ncs | UK National Crystallography Service

Visualising structures using Mercury

CCDC
advancing structural science

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

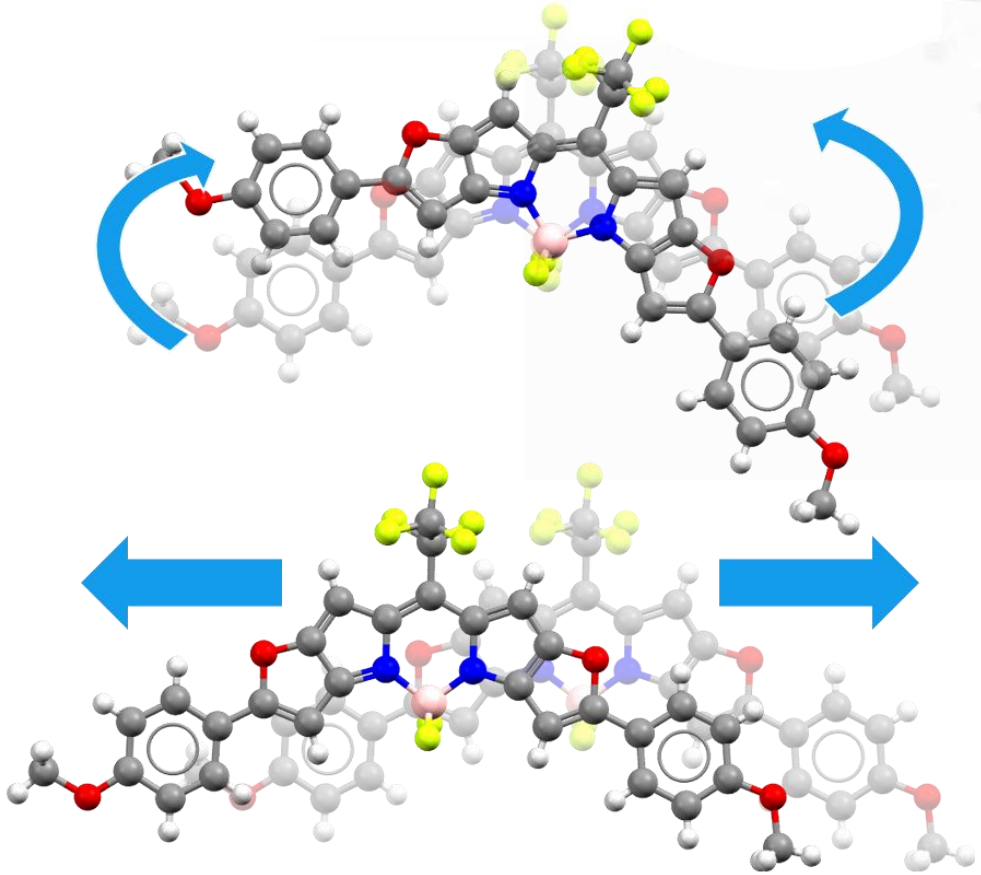
Mouse basics

- 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

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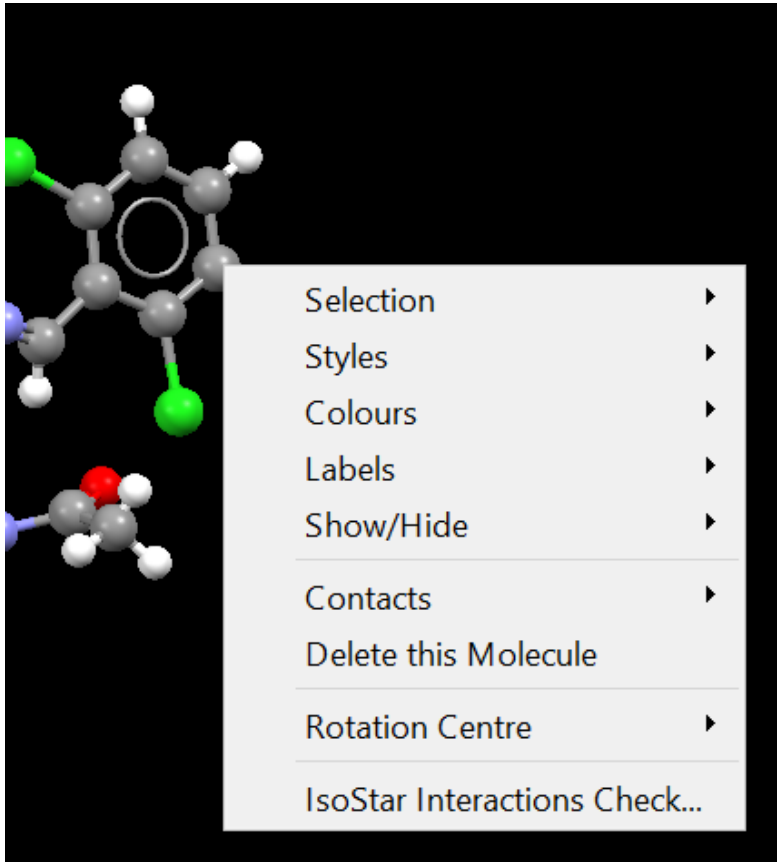
Right mouse click

