

Visualising structures using Mercury



Learning outcomes for Workshop

- Familiarise yourself with the Mercury interface
- Learn the basic options to visualise small molecule crystal structures
- Visualise the packing of a structure effectively
- Obtain extra information from a structure
- Create high quality images of crystal structures

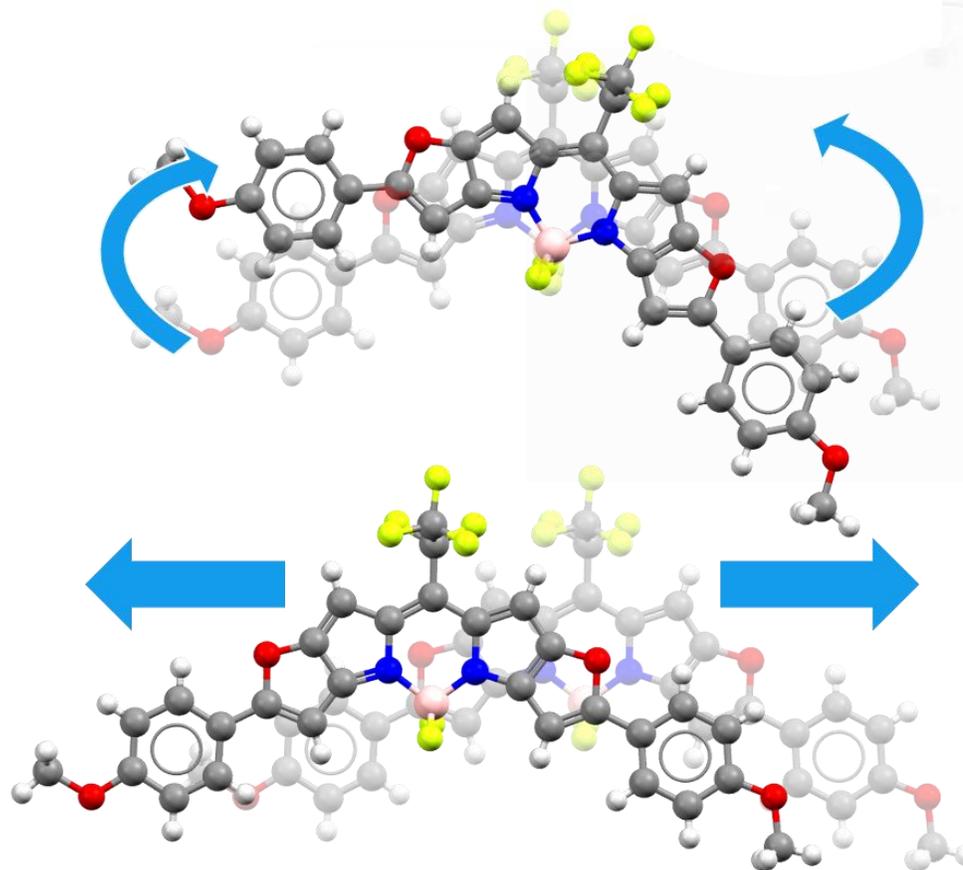
Mouse basics

- **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



Moving and rotating on the plane

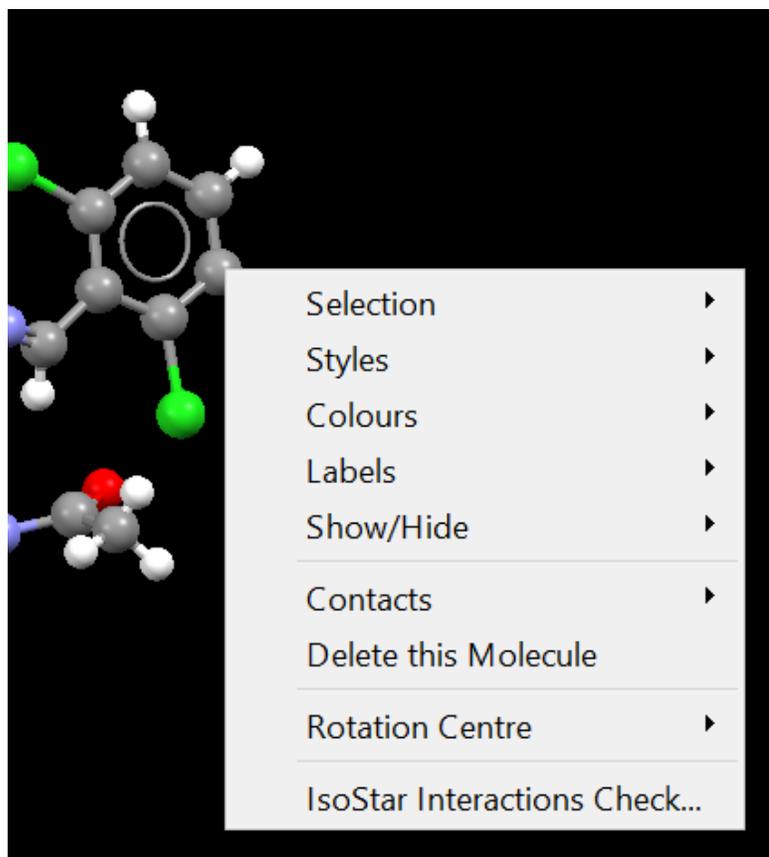
With the keyboard:



CSD Refcode: GIMXUY

Right mouse click

Near a molecule



Away from a molecule



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

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

AACRUB

Find

Crystal Structures

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

<<

>>

 Tree View Multiple Structures

Structures...

