

Visualising structures using Mercury

CCDC Virtual Workshop 2020 – Session 2

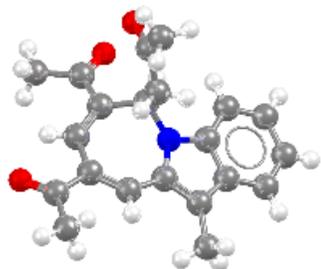
Ilaria Gimondi, Suzanna Ward, Yinka Olantunji-Ojo, Natalie Johnson, Eva Myers

November 2020

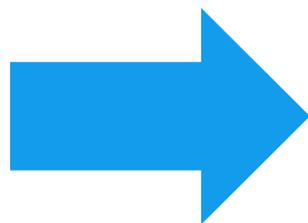
Learning outcomes for today

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

CSD Refcodes



CSD Refcode -
XOPCAJ



What is XOPCAJ?

- 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

The CSD software

CSDEnterprise.

CSDMaterials.



CSDDiscovery.



CSDSystem.



Professional Services

Research & Knowledge partnerships

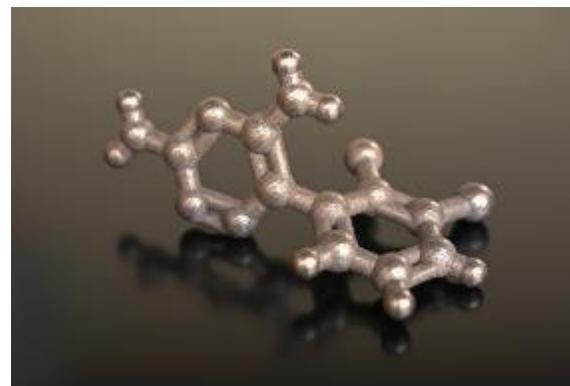
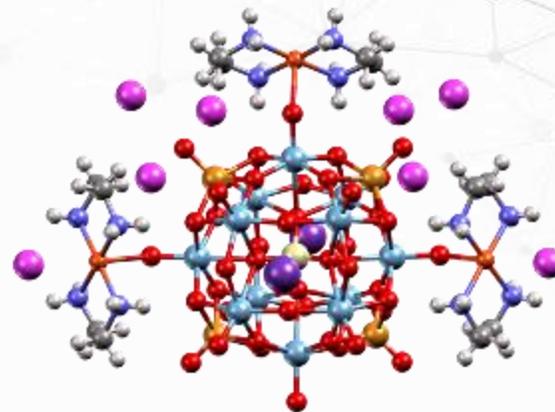
CSDCommunity.



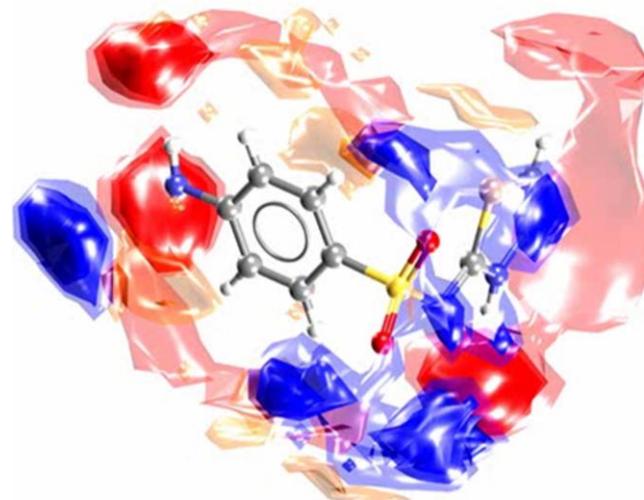
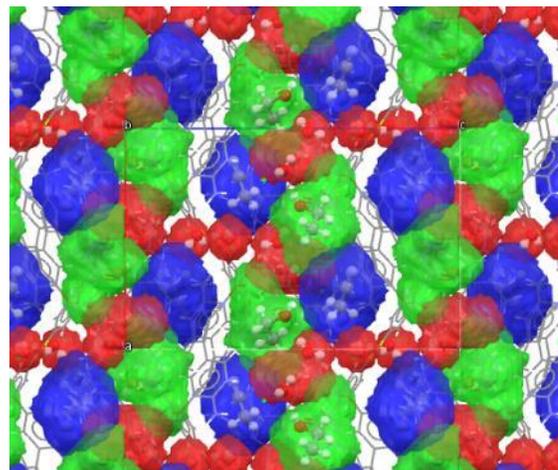
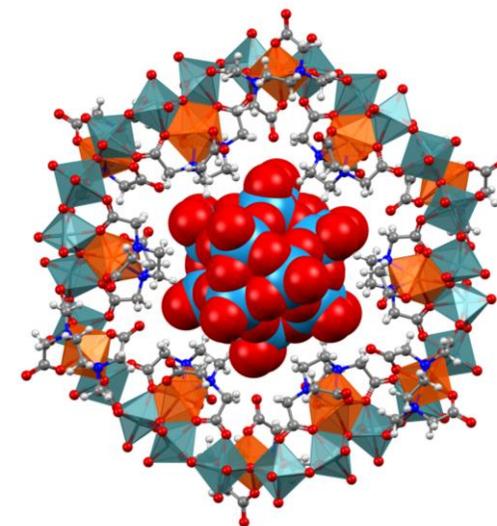
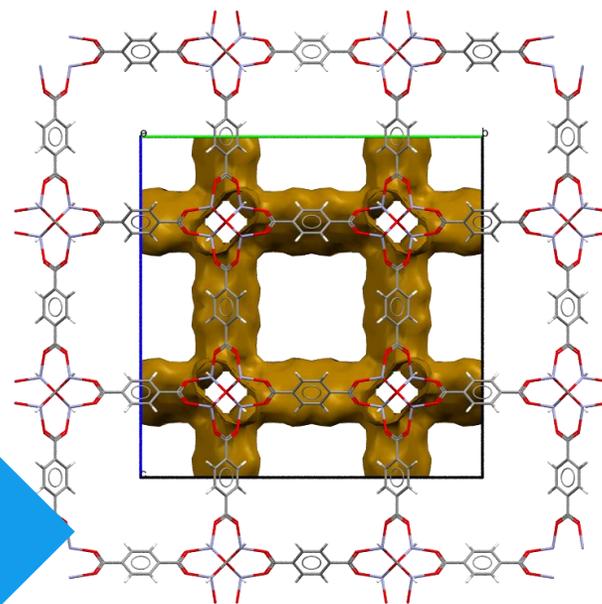
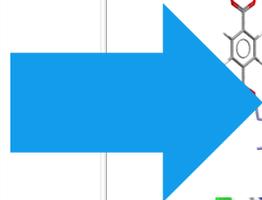
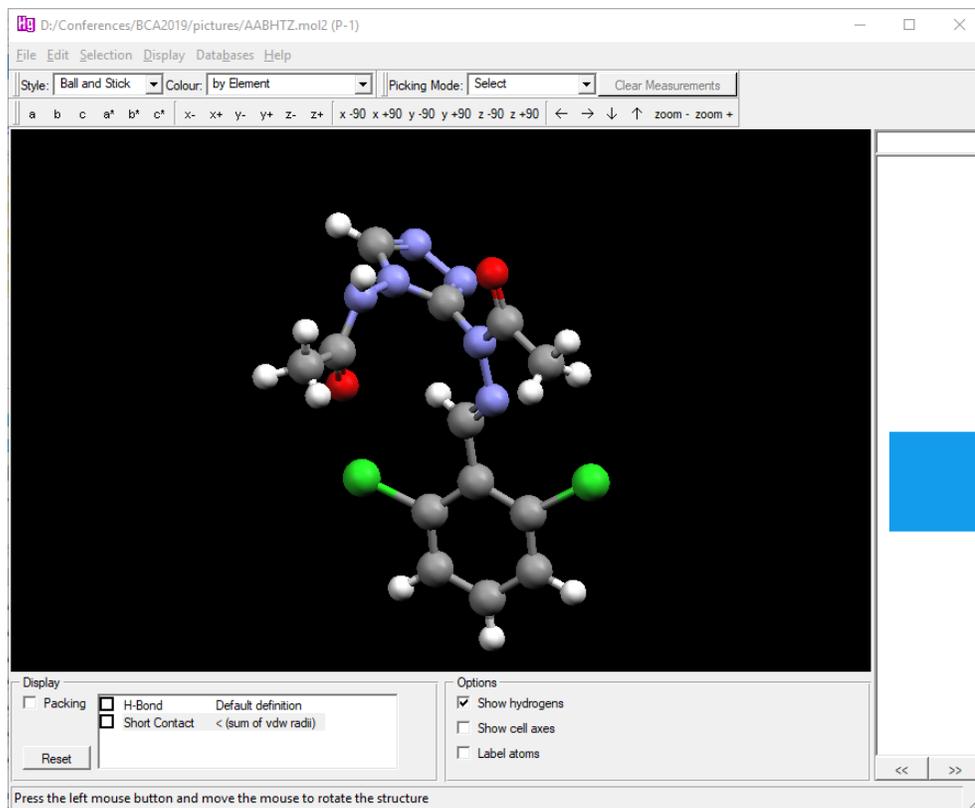
Mercury – Structure visualisation

With Mercury you can:

- Explore [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

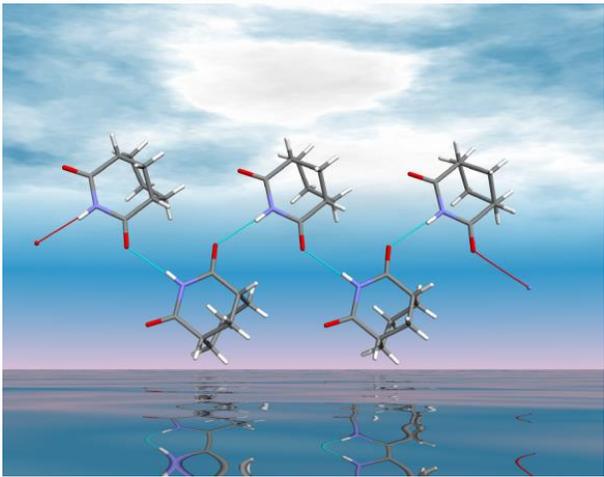
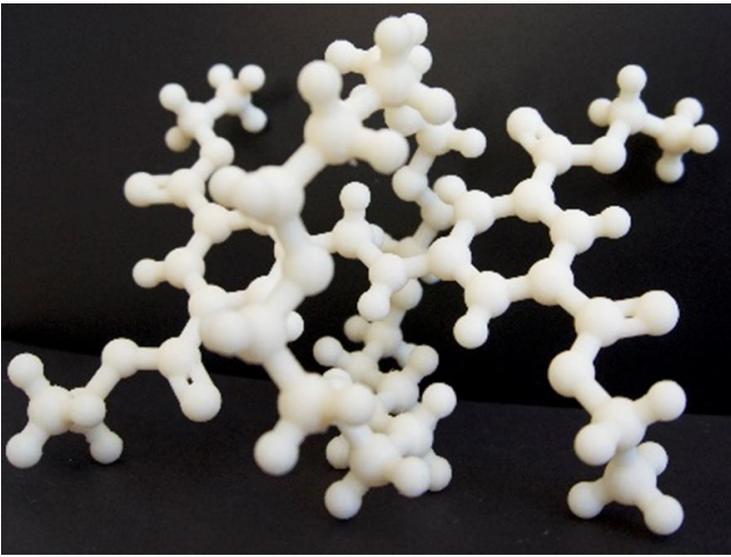
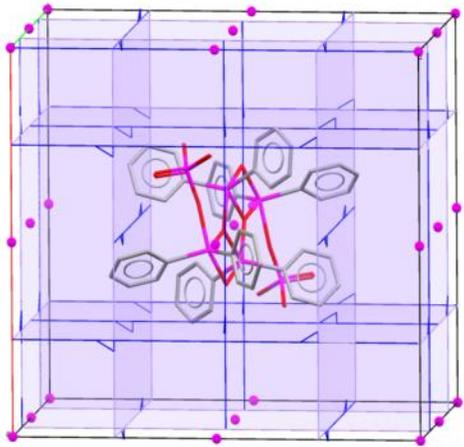
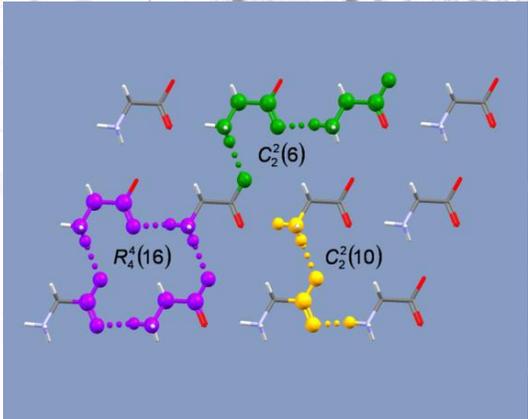
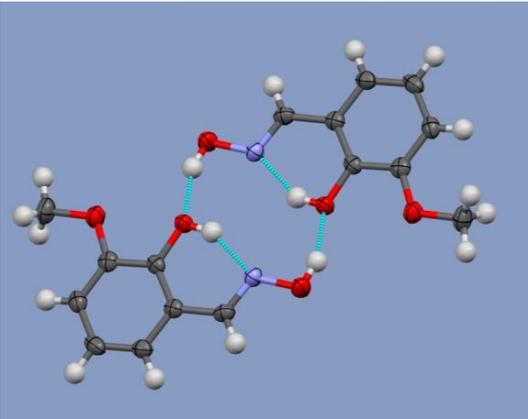


Mercury – first launched in 2001

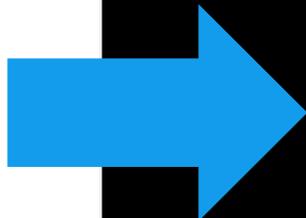


Structure visualisation

- Symmetry elements
- Displacement ellipsoids etc.
- POV-Ray
- 3D printing
- Graph sets
- Movies



Show One: Mercury Demo



AABHTZ (P-1) - Mercury

File Edit Selection Display Calculate CSD-Community CSD-System 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 Select by SMARTS: [c]

Structure Navigator

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
AADMPY	P-1
AADMPY10	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

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
- **Structure Navigator** – Allows you to view any structure in the CSD



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
AADMPY	P-1
AADMPY10	P-1
AADRIB	P21
AAGAGG10	P212121
AAGGAG10	P21

<< >>

Picking Mode: Pick Atoms

Style: Capped Sticks

 Animate... De

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     zoom- >> Select by SMARTS: >>

- 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
AADMPY	P-1
AADMPY10	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
AANHGX	Pna21
AANHGX01	Pna21
AANOPM	P21
AAPUNI	P21/a

Display Options

Display

 Packing Asymmetric Unit Auto centre

Reset

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

Contacts...

