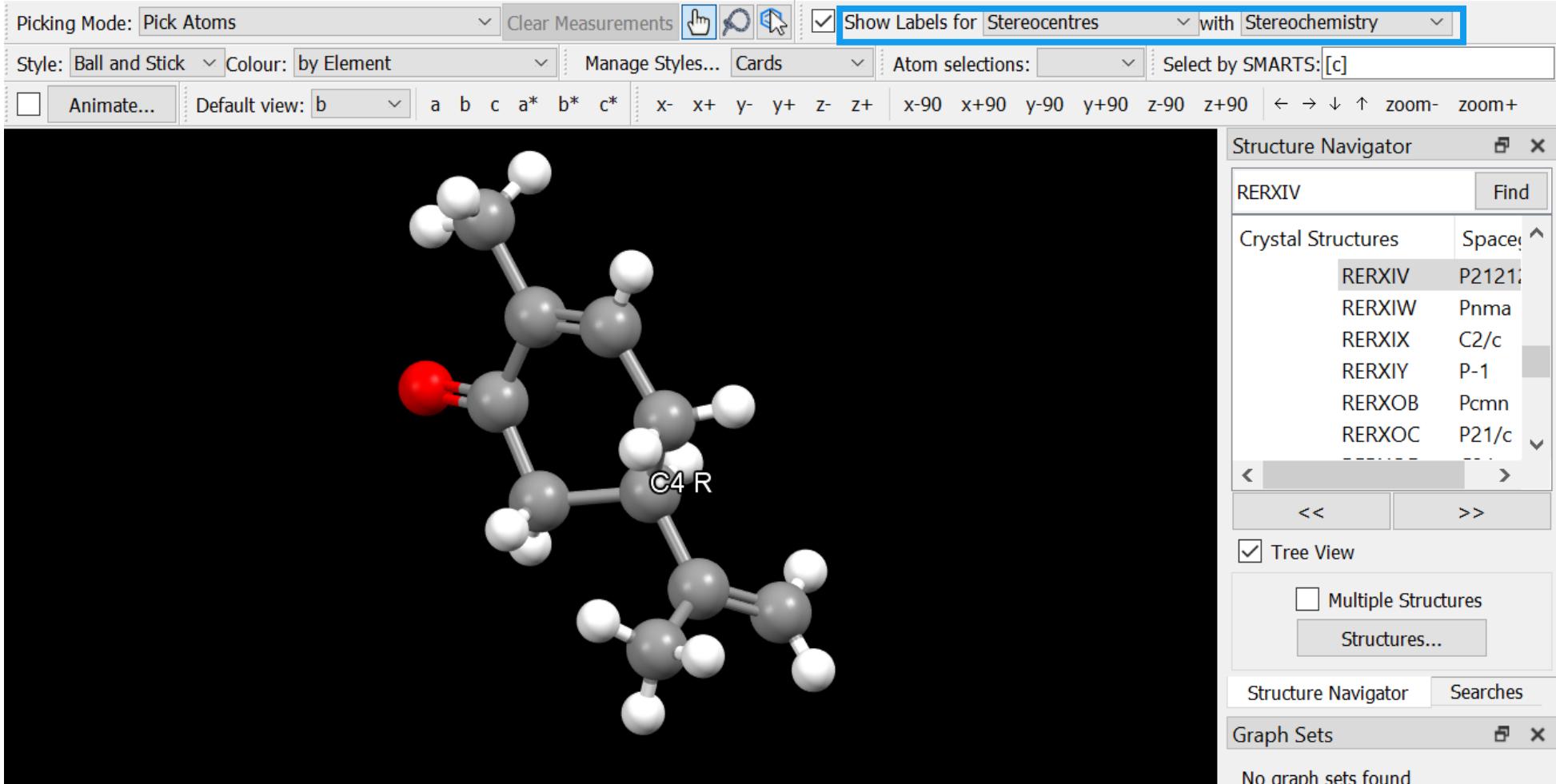
CSD Refcode: ADECIW01

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# Labelling chiral molecules

RERXIV (P212121) - Mercury

File Edit Selection Display Calculate CSD-Community CSD-System CSD-Materials CSD-Discovery CSD Python API Help



CSD Refcode:  
RERXIV

CCDC