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

Picking Mode: Pick Atom

Style: Capped Sticks

 Animate...

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

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

Graph Sets

Intermolecular Potentials

Searches

Post Search Options

 Structure Navigator

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

Changing display - Style

Display Calculate CSD-Community CSD-System CSD-M

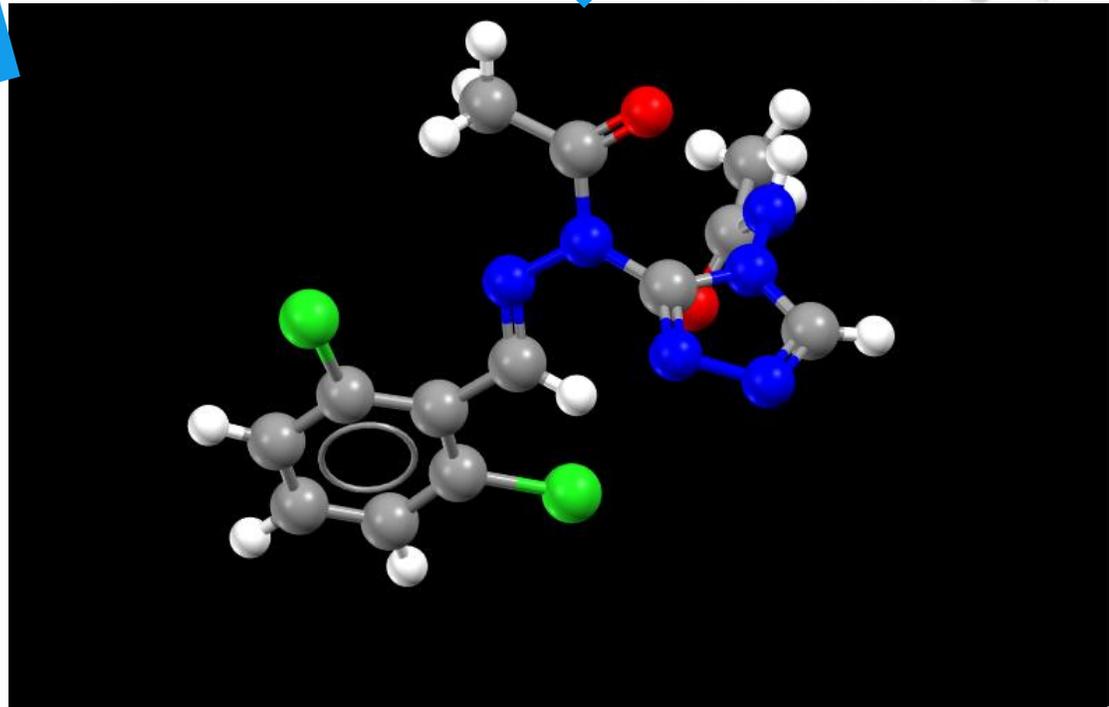
- Styles ▶
 - Wireframe
 - Stick
 - Ball and stick**
 - Spacefill
 - Ellipsoid
 - Polyhedral
- Labels ▶
- Colours ▶
- Show/Hide ▶
- More Information ▶
- Symmetry Elements...
- Voids...
- Display Options...
- Manage Styles...
- View along ▶
- Dial box...
- ✓ Splash screen
- Toolbars ▶

File Edit Selection Display Calculate C...