More Info

Powder...

Options

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

<<

>>

 Tree View Multiple Structures

Structures...

Picking Mode: Pick Atom

Style: Capped Sticks

 Animate... De

Styles

Labels

Colours

Show/Hide

More Information

Symmetry Elements...

Voids...

Display Options...

Manage Styles...

View along

Dial box...

 Splash screen

Toolbars

 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 ← → ↓ ↑ zoom- >> Select by SMARTS: >>

Structure Navigator

AACRUB 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

AADMPY P-1

AADMPY10 P-1

AADRIB P21

AAGAGG10 P212121

AAGGAG10 P21

AALCFE P21/c

AALPRO P21/c

AAMAND P212121

AAMTCO P-1

AAMTCO10 P-1

Display Options

Display

 Packing Asymmetric Unit Auto centre

Reset

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

Contacts...

More Info

Powder...

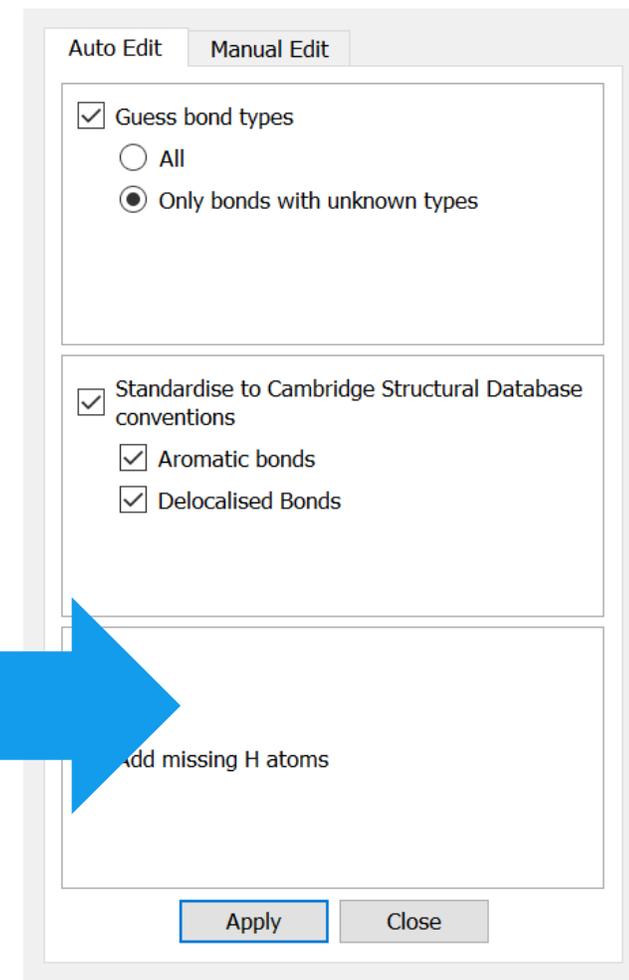
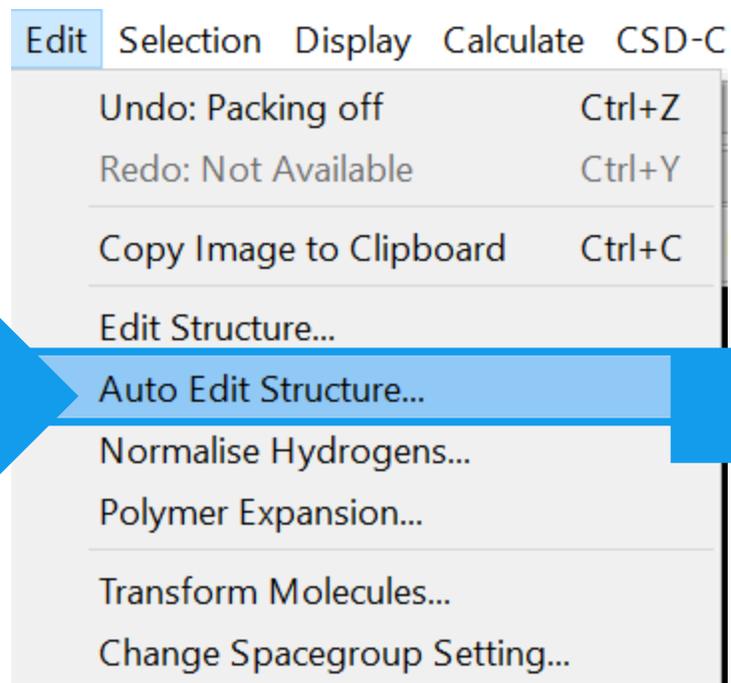
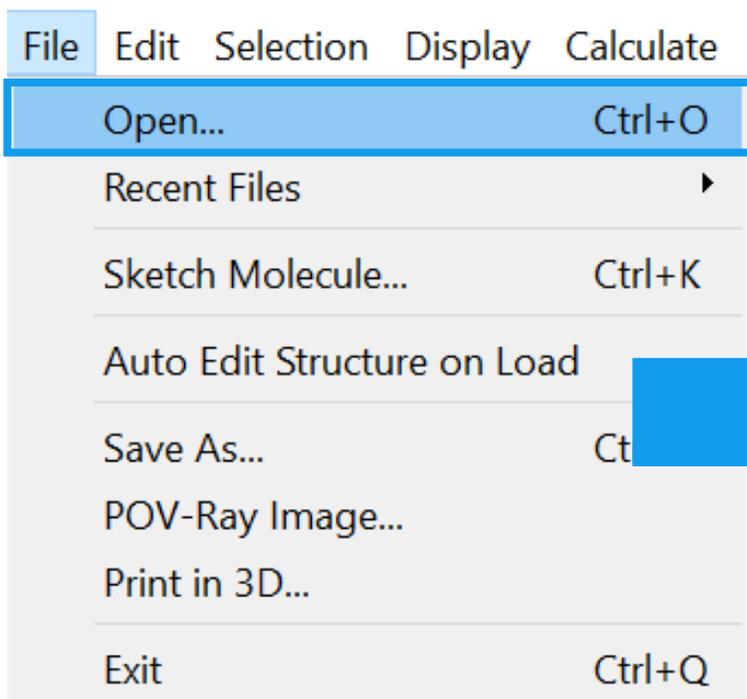
Options

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

Using your own file

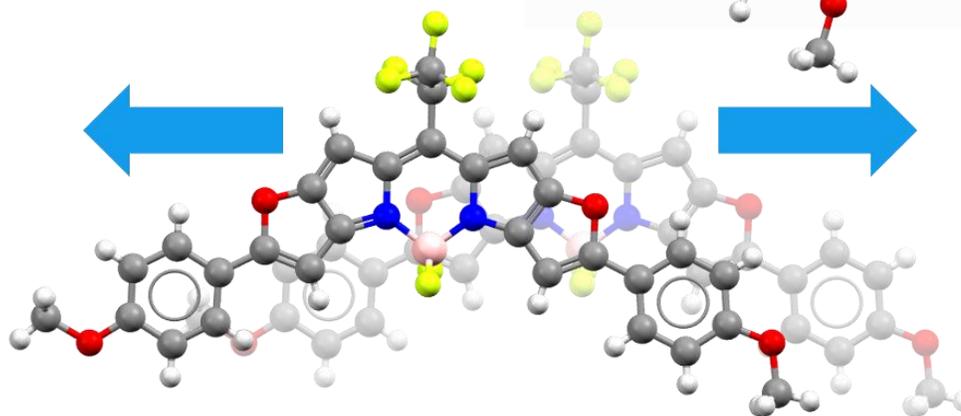
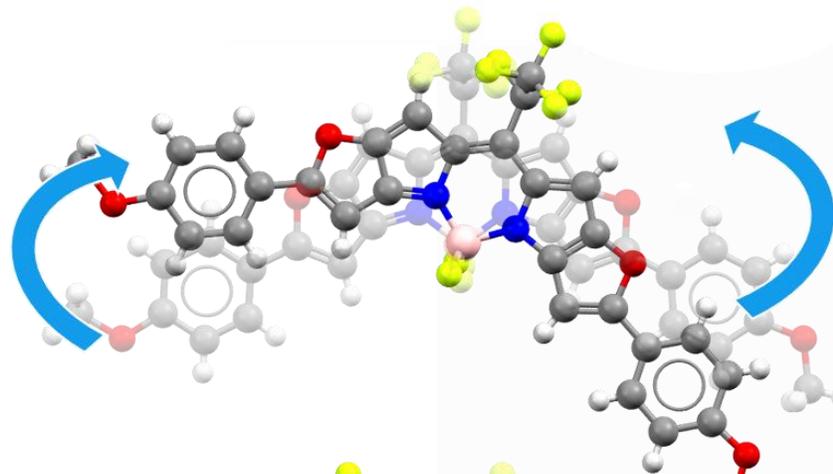
- File > Open – to open one of your own files for example a CIF
- Edit > Auto Edit Structure to assign bond types
- File > Auto Edit Structure on Load to automate

AABHTZ (P-1) - Mercury



Moving and rotating on the plane

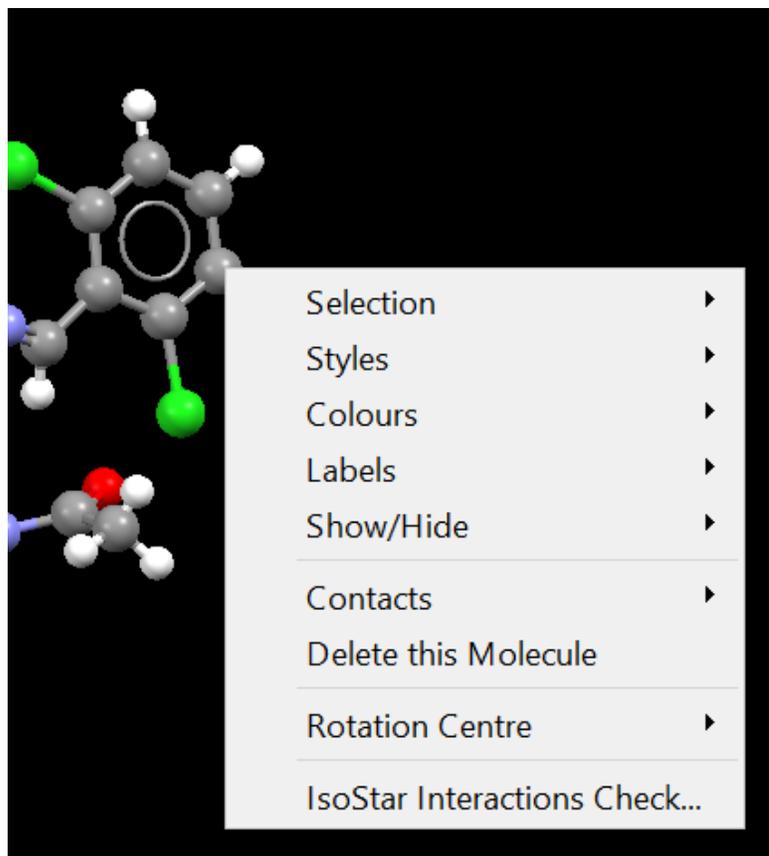
With the keyboard:



CSD Refcode: GIMXUY

Right mouse click

Near a molecule



Away from a molecule



Changing display - Style

Display Calculate CSD-Community CSD-System CSD-M

- Styles ▶
 - Wireframe
 - Stick
 - Ball and stick
 - Spacefill
 - Ellipsoid
 - Polyhedral
- Labels ▶
- Colours ▶
- Show/Hide ▶
- More Information ▶
- Symmetry Elements...
- Voids...
- Display Options...
- Manage Styles...
- View along ▶
- Dial box...
- ✓ Splash screen
- Toolbars ▶