Near a molecule



Away from a molecule

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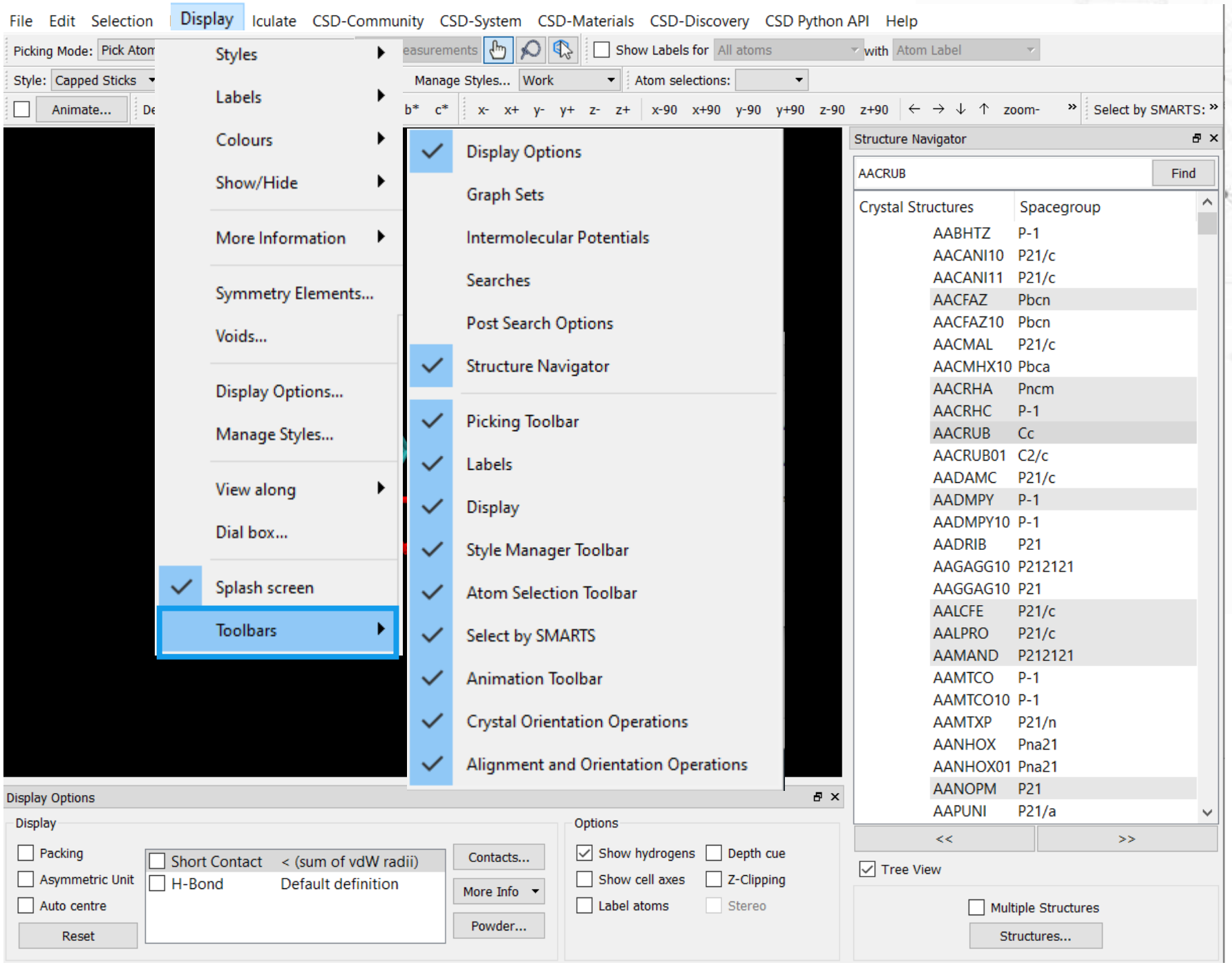
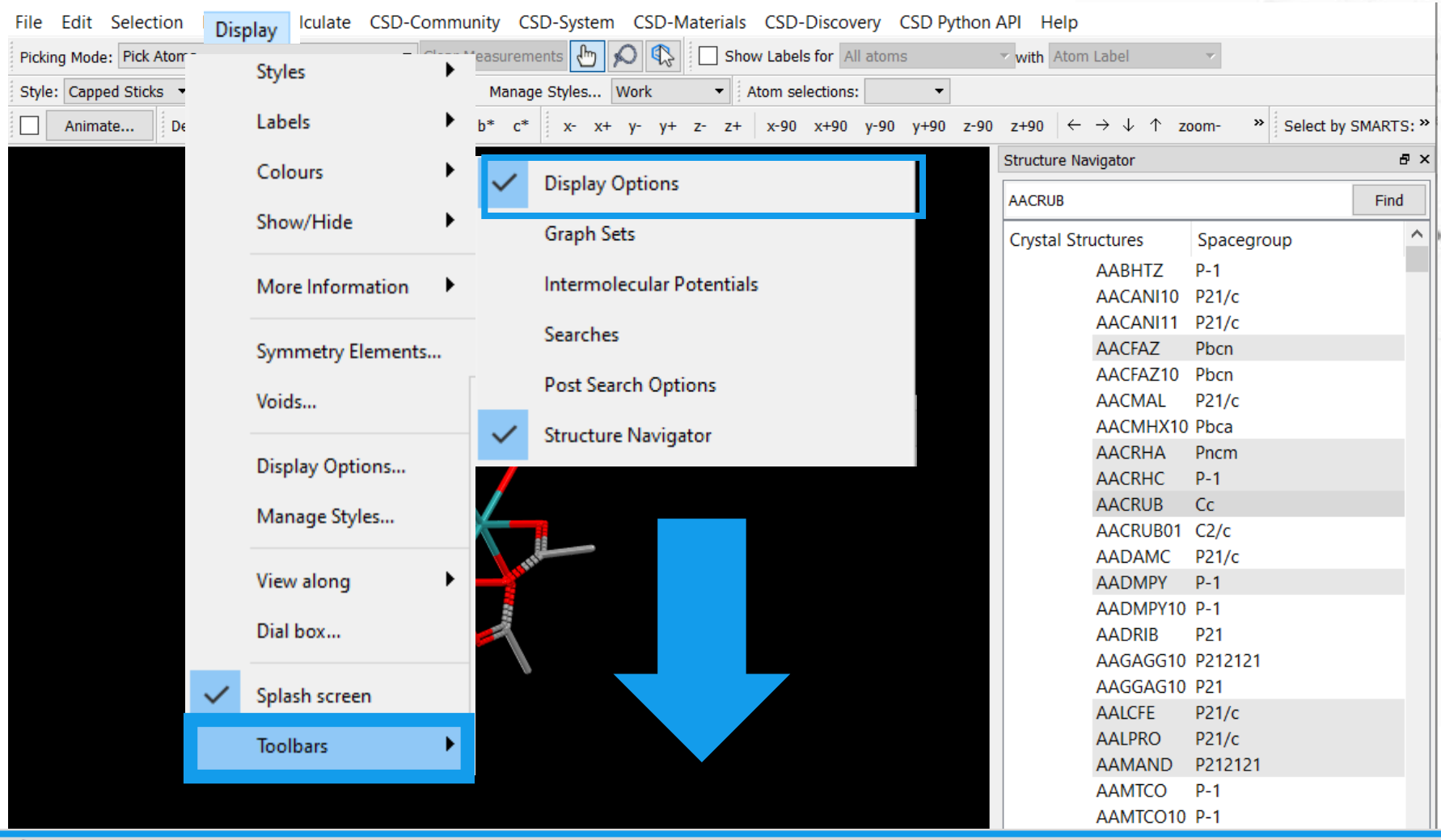

File Edit Selection Display Iculate CSD-Community CSD-System CSD-Materials CSD-Discovery CSD Python API Help
Picking Mode: Pick Atom
Style: Capped Sticks
Animate...
Show Labels for All atoms with Atom Label
Manage Styles... Work
Atom selections:
b* c* x- x+ y- y+ z- z+ x-90 x+90 y-90 y+90 z-90 z+90 zoom-
Select by SMARTS:
Styles
Labels
Colours
Show/Hide
More Information
Symmetry Elements...
Voids...
Display Options...
Manage Styles...
View along
Dial box...
Splash screen
Toolbars
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 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
AANHOX Pna21
AANHOX01 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


File Edit Selection Display Iculate CSD-Community CSD-System CSD-Materials CSD-Discovery CSD Python API Help
Picking Mode: Pick Atom
Show Labels for All atoms with Atom Label
Style: Capped Sticks
Manage Styles... Work
Atom selections:
Animate...
b* c* x- x+ y- y+ z- z+ x-90 x+90 y-90 y+90 z-90 z+90 zoom-
Select by SMARTS:
Styles
Labels
Colours
Show/Hide
More Information
Symmetry Elements...
Voids...
Display Options...
Manage Styles...
View along
Dial box...
Splash screen
Toolbars
Display Options
Graph Sets
Intermolecular Potentials
Searches
Post Search Options
Structure Navigator
Structure Navigator
AACRUB
Find
Crystal Structures
Spacegroup
AABHTZ P-1
AACANI10 P21/c
AACANI11 P21/c
AACFAZ Pbcn
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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
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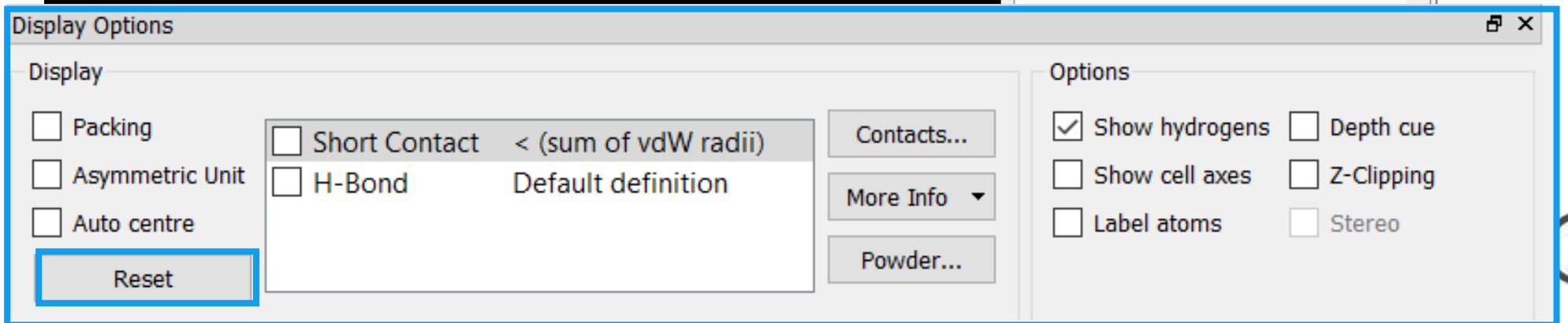
AALPRO P21/c
AAMAND P212121
AAMTCO P-1
AAMTCO10 P-1