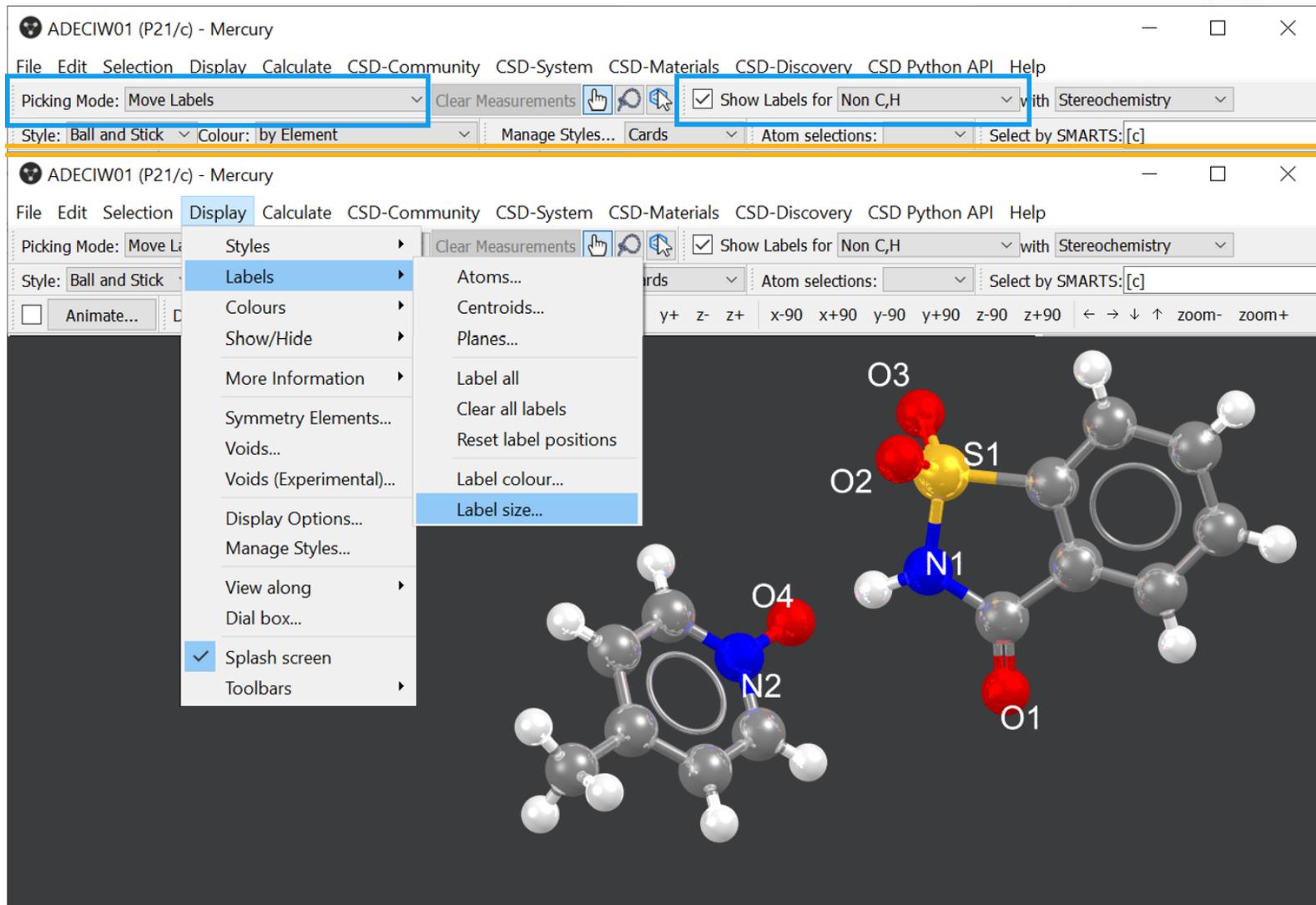
Picking Mode: Pick Atoms

Style: **Ball and Stick** ▼ Colour: by Element

Animate... Fault view: b ▼



Adding, moving and sizing labels



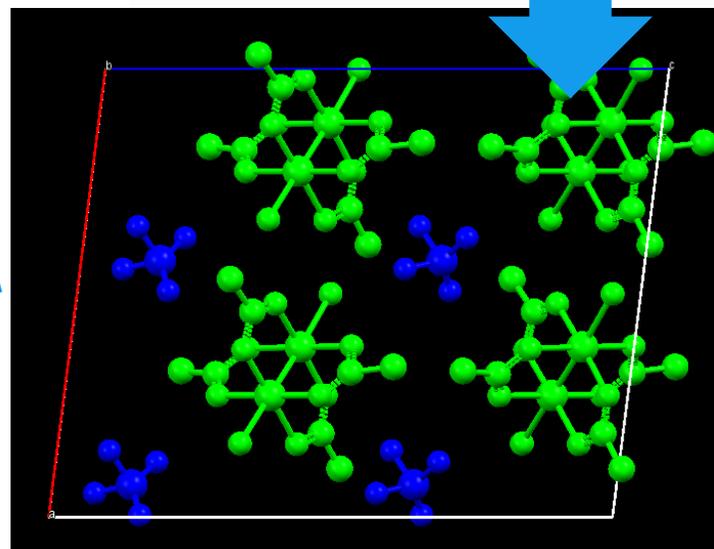
ADECIW01 (P21/c) - Mercury
 File Edit Selection Display Calculate CSD-Community CSD-System CSD-Materials CSD-Discovery CSD Python API Help
 Picking Mode: Move Labels Clear Measurements Show Labels for Non C,H with Stereochemistry
 Style: Ball and Stick Colour: by Element Manage Styles... Cards Atom selections: Select by SMARTS:[c]

ADECIW01 (P21/c) - Mercury
 File Edit Selection **Display** Calculate CSD-Community CSD-System CSD-Materials CSD-Discovery CSD Python API Help
 Picking Mode: Move Labels Styles Labels Colours Show/Hide More Information Symmetry Elements... Voids... Voids (Experimental)... Display Options... Manage Styles... View along Dial box... Splash screen Toolbars
 Labels Atoms... Centroids... Planes... Label all Clear all labels Reset label positions Label colour... **Label size...**