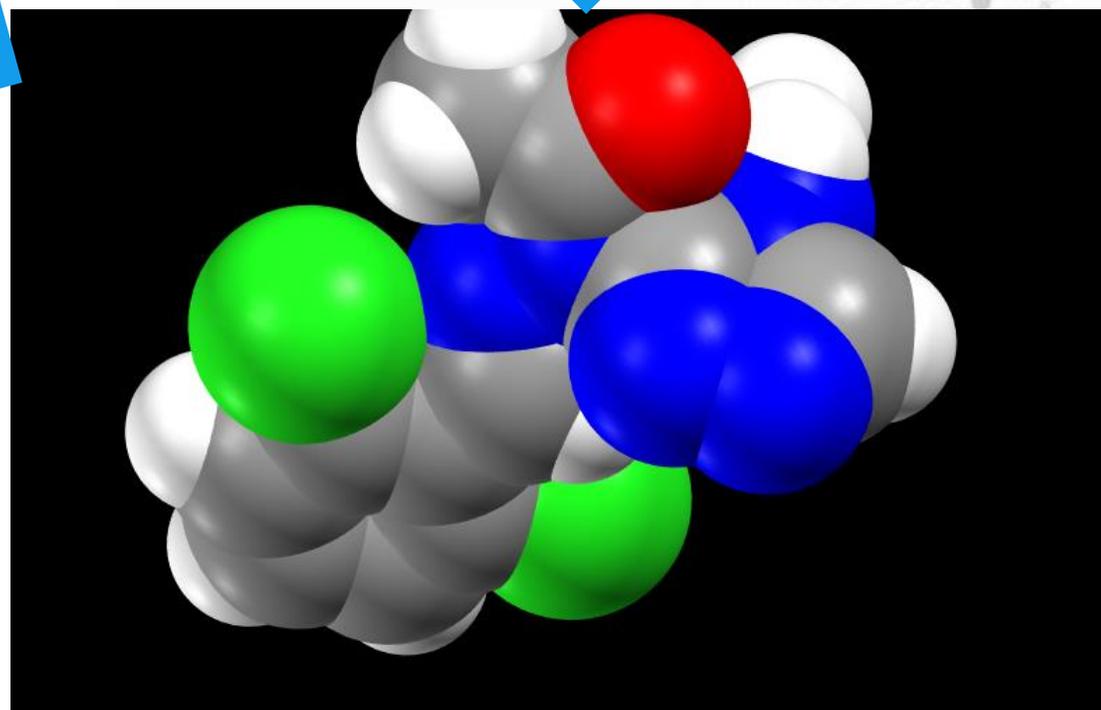
Stick settings...
Ball and Stick settings...
Spacefill settings...
Ellipsoid settings...
Polyhedral settings...
Contact settings...
Measurement settings...
Selected atoms

File Edit Selection Display Calculate C:

Picking Mode: Pick Atoms

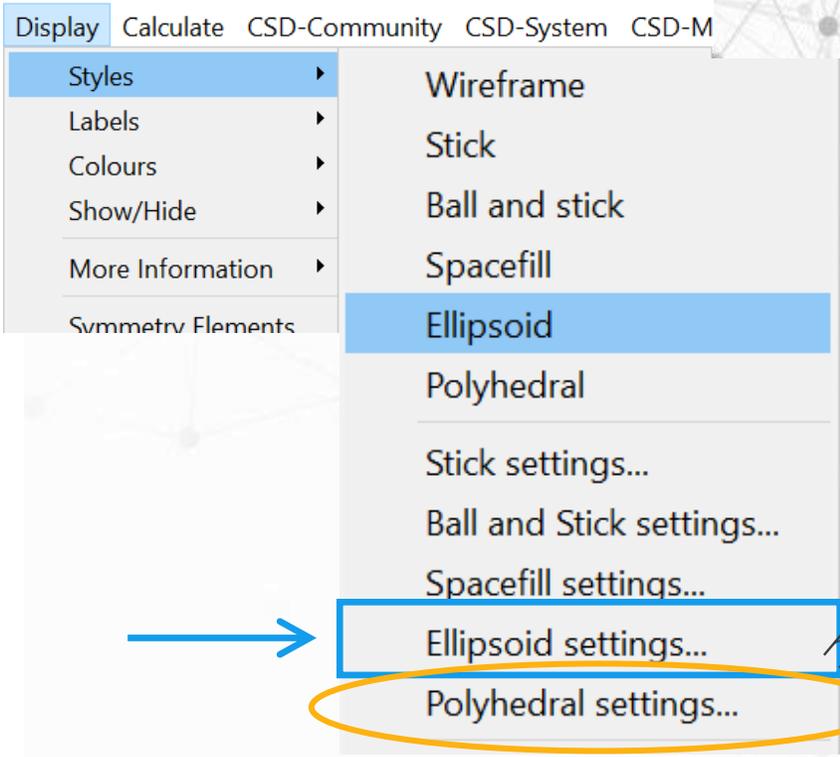
Style: Spacefill Colour: by Element

Animate... Fault view: b



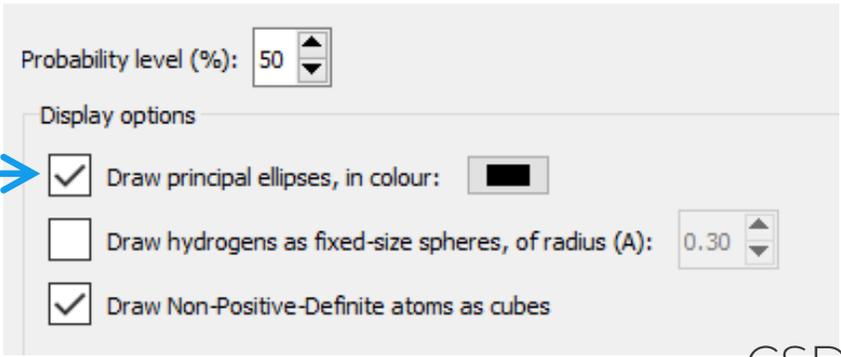
Thermal Ellipsoids

- 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

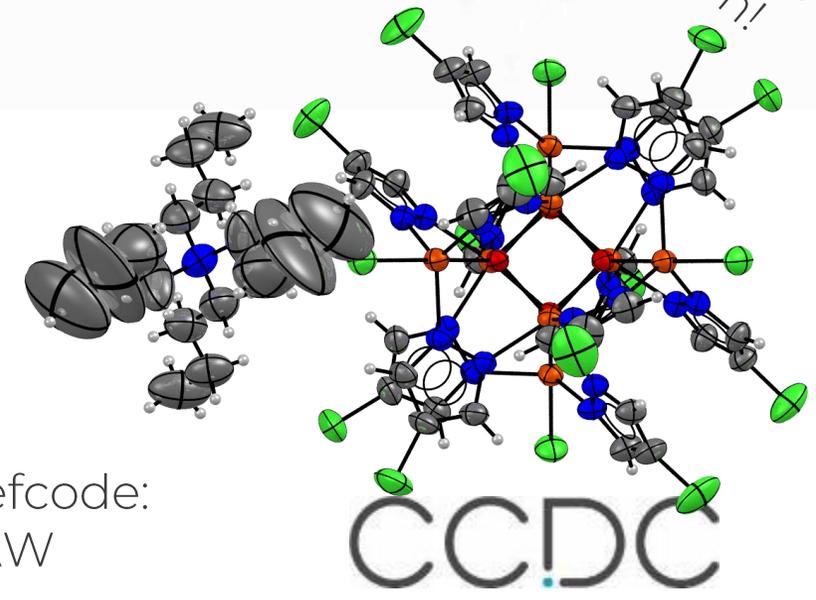


Try it in the hands-on!

Ellipsoid Display Options



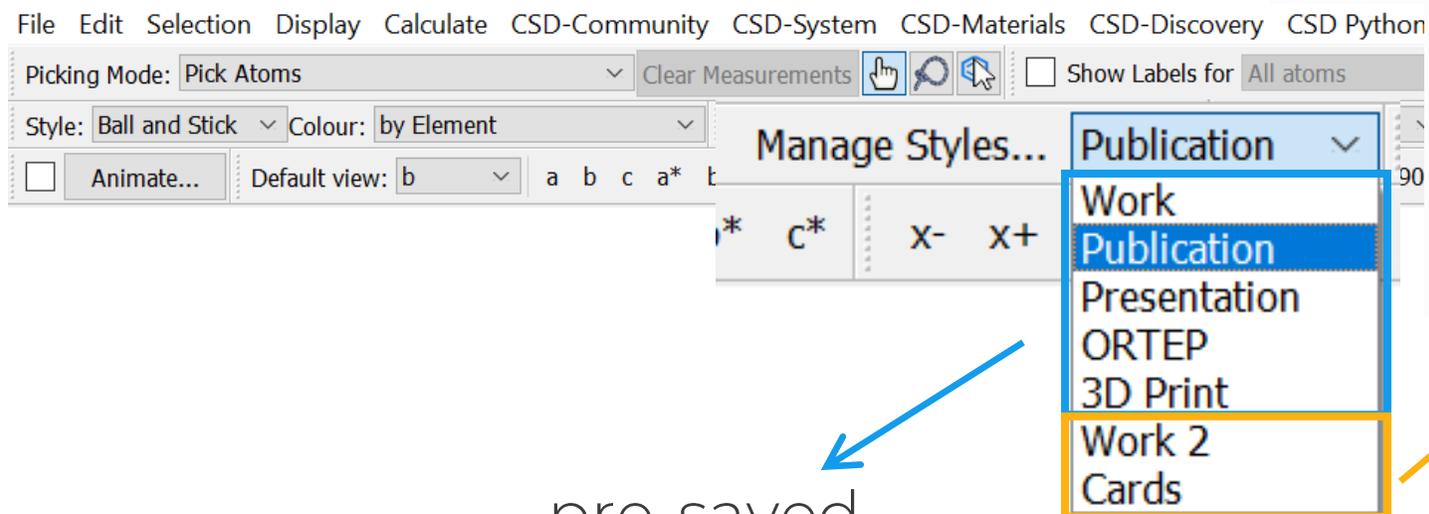
Read more about [ADPs](#) and [Thermal Ellipsoids](#) in the *Dictionary* on the *handout*.



CSD Refcode: LORBAW

Manage Styles

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



pre-saved
options

personalised
options
**Bonus in the
hands-on:**
create your own
style!

Changing display - colours

Display Calculate CSD-Community CSD-System CSD-Materials CSD-Tools

- Styles ▶
- Labels ▶
- Colours ▶**
 - Atoms...
 - Bonds...
 - Centroids...
 - Planes...
 - Contacts...
 - Element colours...
 - Symmetry Equivalence colours...
 - Labels...
 - Background settings...
- Show/Hide ▶
- More Information ▶
- Symmetry Elements...
- Voids...
- Display Options...
- Manage Styles...
- View along ▶
- Dial box...
- Splash screen