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

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 ▸

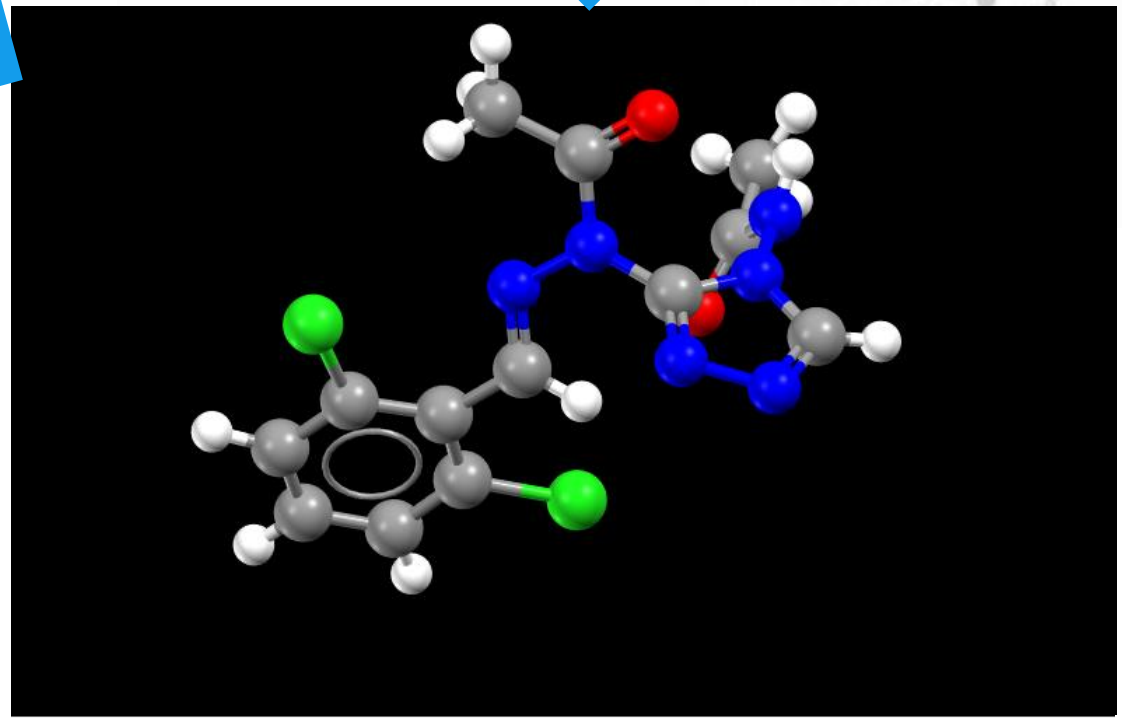
- Stick settings...
- Ball and Stick settings...
- Spacefill settings...
- Ellipsoid settings...
- Polyhedral settings...
- Contact settings...
- Measurement settings...
- Selected atoms