O3 O2 O4 N1 N2 S1 O1

CSD Refcode: ADECIW01

Changing display - colours



CSD Refcode: AACRUB

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

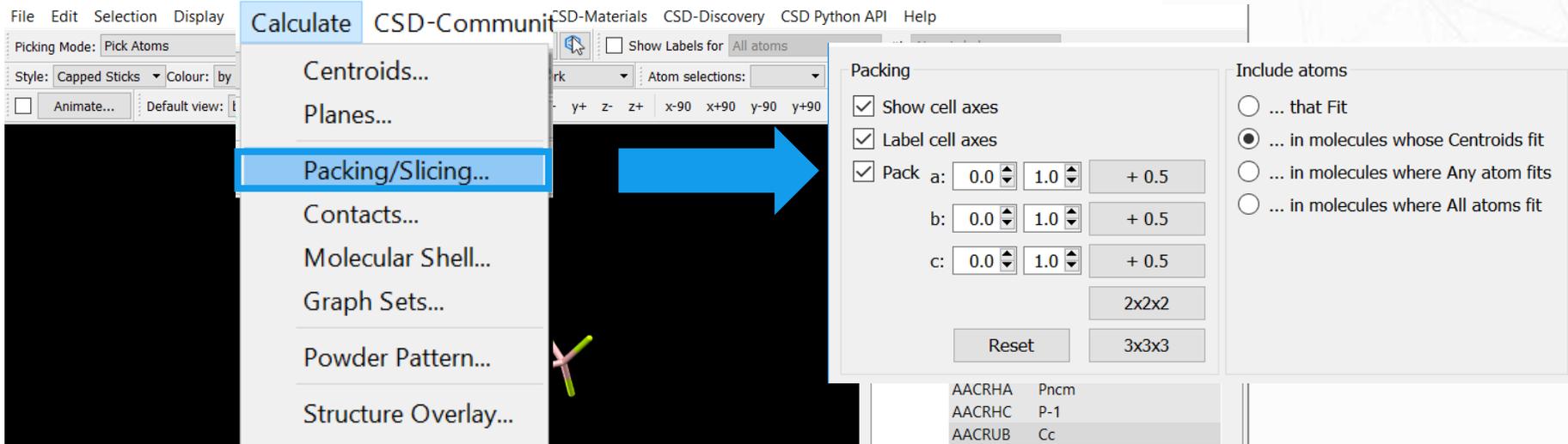
Sat: 0 Green: 255

Val: 255 Blue: 255

HTML: #ffffff

OK Cancel

Packing in a crystal structure



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

Picking Mode: Pick Atoms

Style: Capped Sticks Colour: by

Animate... Default view: t

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

Atom selections: All atoms

Atom selections: y+ z- z+ x-90 x+90 y-90 y+90

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

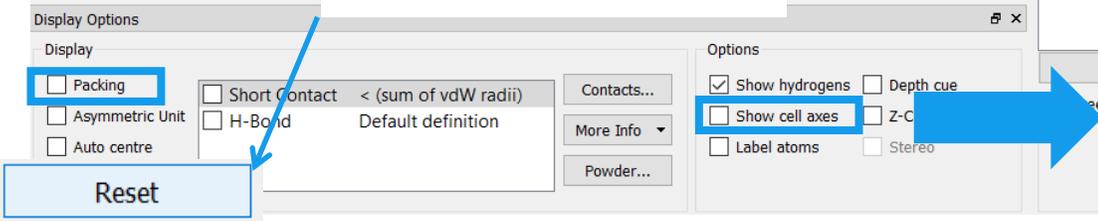
2x2x2
Reset 3x3x3

Include atoms

... that Fit
 ... in molecules whose Centroids fit
 ... in molecules where Any atom fits
 ... in molecules where All atoms fit

AACRHA Pncm
AACRHC P-1
AACRUB Cc

Reset button:
a friend!



Display Options

Display

Packing
 Asymmetric Unit
 Auto centre

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

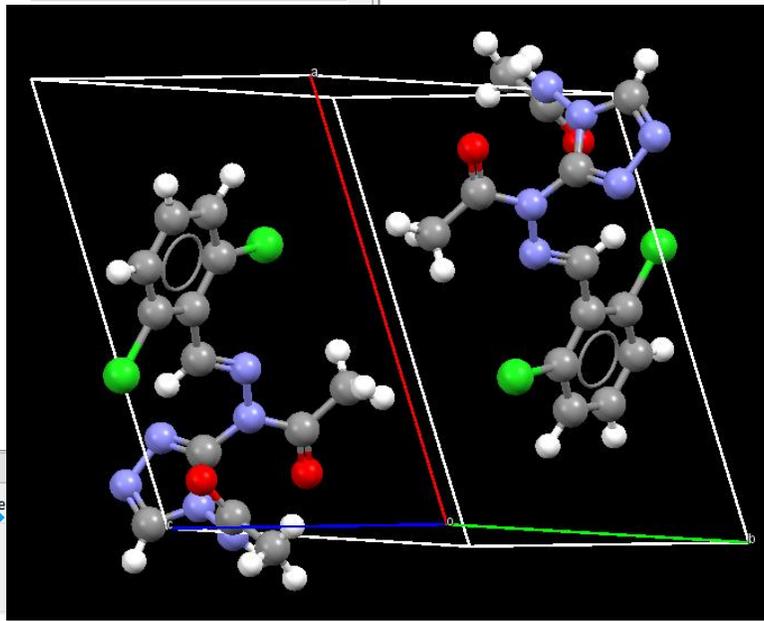
Contacts...
More Info
Powder...