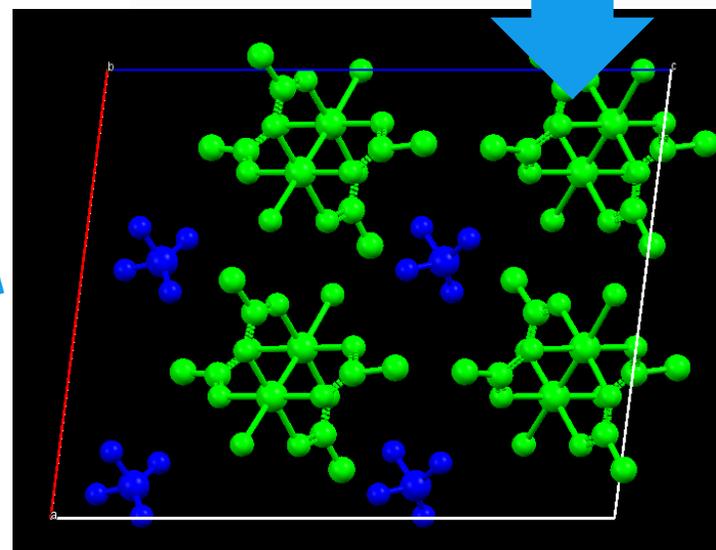
CSD Refcode: AACRUB

File Edit Selection Display Calculate CSD-Community

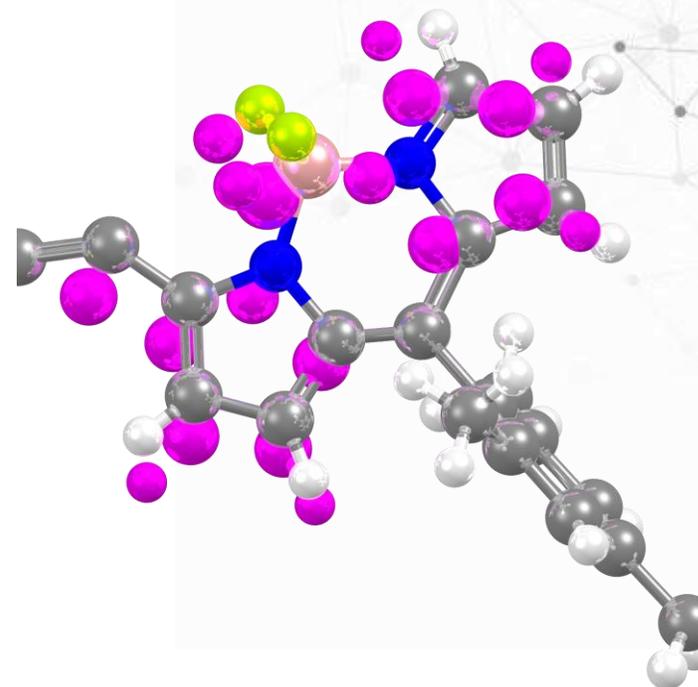
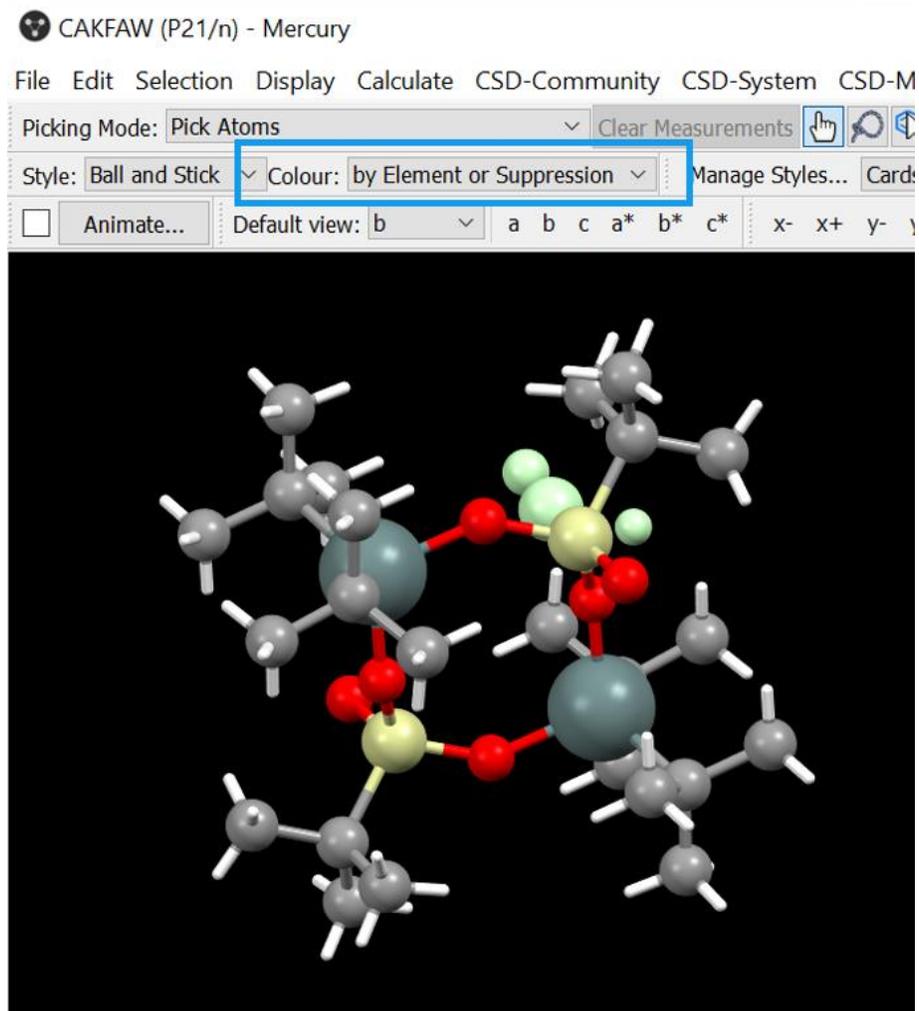
Picking Mode: Pick Atoms Clear M

Style: Ball and Stick Colour: **by Symmetry equivalence**

- by Element
- by Symmetry equivalence**
- by Atomic displacement
- by Symmetry operation
- by Gasteiger charge
- by Partial charge
- by Element or Suppression



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.

Learn more in the *Dictionary* on the handout.

CSD Refcodes: CAKFAW and PIYDEI

Changing background colour

AABHTZ (P-1) - Mercury

File Edit Selection **Display** Calculate CSD-Con

Picking Mode: Pick Atc

Style: Polyhedral

Animate...

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

Display Options

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

Single colour

Gradient

Defaults

Close

Select Color

Basic colors

Pick Screen Color

Custom colors

Add to Custom Colors

Hue: 0 Red: 255

Sat: 0 Green: 255

Val: 255 Blue: 255

HTML: #ffffff

OK Cancel

File Edit Selection Display **Calculate** CSD-CommunitSD-Materials CSD-Discovery CSD Python API Help

Picking Mode: Pick Atoms

Style: Capped Sticks Colour: by E

Animate... Default view: b

Show Labels for All atoms with Atom Label

Atom selections:

y+ z- z+ x-90 x+90 y-90 y+90 z-90 z+90 ← → ↓ ↑ zoom- >> Select by SMARTS: >>

- Centroids...
- Planes...
- Packing/Slicing...**
- Contacts...
- Molecular Shell...
- Graph Sets...
- Powder Pattern...
- Structure Overlay...
- Molecule Overlay...

Packing

Show cell axes

Label cell axes

Pack a: 0.0 1.0 + 0.5

b: 0.0 1.0 + 0.5

c: 0.0 1.0 + 0.5

2x2x2

3x3x3

Reset

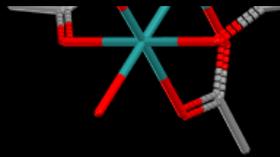
Include atoms

... that Fit

... in molecules whose Centroids fit

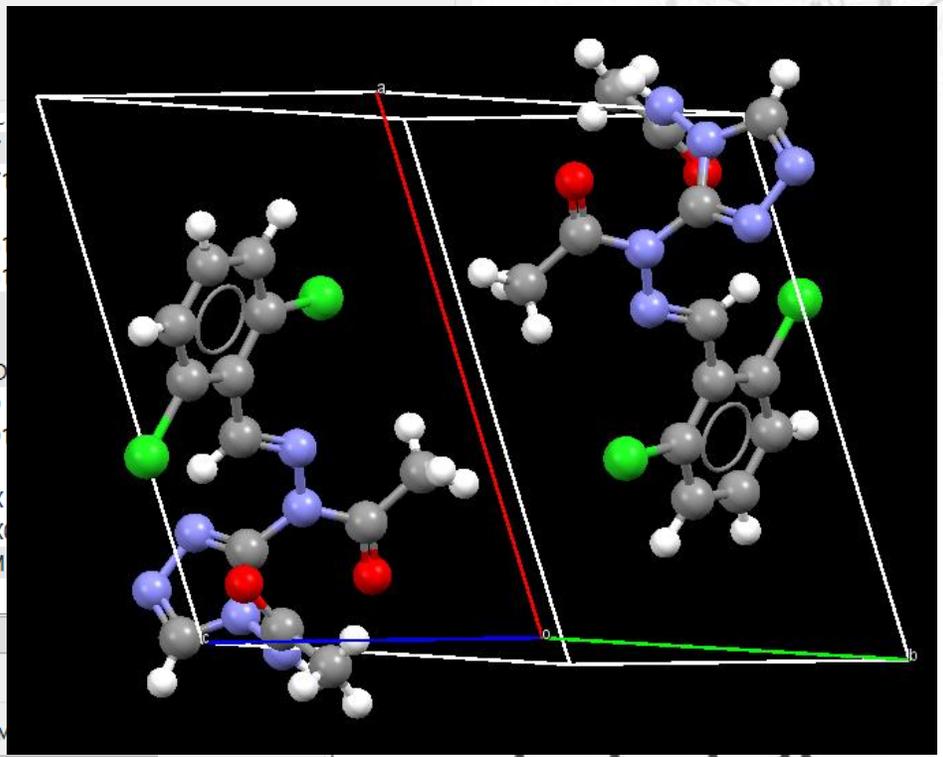
... in molecules where Any atom fits

... in molecules where All atoms fit



Reset button:
a friend!

- AADAMC
- AADMPY
- AADMPY
- AADRIB
- AAGAGG
- AAGGAG
- AALCFE
- AALPRO
- AAMAND
- AAMTCO
- AAMTCO
- AAMTXP
- AANHGX
- AANHGX
- AANOPM
- AAPUNI



Display Options

Display

Packing

Asymmetric Unit

Short Contact < (sum of vdW radii)

H-Bond Default definition

Contacts...

More Info

Powder...

Options

Show hydrogens

Depth

Show cell axes

Z-Clipp

Label atoms

Stereo

Reset



Other display options

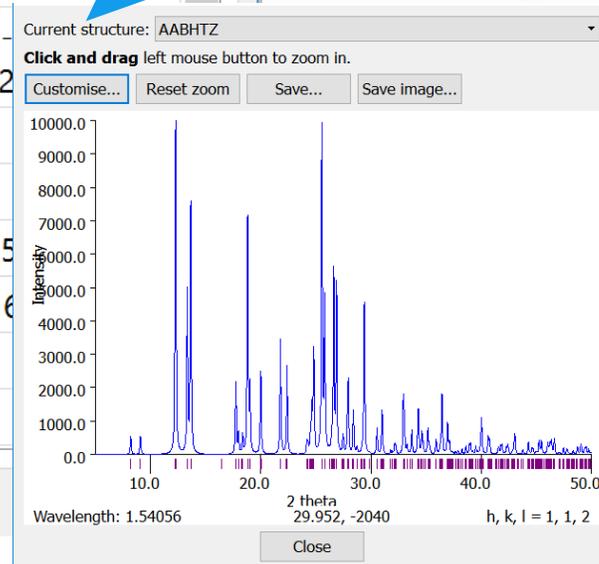
The screenshot displays two main windows from a software application. The top window is titled "Display Options" and contains several sections:

- Display:** Includes checkboxes for "Packing" (checked), "Asymmetric Unit", and "Auto centre". A "Reset" button is located below these options.
- Options:** Includes checkboxes for "Show hydrogens" (checked), "Show cell axes" (checked), "Label atoms", "Depth cue", "Z-Clipping", and "Stereo".
- Short ... < (sum of vdW radii):** A dropdown menu with "More Info" selected.
- H-Bon... Default definition:** A dropdown menu with "Powder..." selected.
- Contacts...:** A button.

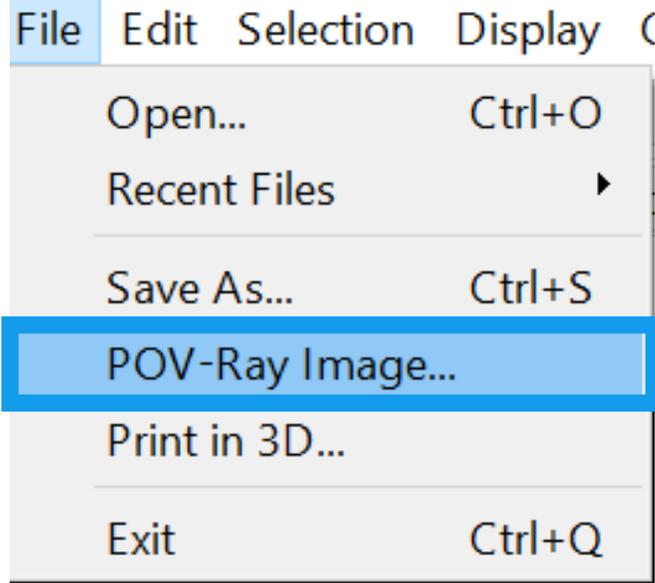
The bottom window is titled "Structure Information" and displays the following data:

- Formula:** $C_{13} H_{12} Cl_2 N_6 O_2$
- 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

Blue arrows highlight the "More Info" dropdown in the "Display Options" window, the "Structure Information..." button in the left sidebar, and the "Powder..." dropdown in the "Display Options" window. A "Close" button is visible at the bottom of the "Structure Information" window.



Generating high quality images



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...

Settings

POV-Ray Executable

Output Directory

In order to run concurrent rendering or generate preview images whilst a render is running, it is necessary to enable multiple instances of POV-Ray. To set this uncheck the "Keep Single Instance" option in the "Options" menu within the POV-Ray user interface.