File | Edit | Selection | Display | Calculate | C

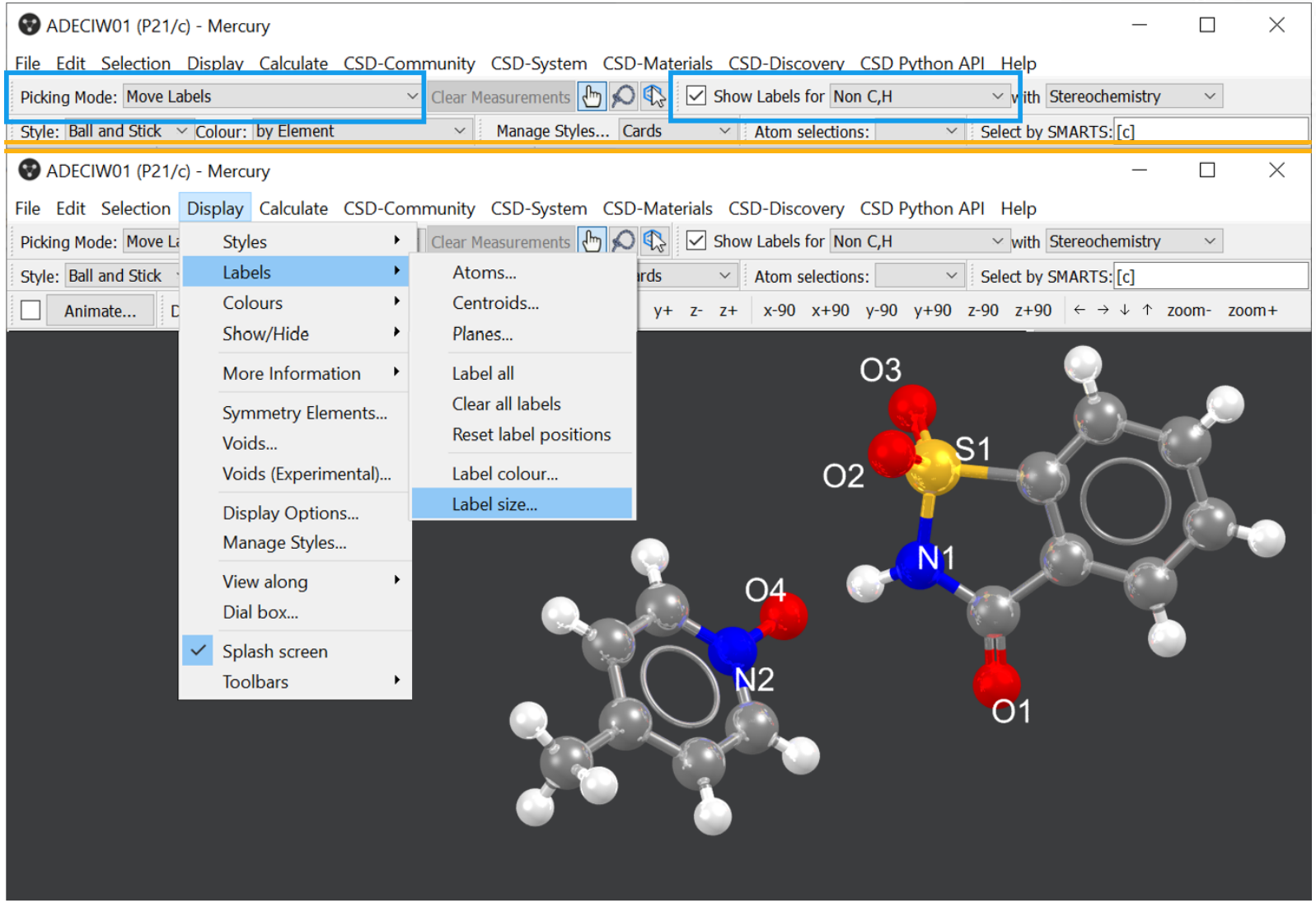
Picking Mode: Pick Atoms

Style: Ball and Stick | Colour: by Element

Animate... | ault view: b



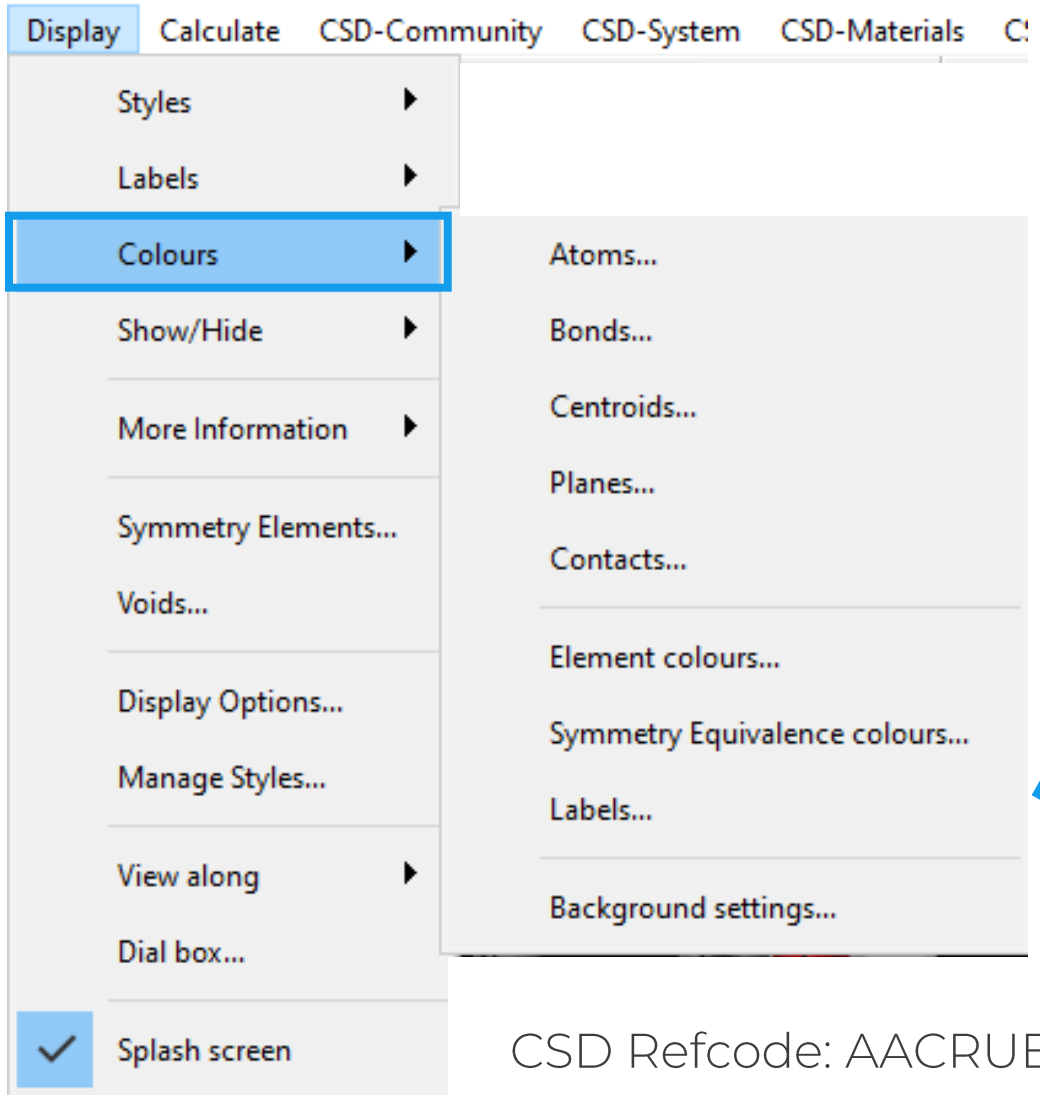
Adding, moving and sizing labels

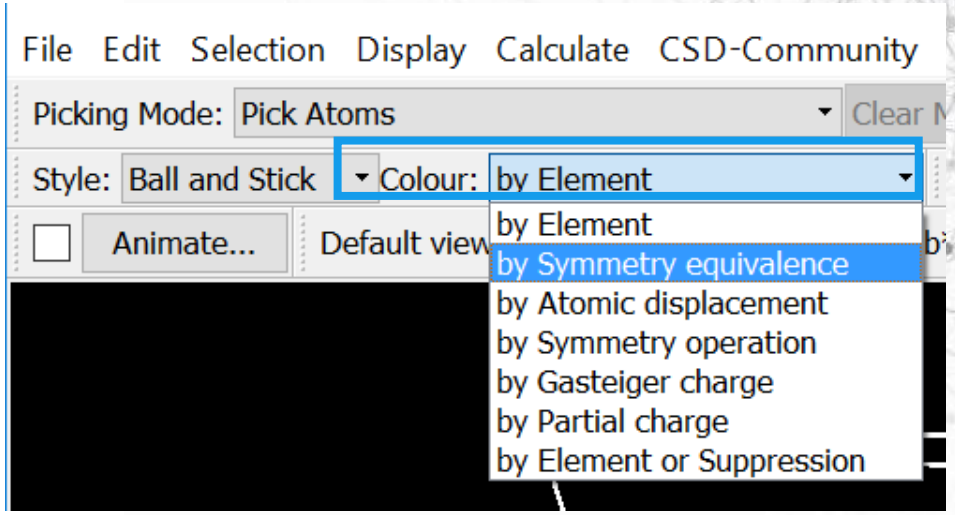


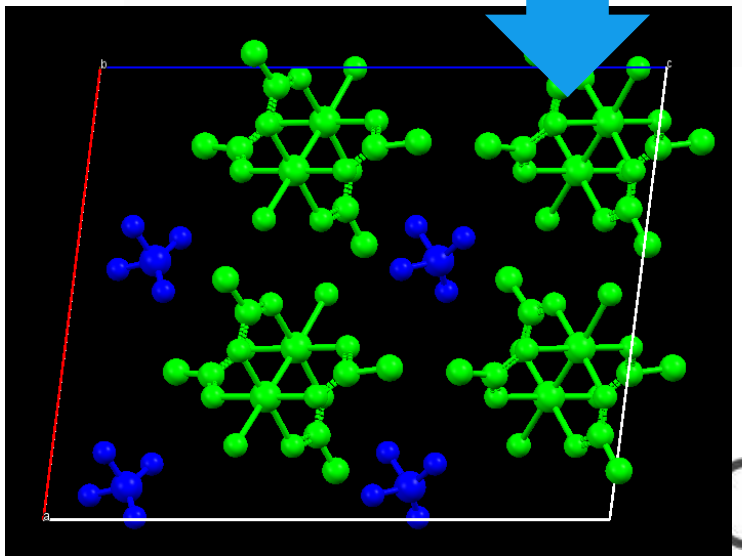
CSD Refcode: ADECIW01

CCDC

Changing display - colours



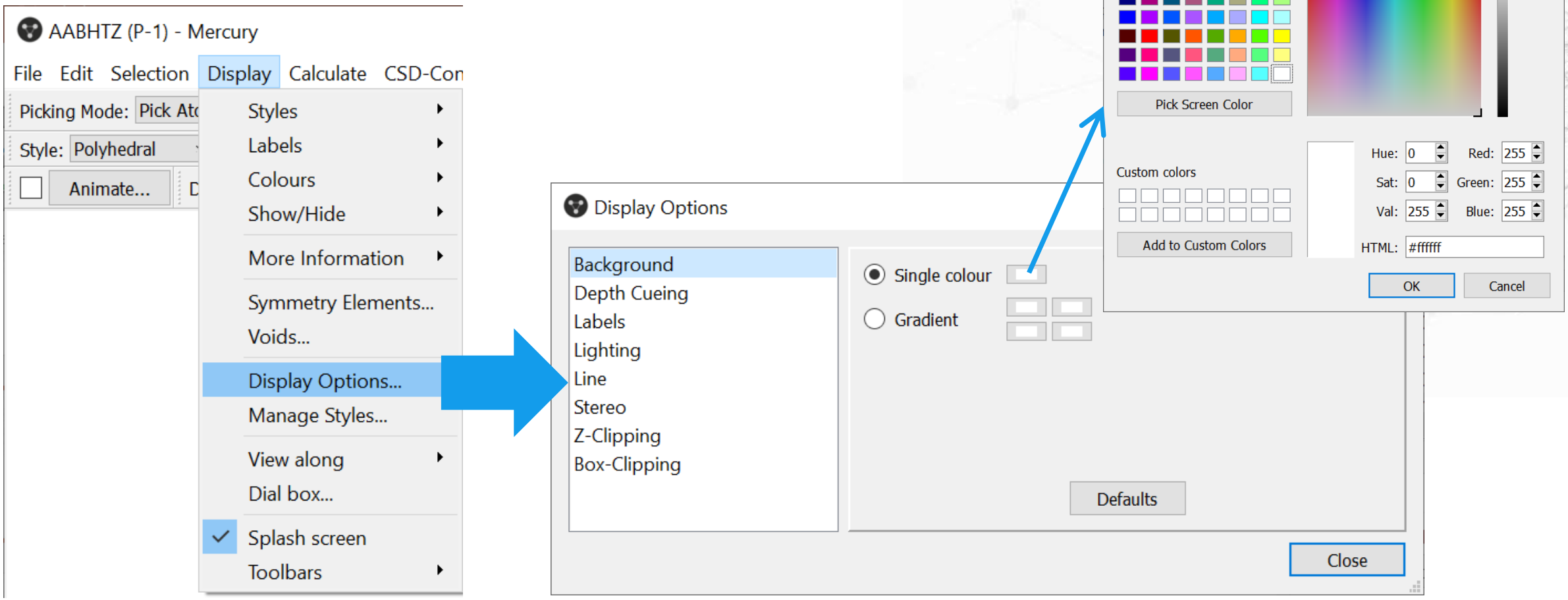




CSD Refcode: AACRUB

CCDC