Options

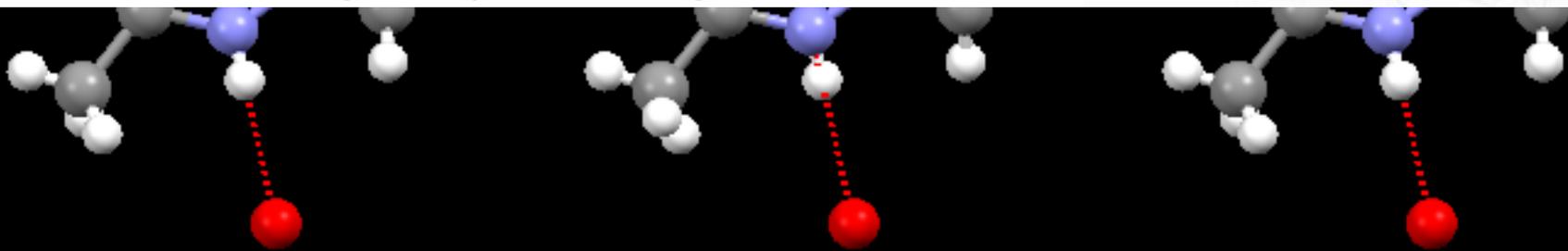
Show hydrogens
 Show cell axes
 Label atoms

Depth cue
 Z-C
 Stereo

Reset



Visualising hydrogen bonds



Display Options

Display

- Packing
- Asymmetric Unit
- Auto centre

Short ... < (sum of vdW radii)
 H-Bon... Default definition

Reset

Contacts...
 More Info ▾
 Powder...

Options

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

Click on a red contact to see the whole molecule

Turn on H-bond interactions using the tick box

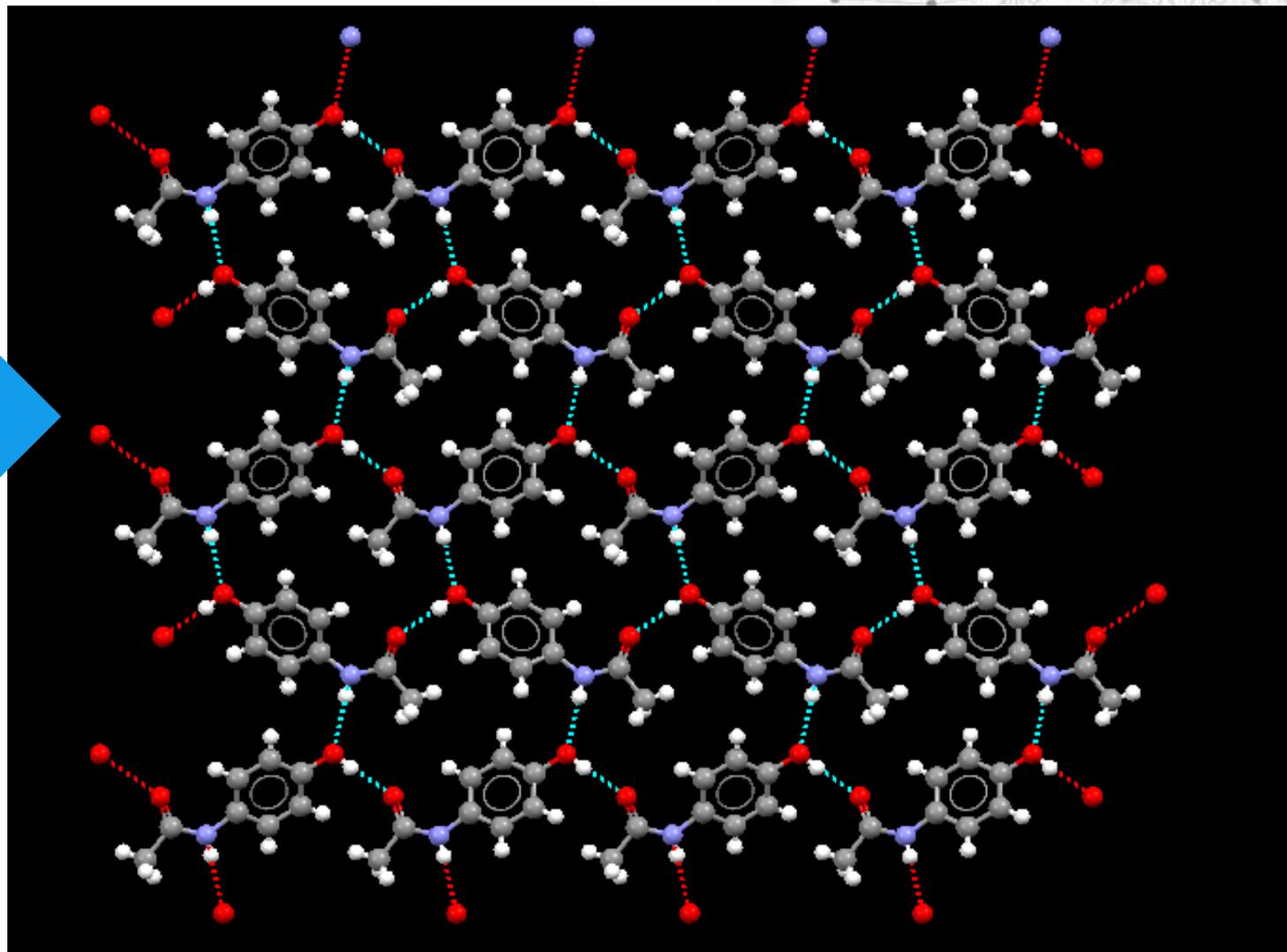
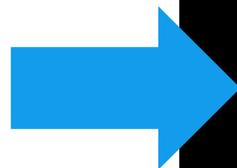
The screenshot shows the CSD software interface. At the top is a menu bar with options like File, Edit, Selection, Display, Calculate, CSD-Community, CSD-System, CSD-Materials, CSD-Discovery, CSD Python API, and Help. Below the menu is a toolbar with various icons and settings, including 'Picking Mode: Expand Contacts', 'Clear Measurements', 'Show Labels for All atoms', 'Style: Ball and Stick', 'Colour: by Element', 'Manage Styles...', 'Work', and 'Atom selections:'. The main window displays a ball-and-stick model of a molecule with several red dashed lines representing hydrogen bonds. A 'Structure Navigator' panel on the right lists crystal structures: HXACAN, HXACAN01, HXACAN02, HXACAN03, HXACAN04, HXACAN05, AN06, AN07, AN08, AN09, and AN10. The 'Display Options' panel at the bottom left has a 'Display' section with checkboxes for 'Packing', 'Asymmetric Unit', and 'Auto centre'. A 'Short < (sum of vdW radii)' checkbox is also present. The 'H-Bon... Default definition' checkbox is checked and highlighted with a blue box. A blue arrow points from the text 'Turn on H-bond interactions using the tick box' to this checkbox. Another blue arrow points from the text 'Expand the H-bonds by clicking on the atoms at the end of the dashed lines.' to one of the red dashed lines in the molecular model. At the bottom of the interface, there is a text prompt: 'Click on a red contact to see the whole molecule'.