File > POV-Ray Image

Change Resolution

Width = 4000

Height = 3000

Change 'Material Properties' to 'Metallic'

Set 'Background' to 'Transparent'

Press 'Preview'

Previewing and rendering an image

Width (pixels) Height (pixels)

Material Properties File Format

Background Custom Color

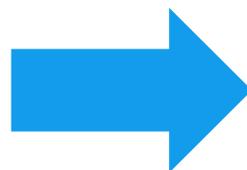
Generate Animation Frames

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

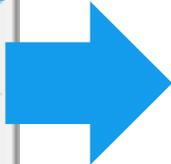
Number of Frames

Preview

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

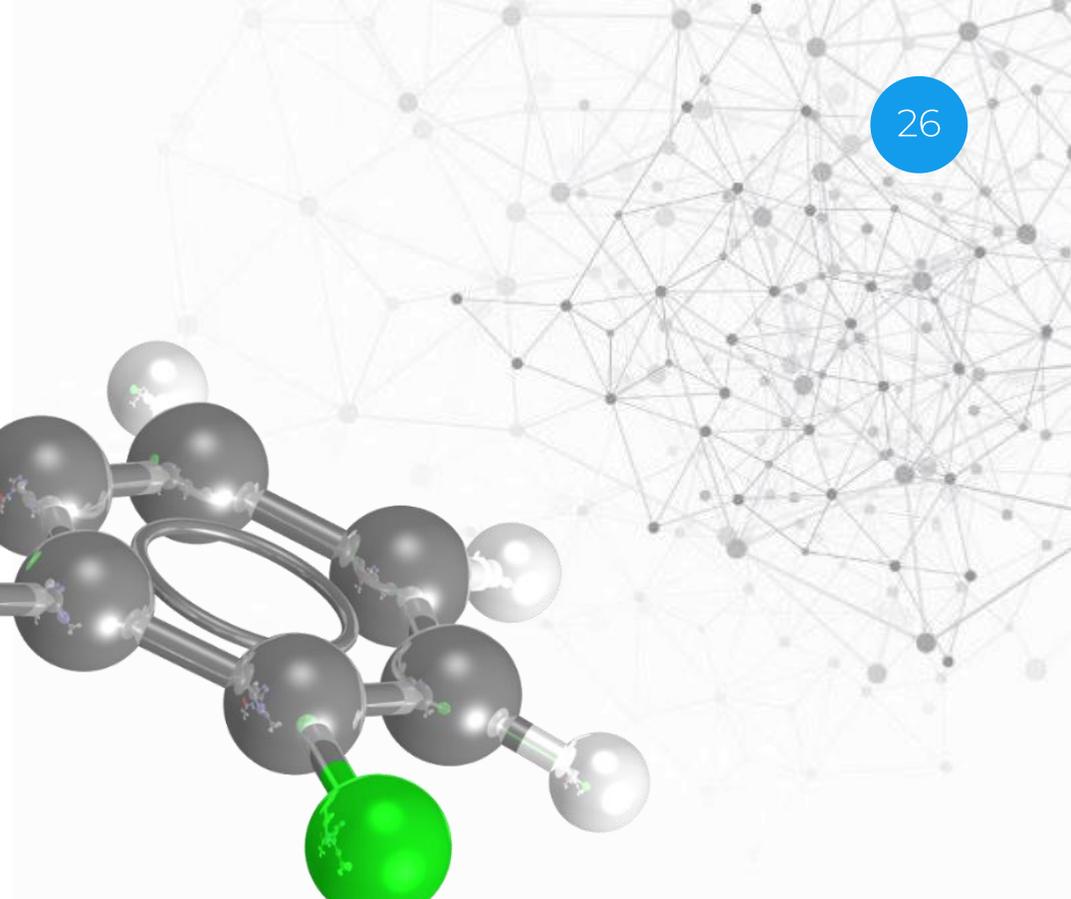
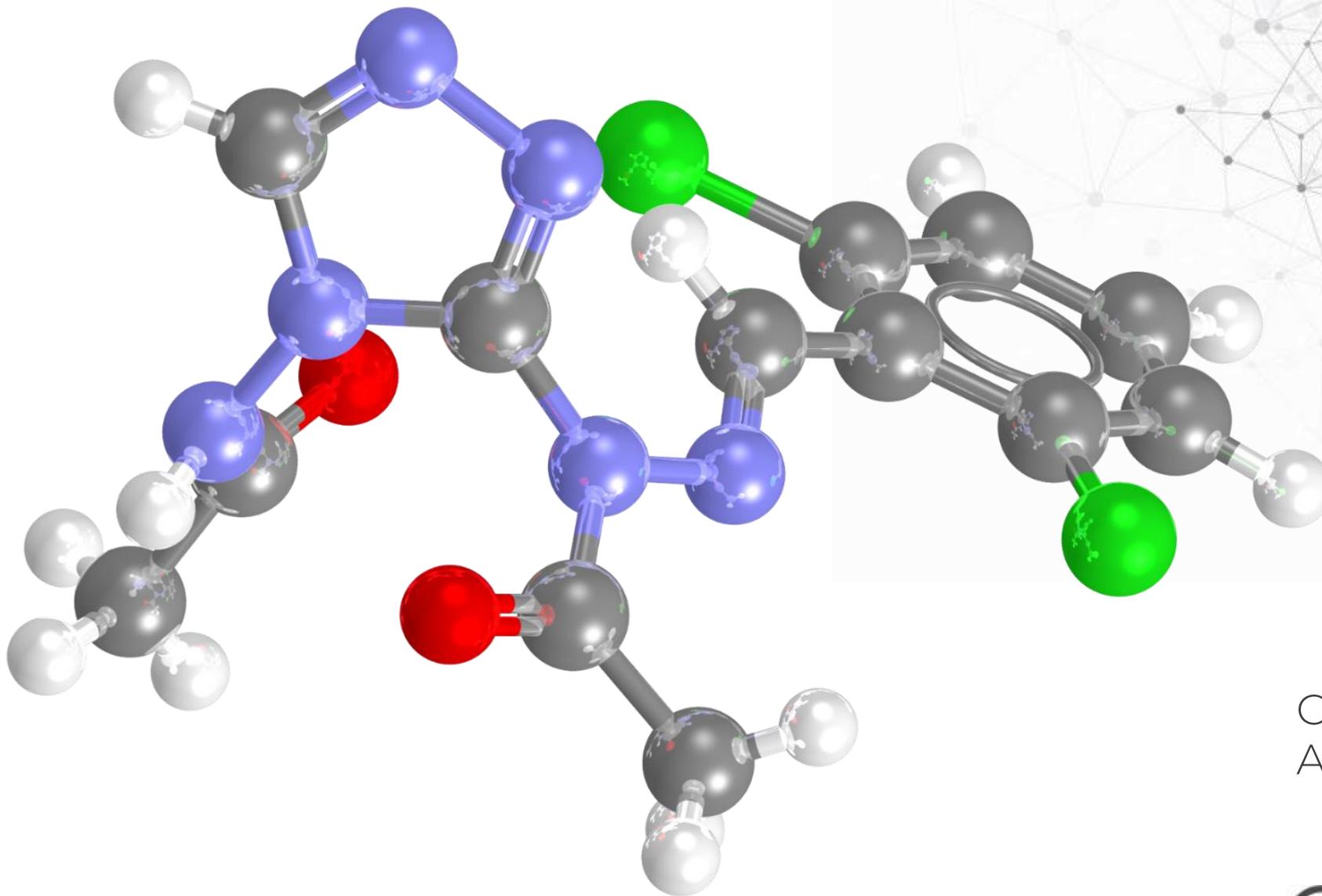
Enabled Diffuse colour: Specular colour:
Position: x: y: z:

Ambient Light
 Enabled Diffuse ambient colour:

Defaults

Close



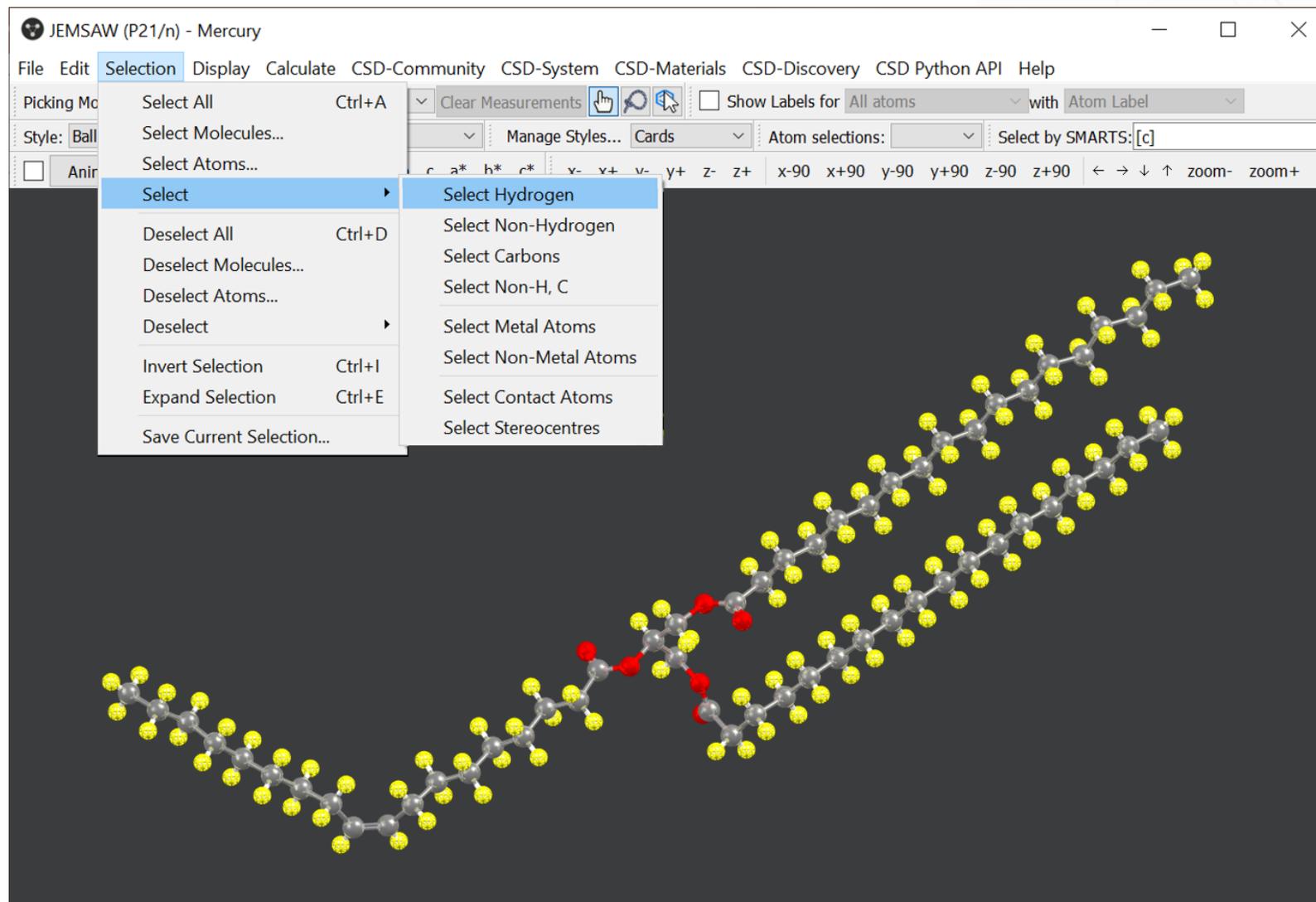


CSD Refcode:
AABHTZ

Explore More: A selection of our Top Tips for Mercury

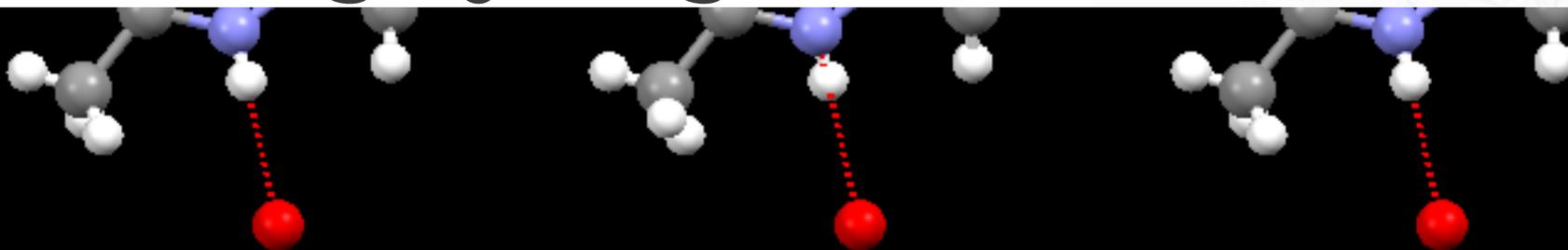
- Not enough time to explore all the things that Mercury can do...
- But here are a selection of [advanced tips and tricks](#)
- You can find more tips on social media with our [#CSDTopTipTuesday](#) series

Selection



CSD Refcode:
JEMSAW

Visualising hydrogen bonds



Display Options

Display

Packing

Asymmetric Unit

Auto centre

Reset

Short ... < (sum of vdW radii)

H-Bon... Default definition

Contacts...

More Info ▾

Powder...