Changing background colour



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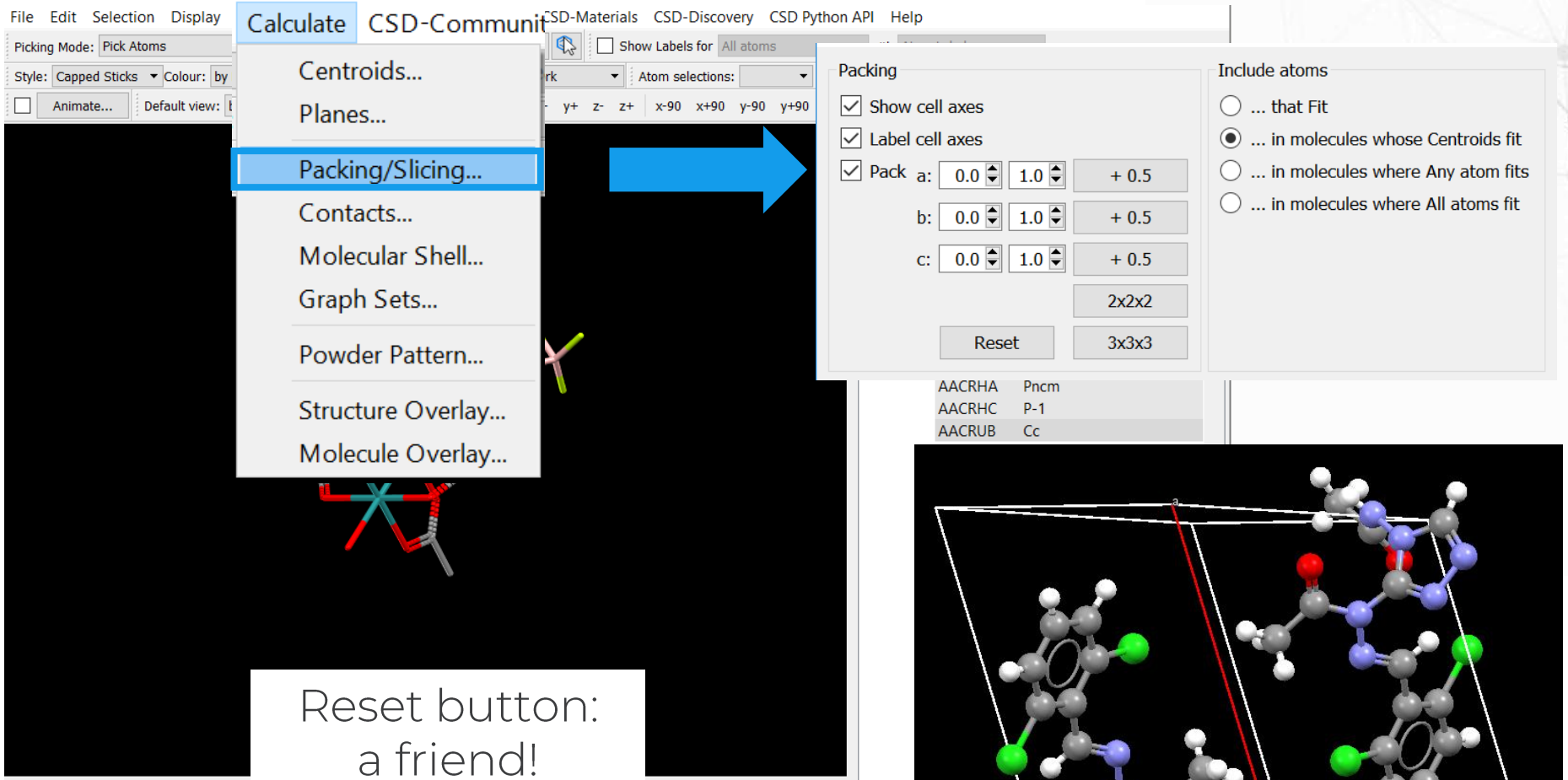
Packing in a crystal structure



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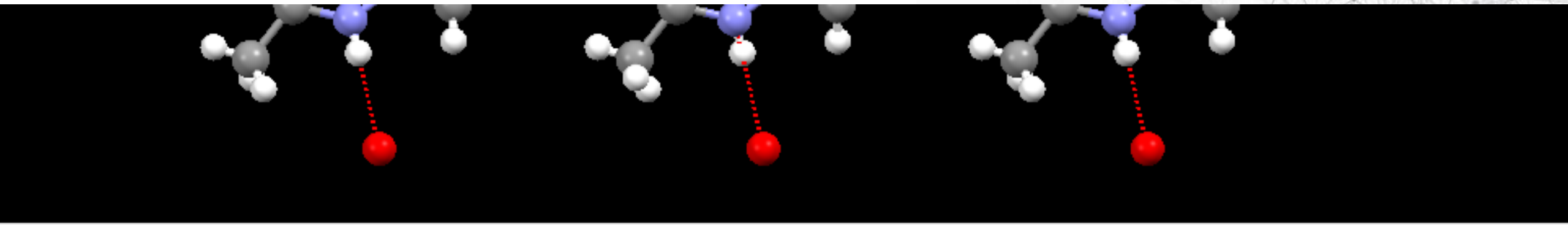
Visualising hydrogen bonds



Display Options

Display

- [ ] Packing
- [ ] Asymmetric Unit
- [ ] Auto centre

Reset

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

Contacts...

More Info

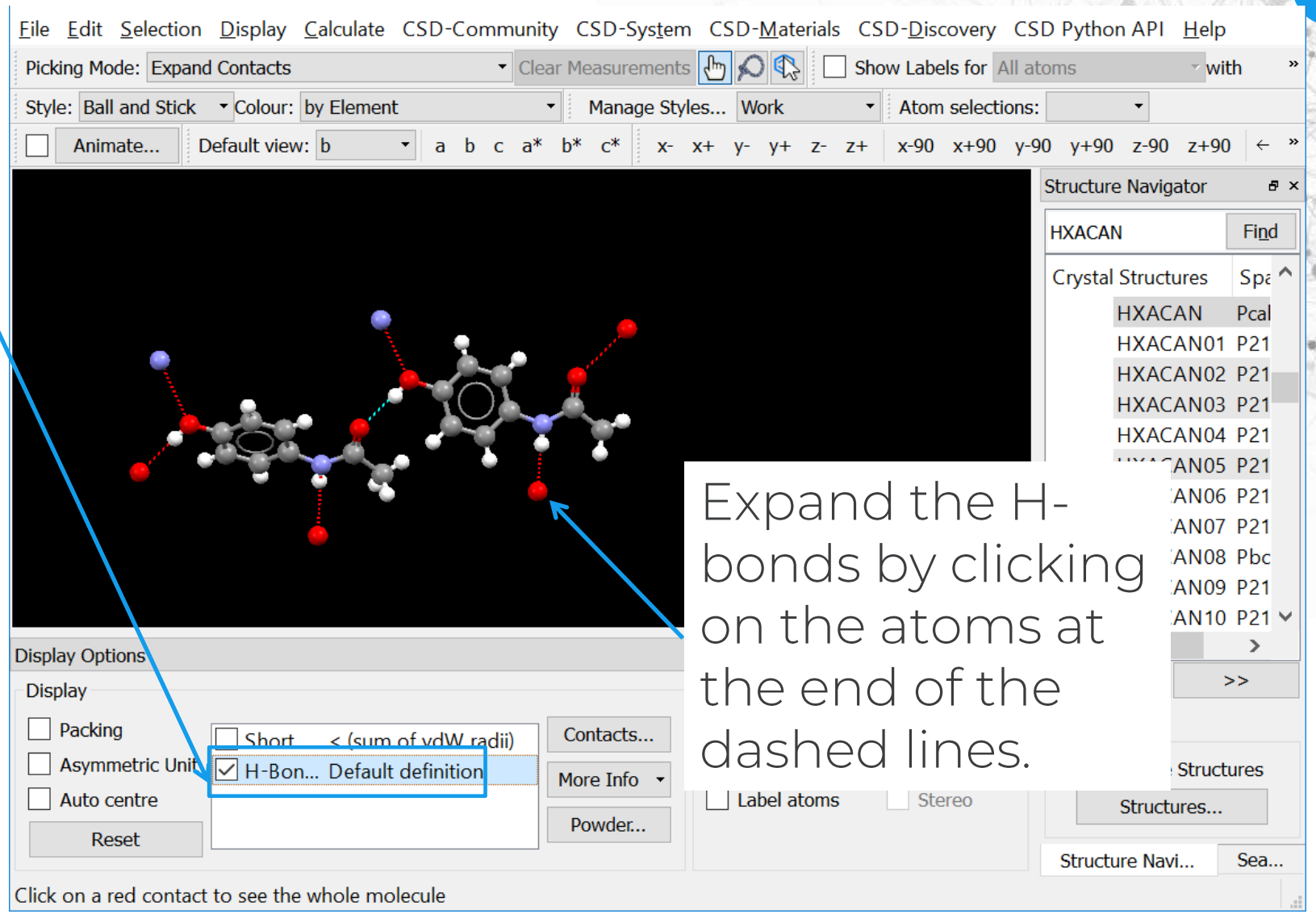
Powder...