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

CSD Refcode: HXACAN

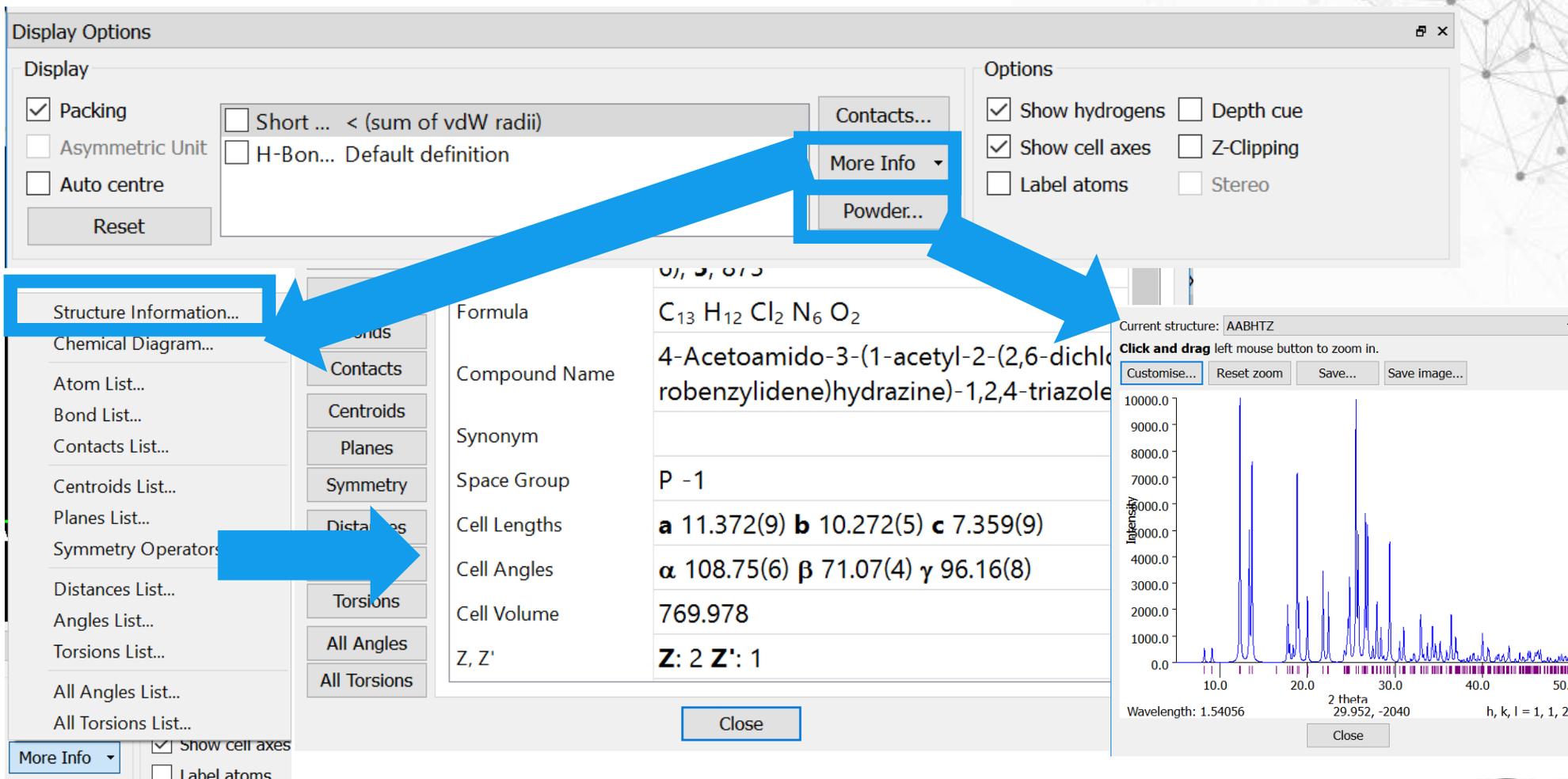
Building the H-bond network

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



CSD Refcode: HXACAN

Generating a powder pattern



The screenshot shows the 'Display Options' window with the 'More Info' dropdown menu open. The 'More Info' menu is highlighted with a blue box, and a blue arrow points from it to the 'Structure Information...' dialog box. Another blue arrow points from the 'Powder...' button in the 'More Info' menu to the powder pattern plot.

Display Options

Display

- Packing
- Asymmetric Unit
- Auto centre
- Reset

Options

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

Structure Information...

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

Compound Name: 4-Acetoamido-3-(1-acetyl-2-(2,6-dichlorobenzylidene)hydrazine)-1,2,4-triazole

Synonym:

Space Group: P -1

Cell Lengths: **a** 11.372(9) **b** 10.272(5) **c** 7.359(9)

Cell Angles: α 108.75(6) β 71.07(4) γ 96.16(8)

Cell Volume: 769.978

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

Close

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

Calculating centroids

The screenshot shows the Mercury software interface for calculating centroids. The 'Calculate' menu is open, and 'Centroids...' is selected. The 'Centroids' dialog box is open, and the 'New Centroid...' button is highlighted. The 'Centroid Properties' dialog box is also open, showing options to create a centroid from a picked atom, molecule, or ring. The main window displays a 3D ball-and-stick model of a molecule with a red centroid point labeled 'centroid: 1' and a blue dashed circle around it.

CSD Refcode:
YAKBES

Calculating and visualising planes

WUTTEM (Pbca) - Mercury

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

Picking Mode: Pick Atoms

Style: Ball and Stick Colour: Centroids... Planes... Packing/Slicing... Contacts...

Show Labels for All atoms with Atom Label

Manage Styles... Cards Atom selections: Select by SMARTS: [c]

b* c* x- x+ y- y+ z- z+ x-90 x+90 y-90 y+90 z-90 z+90 ← → ↓ ↑ zoom- zoom+

mean: C9 C6 C11

Planes

Pick an object from the list below, or graphics window, or right-click on a

mean: C9 C6 C11

New Plane... Edit... Close

Plane Properties

Mean plane hkl

Select at least three atoms to calculate least squares plane:

Pick atom to select:

Picked atom
 Picked molecule
 Ring

Or select:

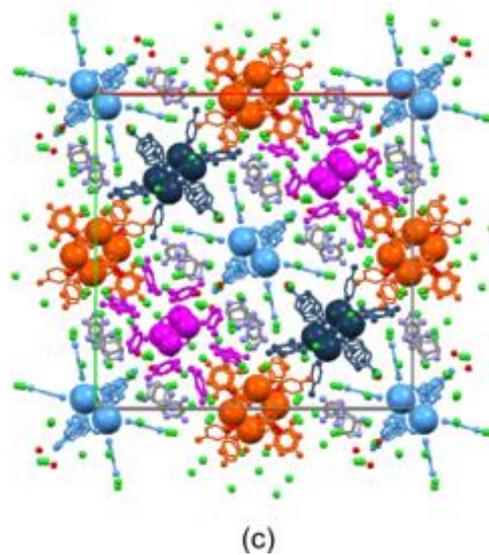
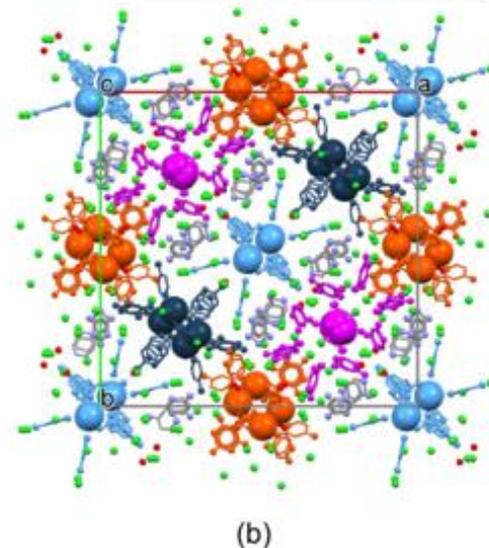
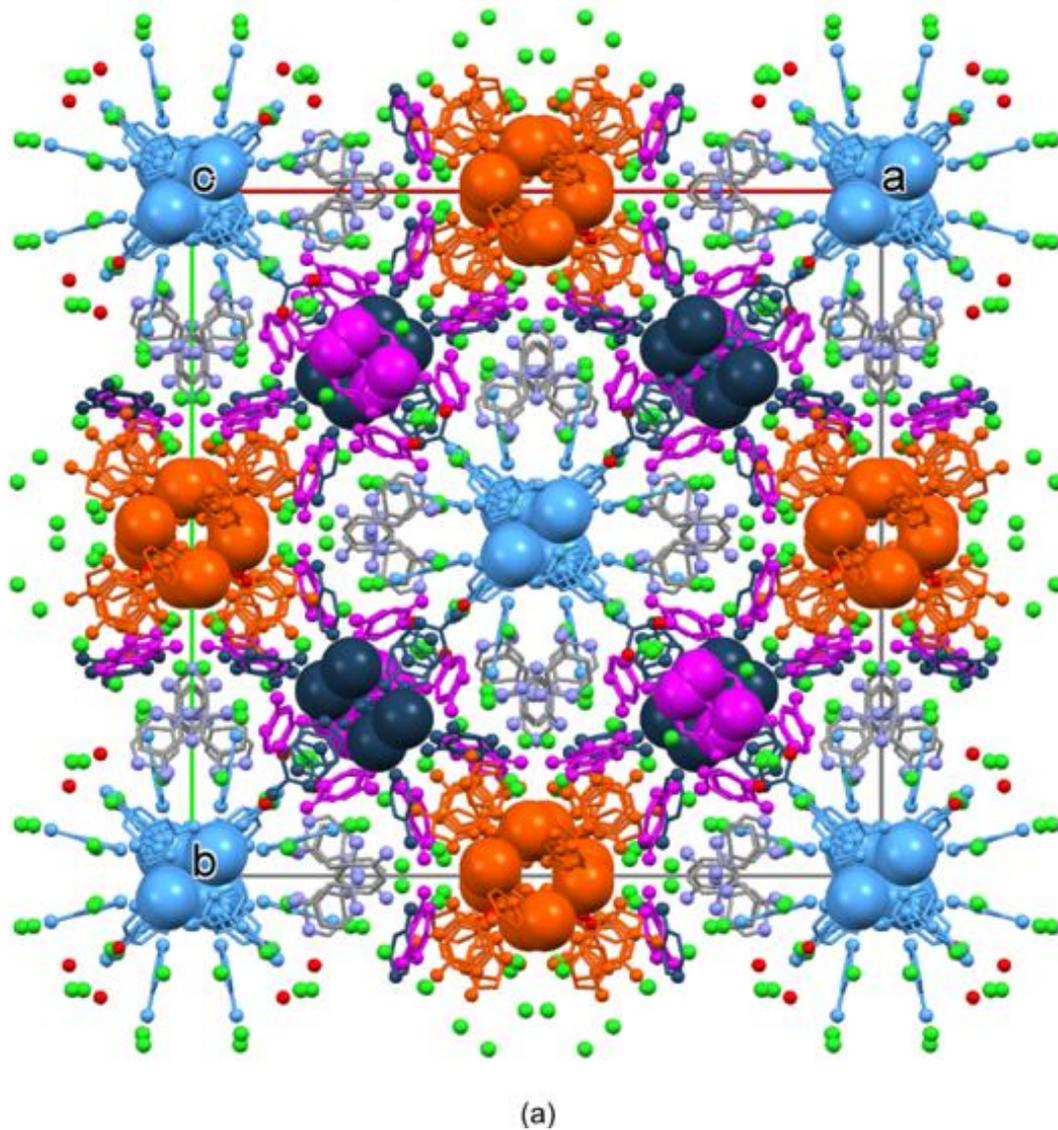
All
 Non-hydrogen
 Hydrogen

Show
 Label mean:
 Transparent
 Colour:

OK Cancel

CSD Refcode:
WUTTEM

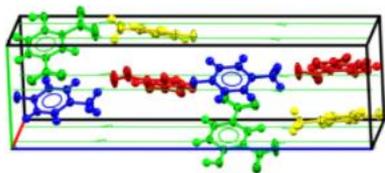
What is possible?



Nature 590, 275–278 (2021).
<https://doi.org/10.1038/s41586-021-03194-y>

Want to explore more?

Educational Resources



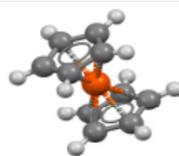
CSD-System

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.

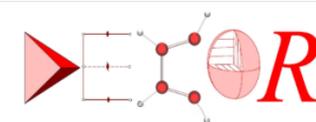
If you are an educator looking for supplementary teaching materials, find out more about the Teaching Database [here](#). If you have developed your own modules using the CSD and would like to share them with the broader community, please contact us at education@ccdc.cam.ac.uk.



Information on the Teaching Subset



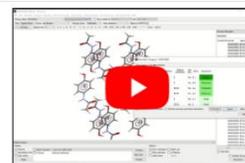
Access a series of teaching modules for use in the classroom



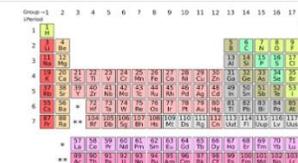
DECOR: Educational Resources for Teaching Crystallography



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/>