Options

Show hydrogens Depth cue

Show cell axes Z-Clipping

Label atoms Stereo

Click on a red contact to see the whole molecule

Turn on H-bond interactions using the tick box

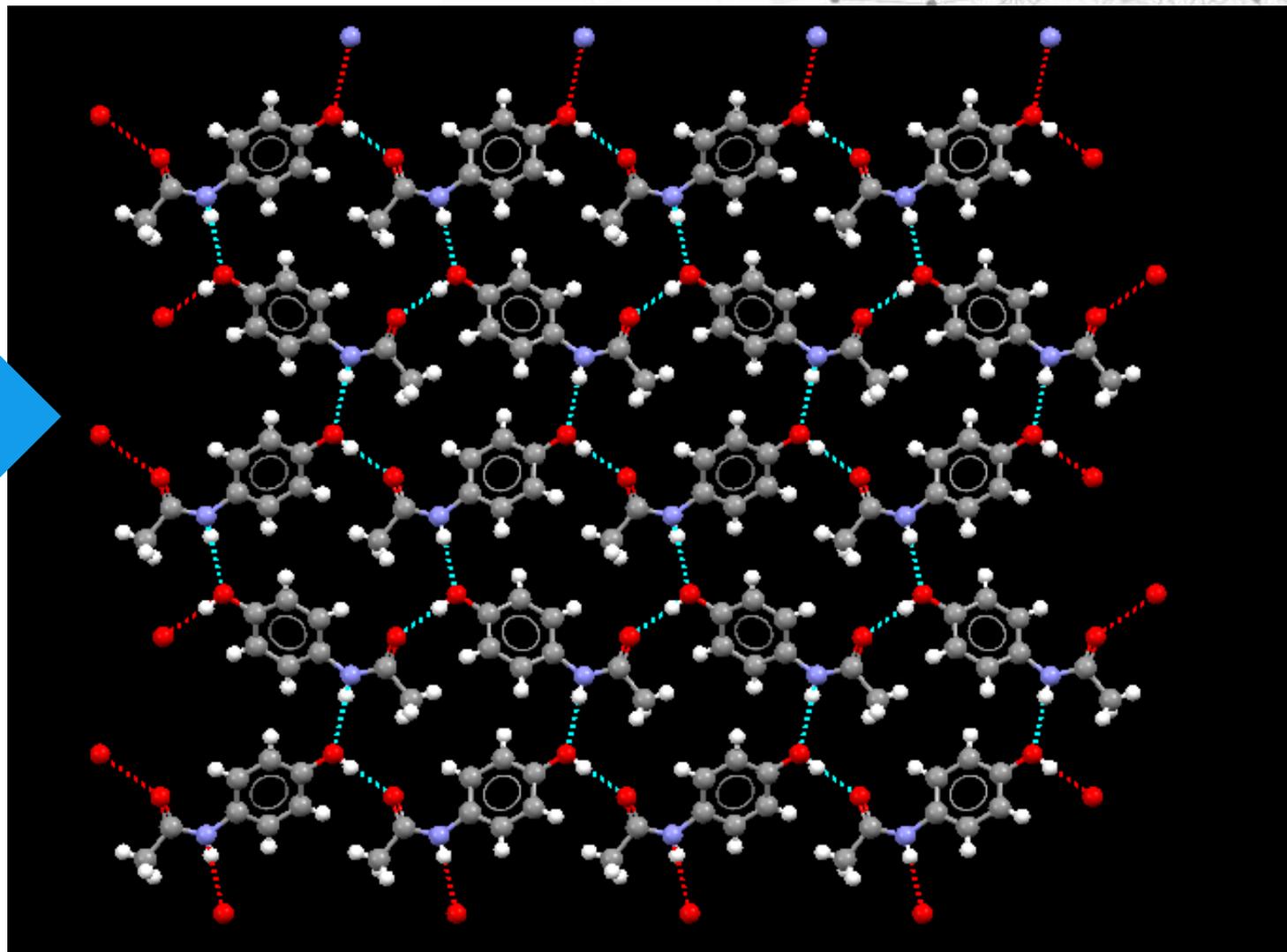
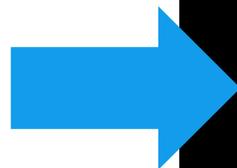
The screenshot shows the CSD software interface. At the top is a menu bar with options: File, Edit, Selection, Display, Calculate, CSD-Community, CSD-System, CSD-Materials, CSD-Discovery, CSD Python API, Help. Below the menu is a toolbar with 'Picking Mode: Expand Contacts', 'Clear Measurements', and 'Show Labels for All atoms'. The main window displays a ball-and-stick model of a molecule with red dashed lines representing hydrogen bonds. The 'Display Options' panel is open, showing 'H-Bon... Default definition' checked. The 'Structure Navigator' panel on the right lists crystal structures: HXACAN, HXACAN01, HXACAN02, HXACAN03, HXACAN04, HXACAN05, AN06, AN07, AN08, AN09, AN10.

Expand the H-bonds by clicking on the atoms at the end of the dashed lines.

CSD Refcode: HXACAN

Building the H-bond network

By clicking on the atoms at the end of the dashed lines



CSD Refcode: HXACAN

Colour H-bonds by distance

The screenshot shows the Mercury software interface. The 'Display' menu is open, and 'Contacts...' is selected. The 'Contact Colours' dialog box is also open, showing the 'Colour by distance' option selected. The main window displays a 3D molecular model with hydrogen bonds colored by distance.

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

Picking Mode: Expand Styles Labels Colours Show/Hide More Information Symmetry Elements... Voids... Voids (Experimental)... Display Options...

Style: Capped Sticks Animate... Clear Measurements Show Labels for Stereocentres with Stereochemistry Manage Styles... Cards Atom selections: Select by SMARTS:[c]

x-90 x+90 y-90 y+90 z-90 z+90 ← → ↓ ↑ zoom- zoom+

Contact Colours

Contact Colours

By expanded/hanging

Colour

select colour:

Colour by distance

short: mid: long:

Apply to:

All Contacts

Expanded Contacts

Hanging Contacts

Close

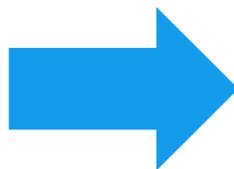
CSD Refcode:
HXACAN

Bonus: Graph Sets

CSD Refcode: SALMID02

Calculate CSD-Community

- Centroids...
- Planes...
- Packing/Slicing...
- Contacts...
- Molecular Shell...
- Graph Sets...**
- Powder Pattern...
- Structure Overlay...
- Molecule Overlay...



SALMID02 (I2/a) - Mercury

File Edit Selection Display Calculate CSD-Community CSD-System 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 Manage Styles... Cards Atom selections: Select by SMARTS:[c]

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+

Structure Navigator

SALMID02 Find

Crystal Structures Space: SALMID02 I2/a SALMID02 I2/a

Tree View

Multiple Structures Structures...

Graph Sets

descriptor ^	level
R2,2(8) >a>a	1
C1,1(6) b	1
S1,1(6) c	1
C2,2(8) >a<b	2
C2,2(10) >a>b	2
C4,4(18) >a>b<a<b	2
R6,6(28) >a<ba<b<b	2
R6,6(30) >a>b>b<a>b>b	2
R6,6(32) >a>b>b>a>b>b	2

Options

Graph Sets describe the H-bonds pattern. Learn more in the *Dictionary* on the handout.

Adding, moving and sizing labels

The screenshot displays the Mercury software interface for the structure ADECIW01 (P21/c) - Mercury. The top menu bar includes File, Edit, Selection, Display, Calculate, CSD-Community, CSD-System, CSD-Materials, CSD-Discovery, CSD Python API, and Help. The 'Display' menu is open, showing options like Styles, Labels, Colours, Show/Hide, More Information, Symmetry Elements..., Voids..., Voids (Experimental)..., Display Options..., Manage Styles..., View along, Dial box..., Splash screen, and Toolbars. The 'Labels' sub-menu is also open, listing Atoms..., Centroids..., Planes..., Label all, Clear all labels, Reset label positions, Label colour..., and Label size... (which is highlighted). The main window shows a ball-and-stick model of a molecule with atoms labeled O1, O2, O3, O4, N1, N2, and S1. The interface includes a toolbar with 'Picking Mode: Move Labels', 'Clear Measurements', and 'Show Labels for Non C,H' (checked). The style is set to 'Ball and Stick' and the color is 'by Element'. The 'Select by SMARTS' field contains '[c]'.

CSD Refcode: ADECIW01

Labelling chiral molecules

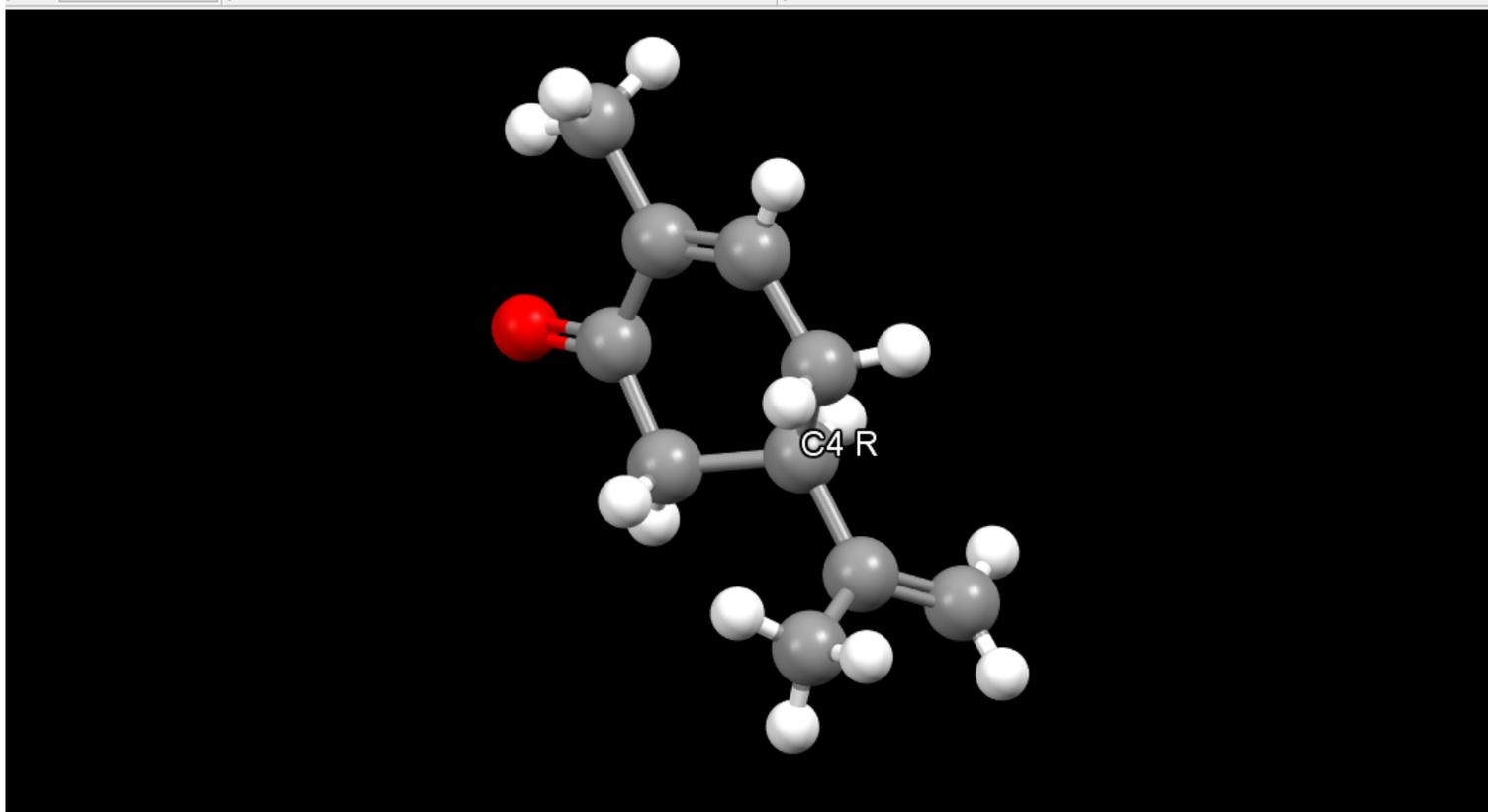
RERXIV (P212121) - Mercury

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

Picking Mode: Pick Atoms Clear Measurements Show Labels for Stereocentres with Stereochemistry

Style: Ball and Stick Colour: by Element Manage Styles... Cards Atom selections: Select by SMARTS: [c]

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+



Structure Navigator

RERXIV	Find
Crystal Structures	Space
RERXIV	P2121
RERXIW	Pnma
RERXIX	C2/c
RERXIY	P-1
RERXOB	Pcmn
RERXOC	P21/c

Tree View

Multiple Structures

Structures...

Structure Navigator Searches

Graph Sets

No graph sets found

CSD Refcode:
RERXIV

Symmetry

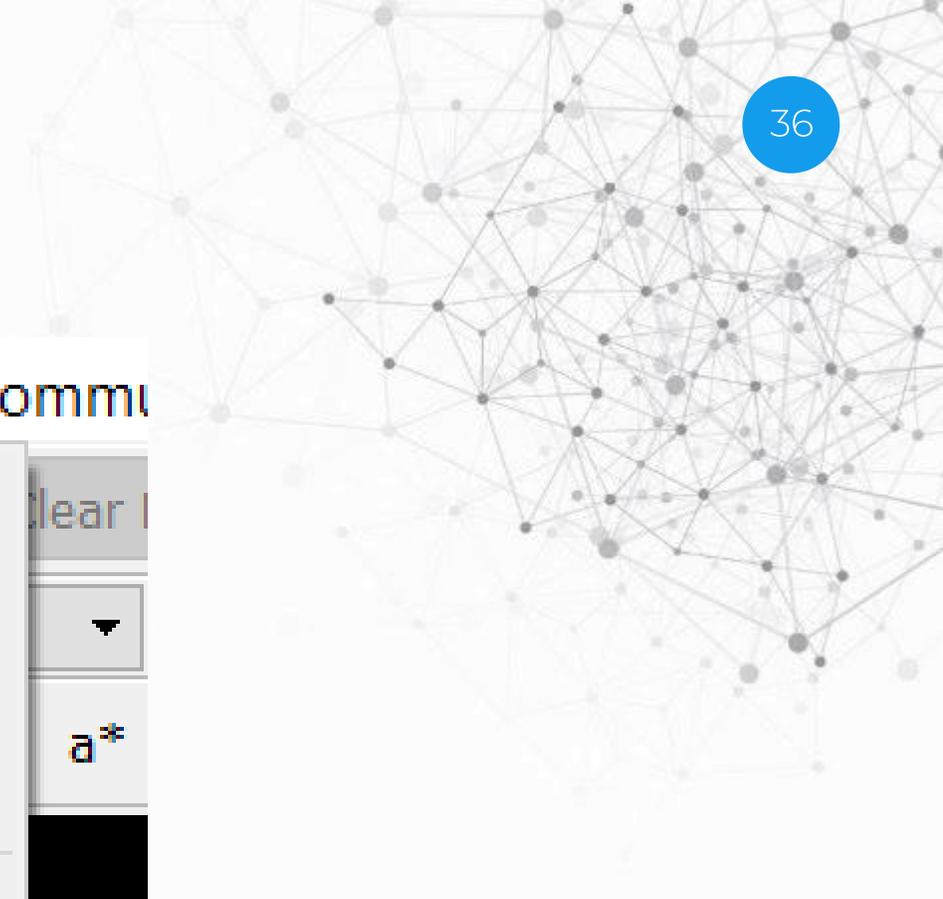
File Edit Selection **Display** Calculate CSD-Comm

Picking Mode: Pick Atoms

Style: Capped Sticks

Animate... Def

- Styles
- Labels
- Colours
- Show/Hide
- More Information
- Symmetry Elements...**
- Voids...