Options

- [x] 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

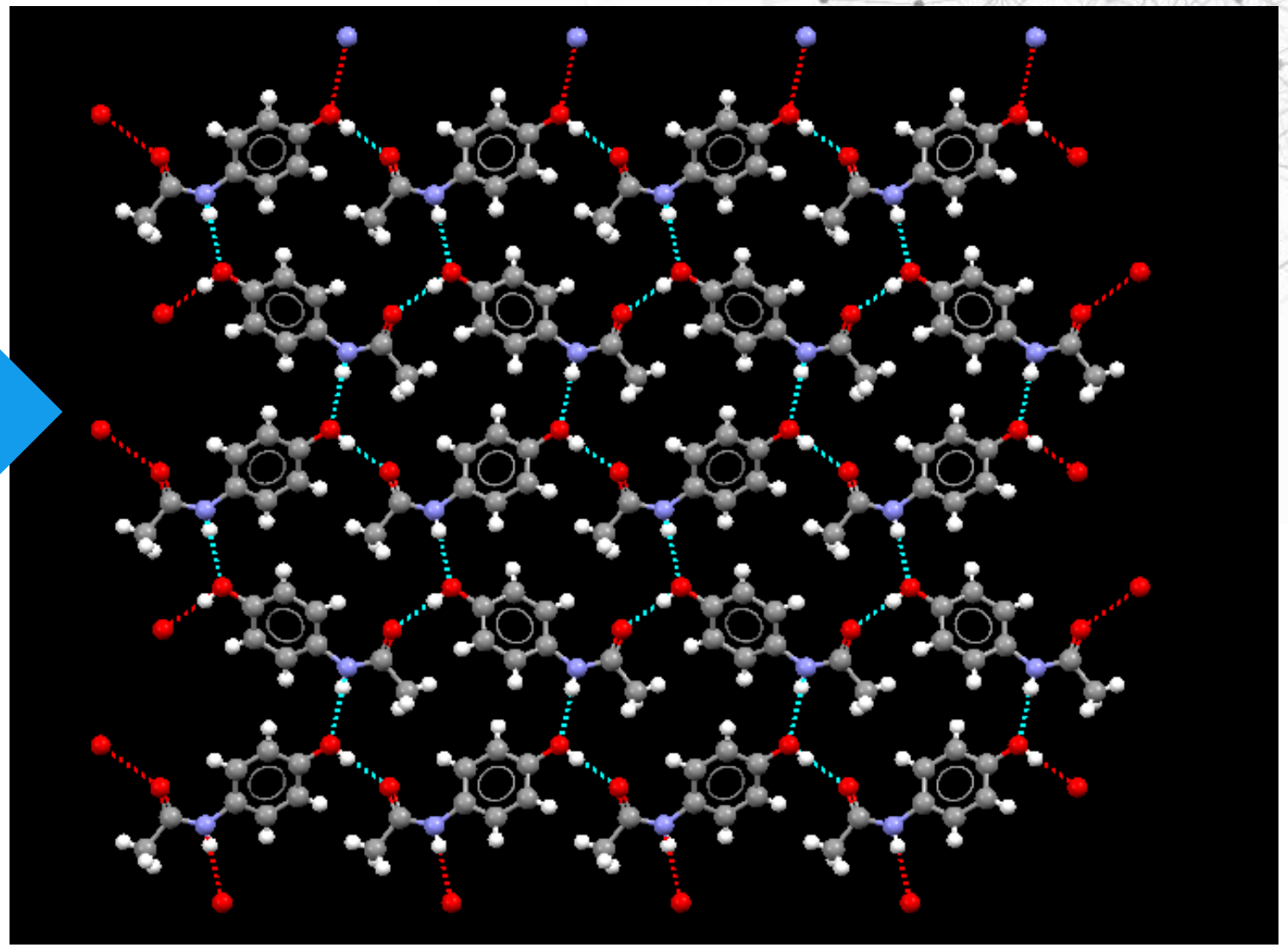


Expand the H-bonds by clicking on the atoms at the end of the dashed lines.

CSD Refcode: HXACAN

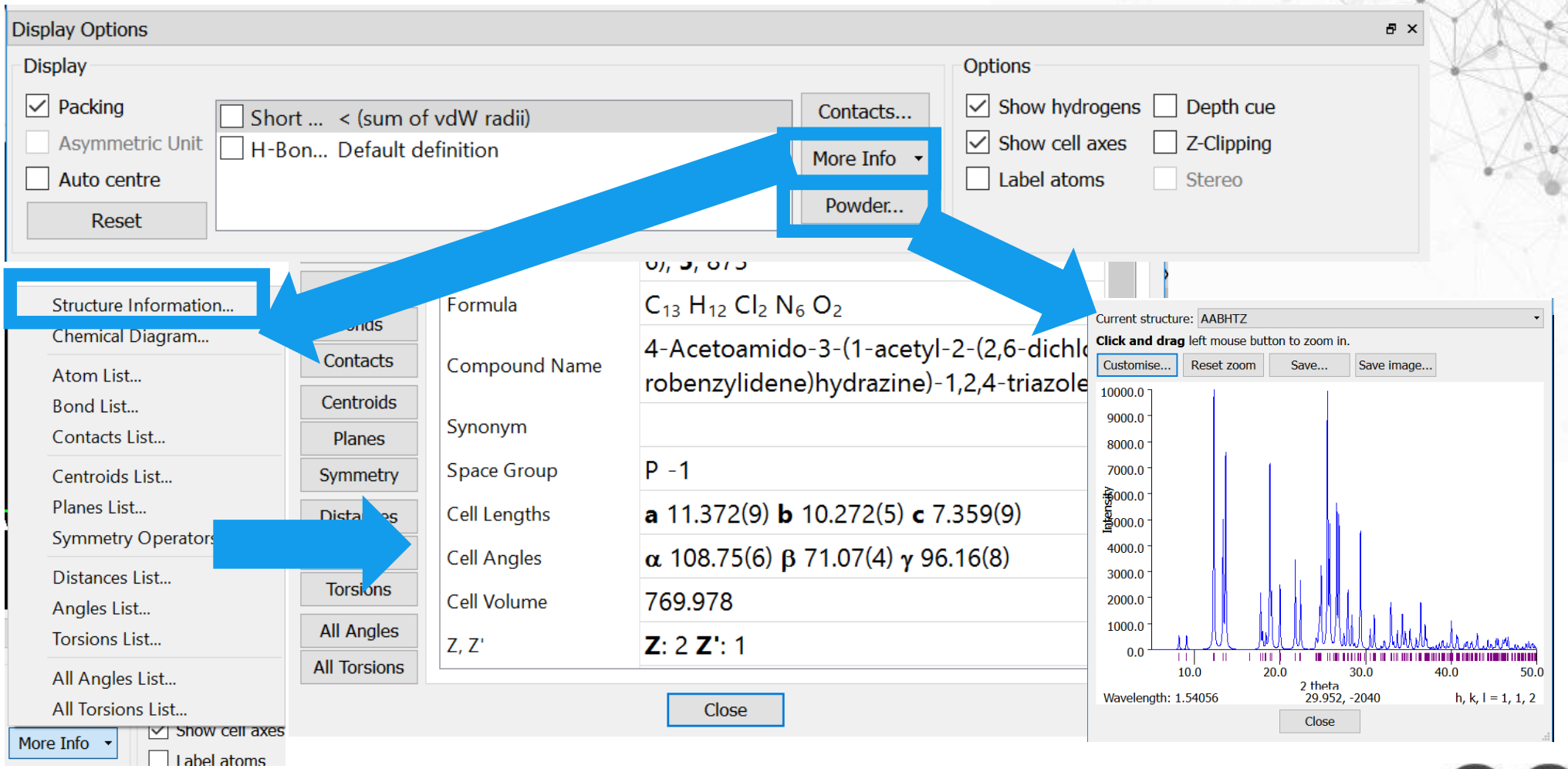
Building the H-bond network

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

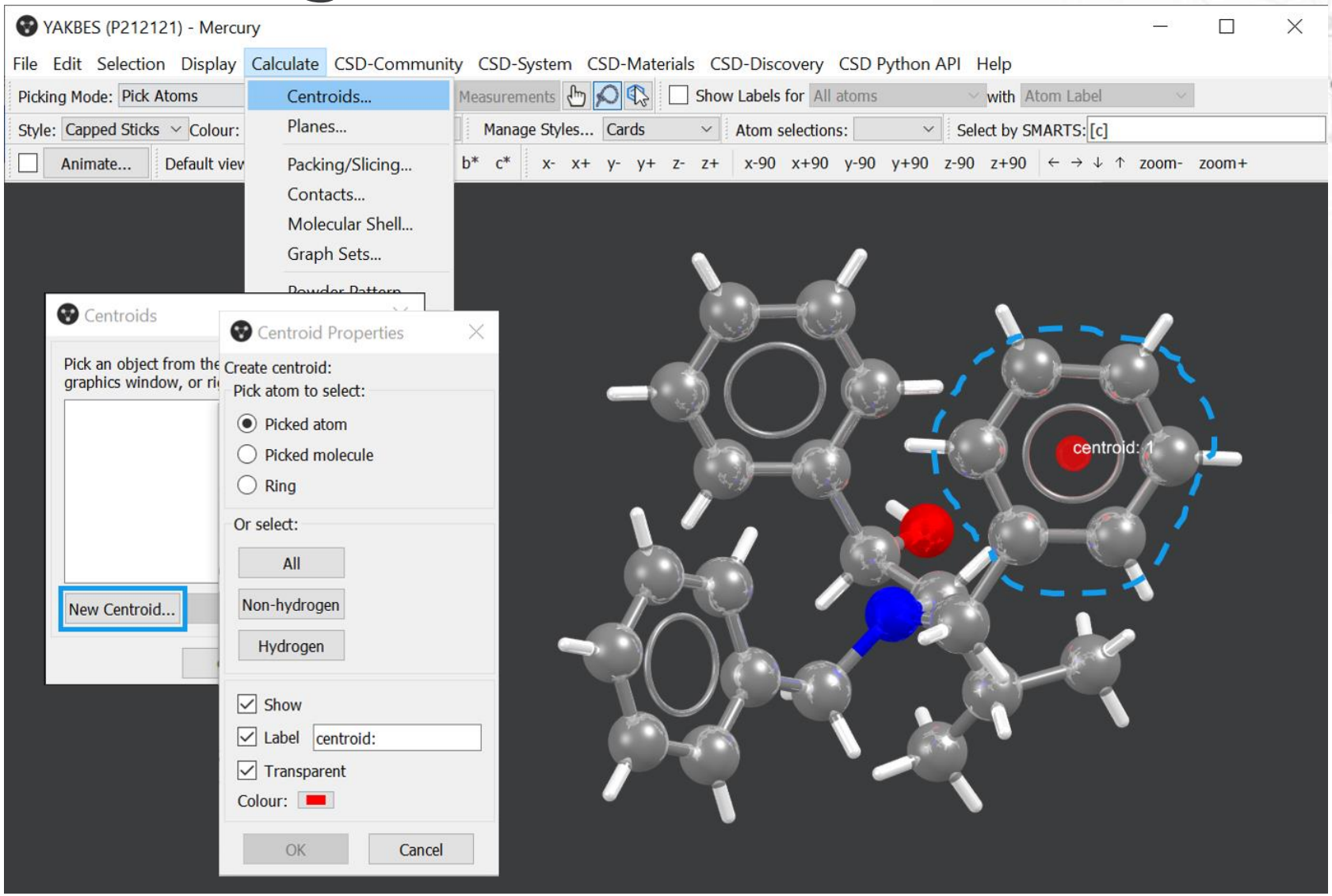


CSD Refcode: HXACAN

Generating a powder pattern



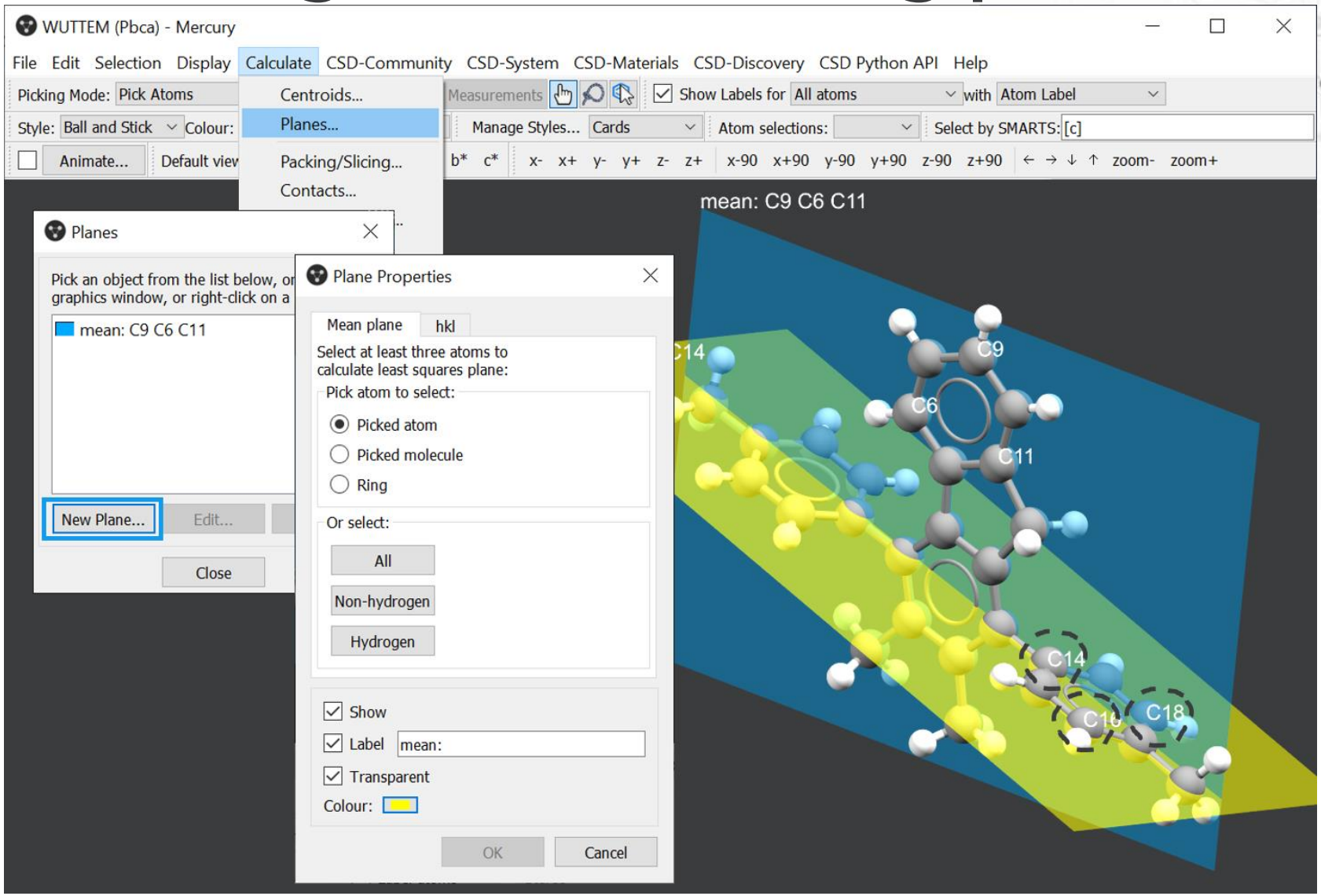
Calculating centroids



CSD Refcode:
YAKBES

CCDC

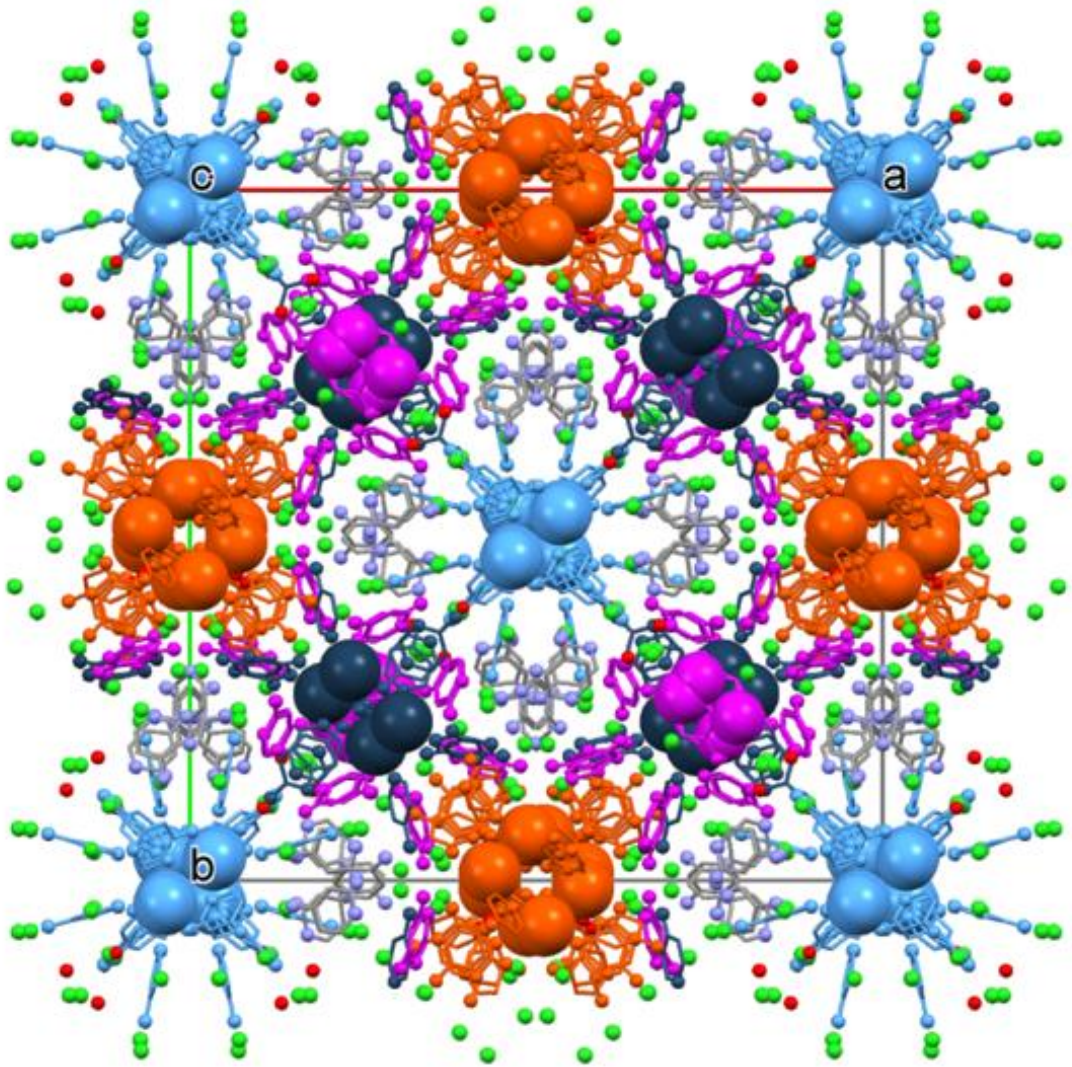
Calculating and visualising planes



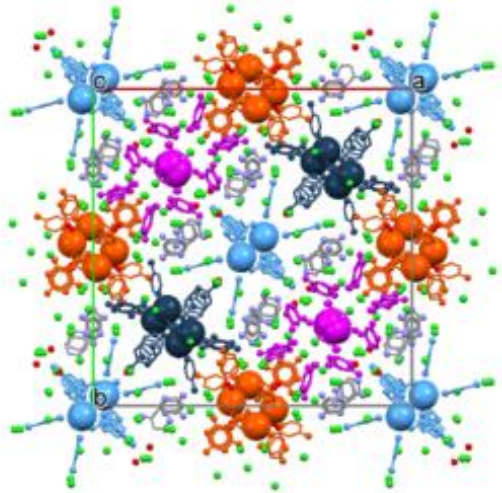
CSD Refcode:
WUTTEM

CCDC

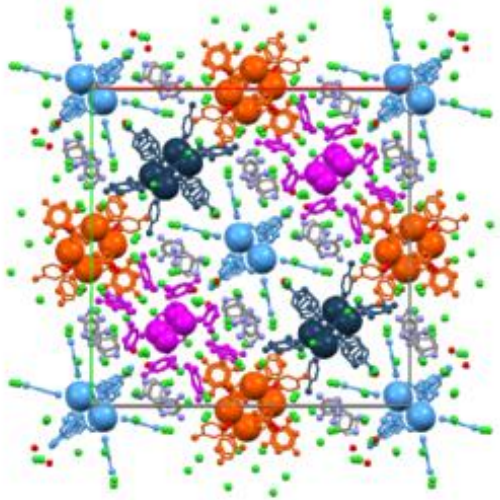
What is possible?



(a)



(b)



(c)

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

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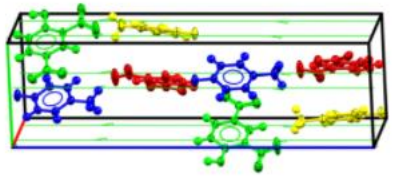
Want to explore more?



CSD-System

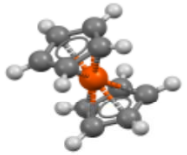
Essential crystallographic and structural chemistry capabilities.

Educational Resources

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.

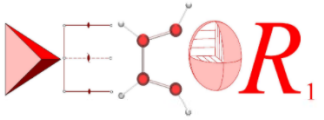
The CCDC and our colleagues continually produce educational materials for use in classroom and computer lab settings, or as independent study modules. Many of these materials make use of the Teaching Subset - a freely available set of over 750 structures that can be investigated with the free version 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.



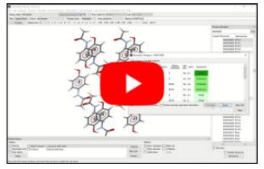
Information on the Teaching Subset

Access a series of teaching modules for use in the classroom

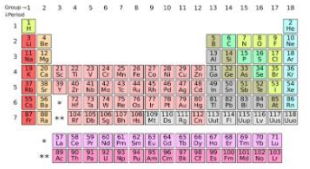


DECOR: Educational Resources for Teaching Crystallography

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/