Show Symmetry Elements

Show Inversions

Show Colour Size 0.22

Show Axes

Show proper rotation axes

Show screw axes Show arrows

Show rotoinversion axes

2-fold Colour 3-fold Colour

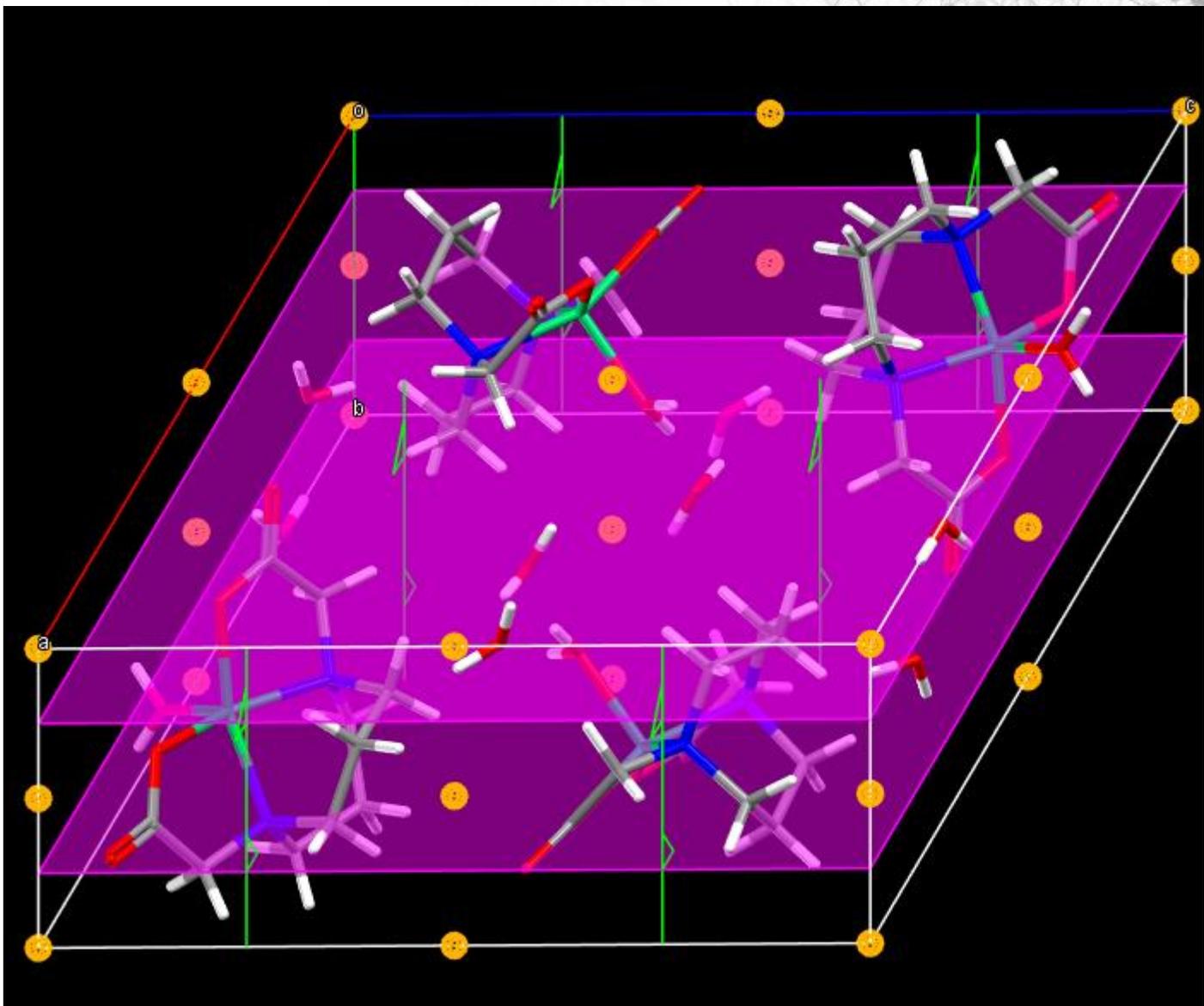
4-fold Colour 6-fold Colour

Show Glide & Mirror Planes

Show mirrors Colour 0.51

Show glides Colour 0.49

Shadows



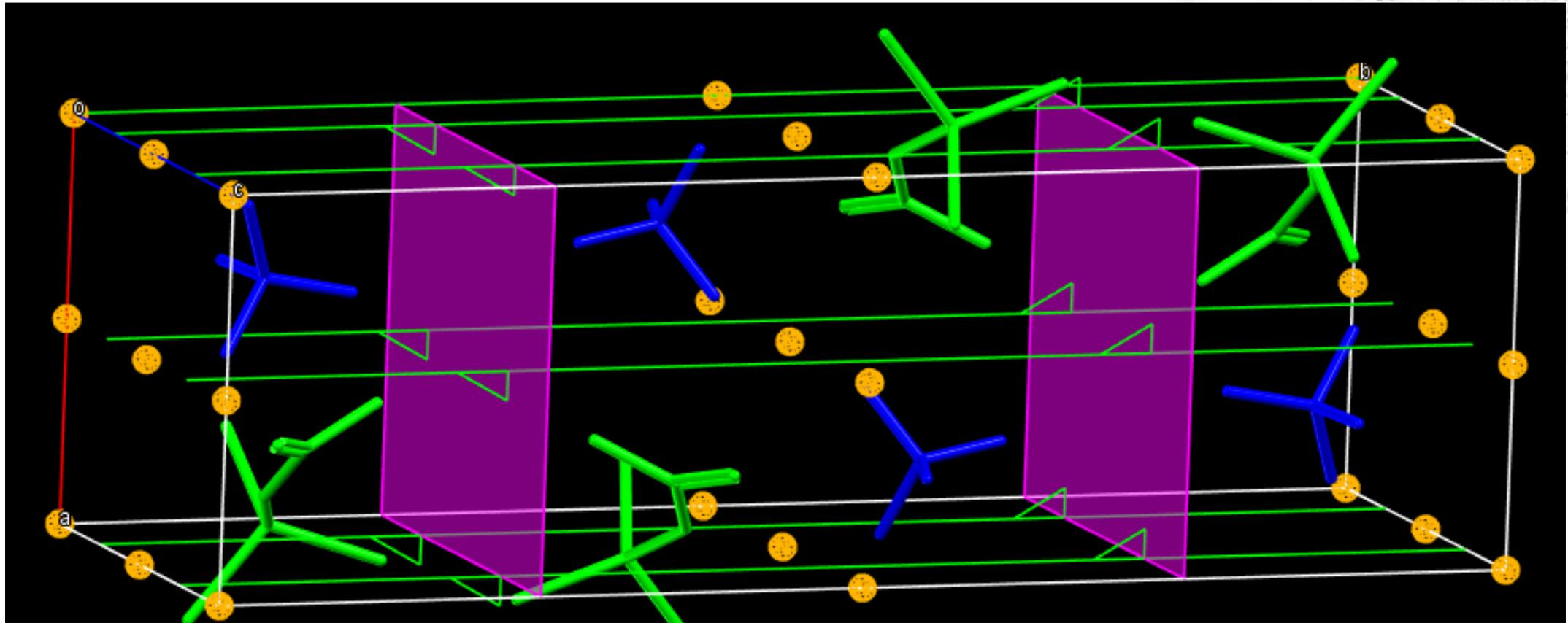
File Edit Selection Display Calculate CSD-Community CSD

Picking Mode: Lasso Atoms Clear Measurement

Style: Capped Sticks Colour: by Element Manage

Animate... Default view b* c*

- by Element
- by Symmetry equivalence**
- by Atomic displacement
- by Symmetry operation
- by Gasteiger charge
- by Partial charge
- by Element or Suppression



Calculating and visualising planes

The screenshot displays the Mercury software interface for the WUTTEM (Pbca) - Mercury structure. The 'Calculate' menu is open, with 'Planes...' selected. A 'Planes' dialog box is open, showing a list of planes with 'mean: C9 C6 C11' selected. The 'Plane Properties' dialog box is also open, showing options for calculating a mean plane from three atoms (C9, C6, C11). The 'Plane Properties' dialog has the following settings:

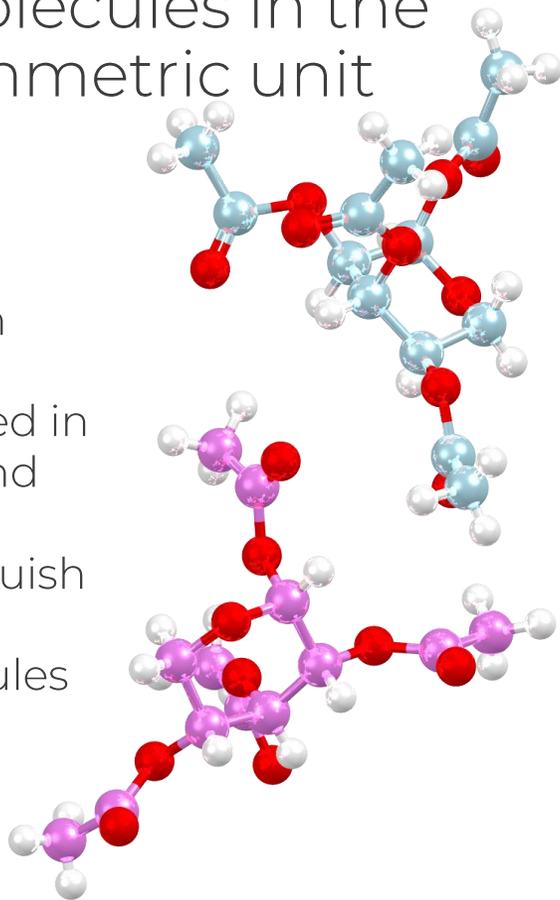
- Mean plane: hkl
- Select at least three atoms to calculate least squares plane:
- Pick atom to select:
 - Picked atom
 - Picked molecule
 - Ring
- Or select:
 - All
 - Non-hydrogen
 - Hydrogen
- Show:
- Label: mean:
- Transparent:
- Colour:

The main window shows a 3D ball-and-stick model of the molecule with a blue and yellow plane overlaid. The plane is labeled 'mean: C9 C6 C11'. Atoms C9, C6, and C11 are highlighted with dashed circles. Other atoms shown include C14, C16, and C18.

CSD Refcode:
WUTTEM

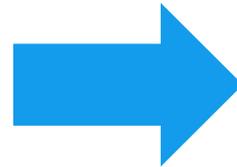
Molecule overlay

2 molecules in the asymmetric unit



Carbon atoms coloured in blue and pink to distinguish the molecules

compare their conformation overlapping them



File Edit Selection Display Calculate CSD-Community

Picking Mode: Pick Atoms

Style: Capped Sticks Colour: by

Animate... Default view: k

Structure Navigator

AAADRIB Find

Crystal Structures Spacegroup

Databases

CSD 5.40

AABHTZ P-1

AACANI10 P21/c

Calculate

- Centroids...
- Planes...
- Packing/Slicing...
- Contacts...
- Molecular Shell...
- Graph Sets...
- Powder Pattern...
- Structure Overlay...
- Molecule Overlay...

Options

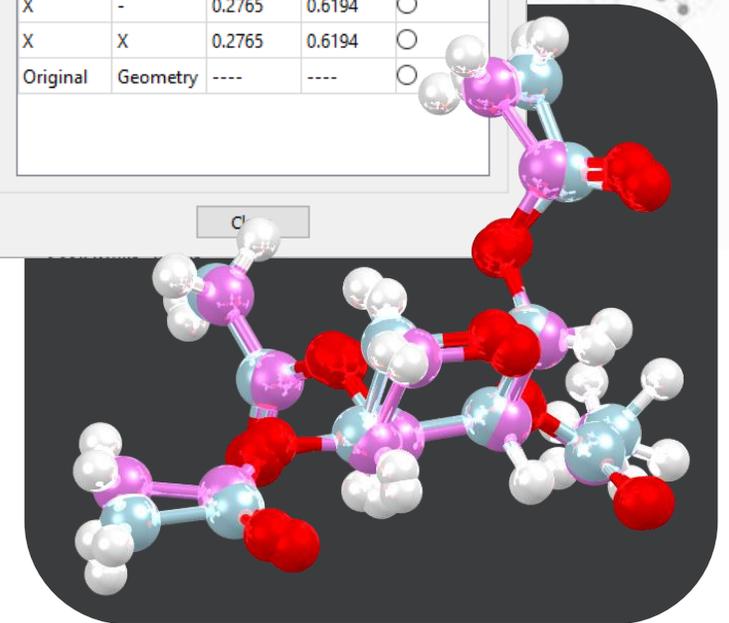
Select **two molecules** (by selecting at least one atom in each) then press **Overlay**. The molecules must have at least three atoms, and the same number of atoms. After overlay is complete you must select **Reset** before repeating the overlay or selecting different molecules.

Reset

Results

Flexibility	Inversion	RMSD	Max. D	Display
-	-	0.5452	1.3503	<input checked="" type="radio"/>
-	X	0.5452	1.3503	<input type="radio"/>
X	-	0.2765	0.6194	<input type="radio"/>
X	X	0.2765	0.6194	<input type="radio"/>
Original	Geometry	----	----	<input type="radio"/>

Overlay



Structure overlay

CSD Refcodes: VIRAZL, FOQROU
(light blue – pink)

Tick Multiple structures to load more than one structure

Structure Navigator

VIRAZL Find

Crystal Structures Spacegr

VIRAZL	P2121;
VIRAZL01	P2121;
VIRBAA	P21/m
VIRBAB	P21/n
VIRBAZ	P-31c
VIRBED	P-1

<< >>

Tree View

Multiple Structures

Structures...

File Edit Selection Display Calculate CSD-Community

Picking Mode: Pick Atoms

Style: Capped Sticks Colour: by

Animate... Default view: b

Structure Navigator

AADRIB Find

Crystal Structures Spacegr

Databases

CSD 5.40

AABHTZ	P-1
AACANI10	P21/c

Centroids...

Planes...

Packing/Slicing...

Contacts...

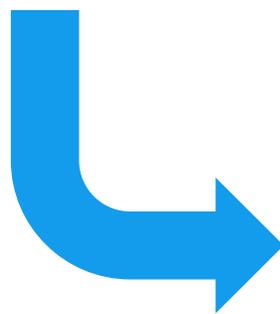
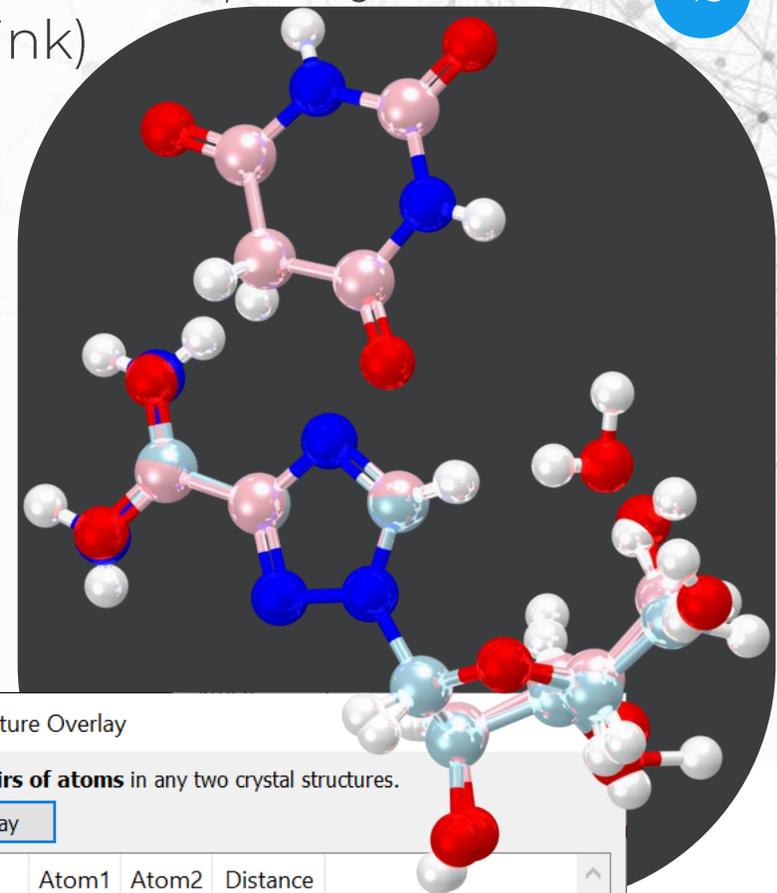
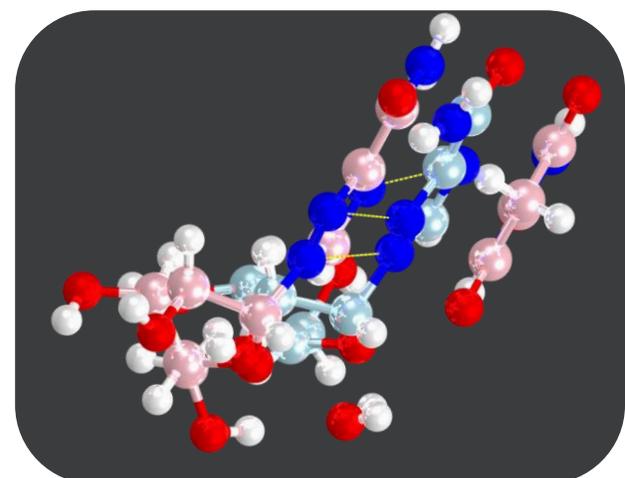
Molecular Shell...

Graph Sets...

Powder Pattern...

Structure Overlay...

Molecule Overlay...



Structure Overlay

Select **pairs of atoms** in any two crystal structures.

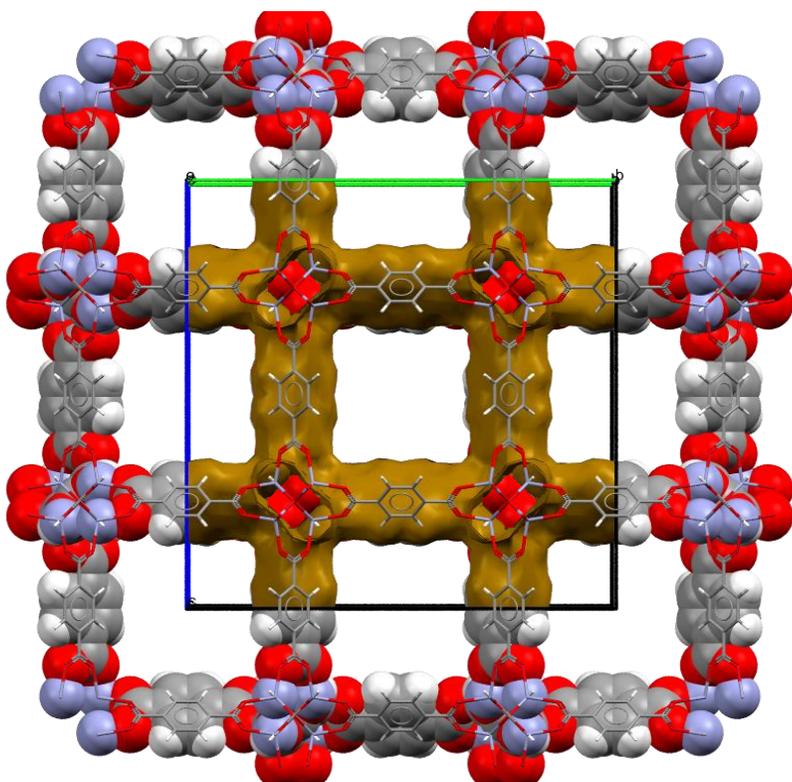
Overlay

	Atom1	Atom2	Distance
1	Delete	N2 N3	0.010
2	Delete	N3 N5	0.001
3	Delete	N1 N2	0.010

RMS: **0.00795**

Close

Empty space visualisation



CSD Refcode: SAHYIK
(MOF5)

Display Calculate CSD-Community

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

Find any empty spaces (**voids**) in crystal unit cells that are big enough to hold a spherical "probe" of the given radius. Decrease the **Probe Radius** to find smaller spaces. Decrease the **Grid Spacing** to create smoother surfaces. To see voids in more than one unit cell, use the **Packing/Slicing** dialog to turn on packing and increase the ranges along a, b and c.

Show

Probe Radius: Å

Approx. Grid Spacing: Å

Calculate using the

Display Options

Outside Colour:

Inside Colour:

Results

Volume % of unit cell volume

Å³

Defaults OK Apply **Cancel**

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

Clear Measurements Show Labels for All atoms with Atom La

Manage Styles... 3D Print Atom selections: Select by SMARTS

a b c a* b* c* x- x+ y- y+ z- z+ x-90 x+90 y-90 y+90 z-90 z+90 ← →

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

Settings

Output Directory documents/Education Browse...

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

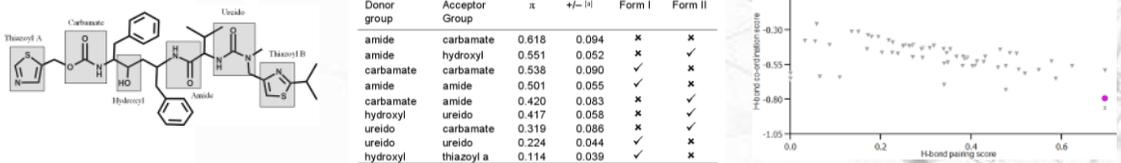


What else can you explore in Mercury?

CSD Python API functionalities

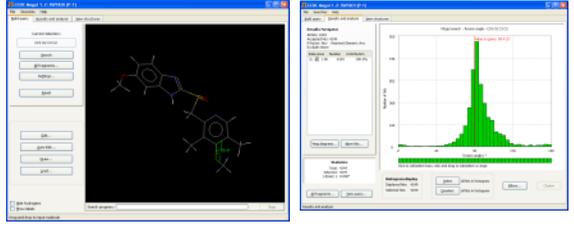
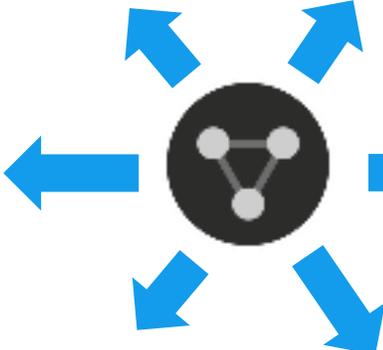


Hydrogen bond propensity

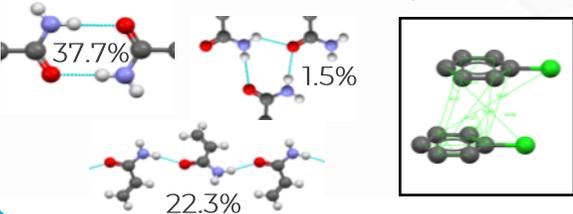


Donor group	Acceptor Group	π	$+/- n $	Form I	Form II
amide	carbamate	0.618	0.094	x	x
amide	hydroxyl	0.551	0.052	x	✓
carbamate	carbamate	0.538	0.090	✓	x
amide	amide	0.501	0.055	✓	x
carbamate	amide	0.420	0.083	x	x
hydroxyl	ureido	0.417	0.058	x	✓
ureido	carbamate	0.319	0.086	x	✓
ureido	ureido	0.224	0.044	✓	✓
hydroxyl	thiazoyl a	0.114	0.039	✓	x

Mogul geometry library

Motif & packing feature frequency



CSD Materials

Videos

POV-Ray Image

Width (pixels) 900 Height (pixels) 900

Material Properties Metallic File Format PNG

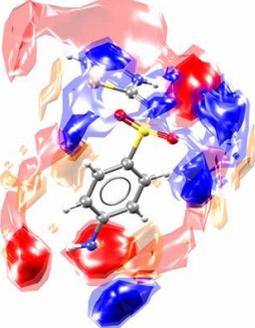
Background Transparent Custom Color

Generate Animation Frames

Rotate around x y z Number of Frames 30

Preview Render Close

Full Interaction Maps



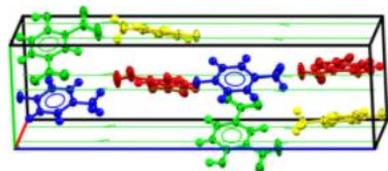
CSD Materials & CSD Discovery

...and more!



Want to explore more?

Educational Resources



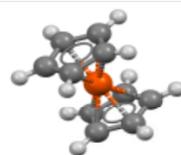
CSD-System

Essential crystallographic and structural chemistry capabilities.

The wealth of information contained within the Cambridge Structural Database (CSD) extends far beyond a collection of crystal structures. Knowledge derived from these materials informs much of chemistry, biochemistry, and biology. Chemical and structural concepts are often difficult to grasp without real world, interactive examples for students to explore.

The CCDC and our colleagues continually produce educational materials for use in classroom and computer lab settings, or as independent study modules. Many of these materials make use of the Teaching Subset - a freely available set of over 750 structures that can be investigated with the free version of our Mercury visualisation and analysis program. Of course, our database of over one million entries are available for free through our Access Structures portal.

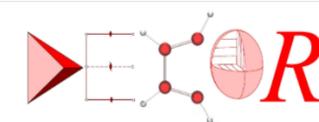
If you are an educator looking for supplementary teaching materials, find out more about the Teaching Database [here](#). If you have developed your own modules using the CSD and would like to share them with the broader community, please contact us at education@ccdc.cam.ac.uk.



Information on the Teaching Subset



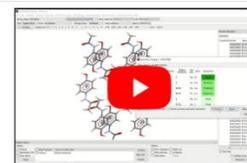
Access a series of teaching modules for use in the classroom



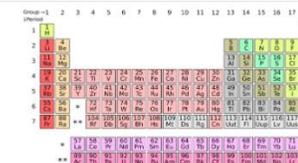
DECOR: Educational Resources for Teaching Crystallography



Download a series of self-guided workshop materials for CCDC tools and features



Watch software training and support videos



Explore the Periodic Table through Crystal Structures



Access fun science activities for kids through the CCDC Home learning page

Self-guided workshops
<https://www.ccdc.cam.ac.uk/Community/educationalresources/workshop-materials/>

YouTube and LabTube channels links from
<https://www.ccdc.cam.ac.uk/Community/educationalresources/ccdc-videos/>