Visualising structures using Mercury

CCDC Virtual Workshop 2020 – Session 2

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CCDC
advancing structural science

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

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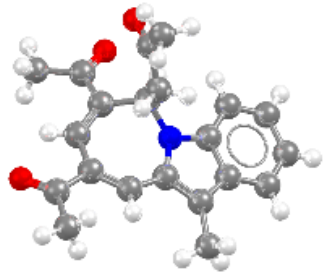
CSD Refcodes



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

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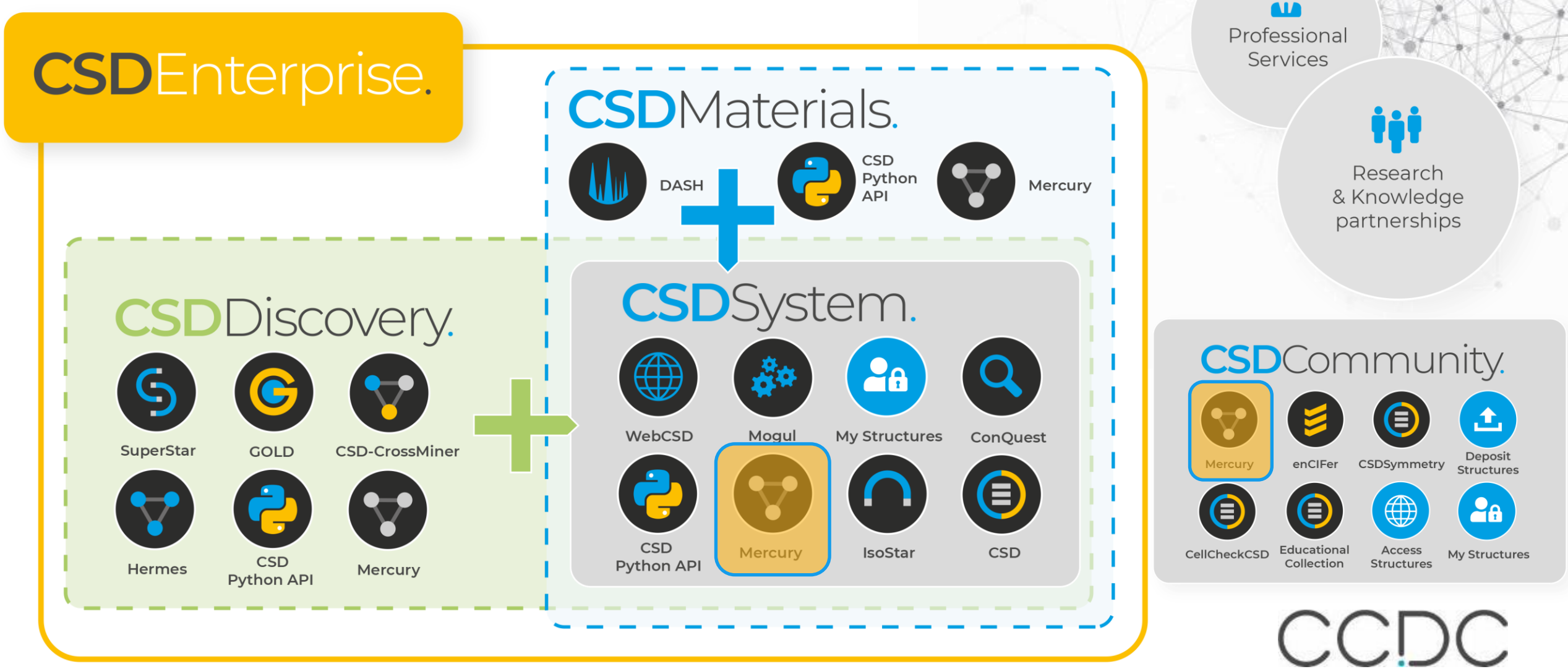
The CSD software



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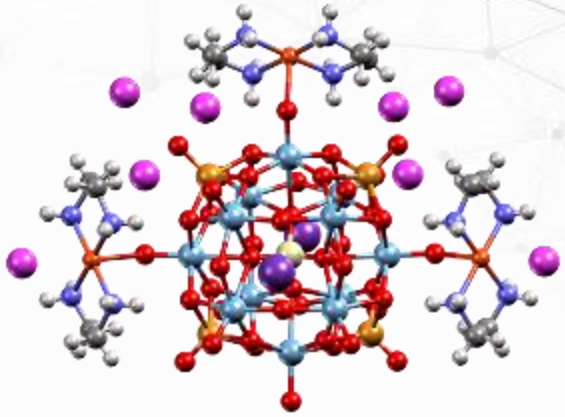
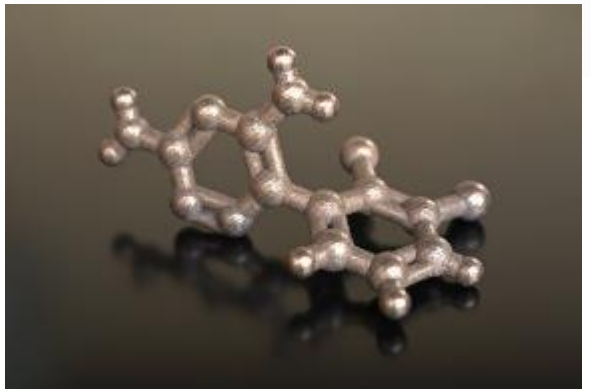
Mercury – Structure visualisation

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





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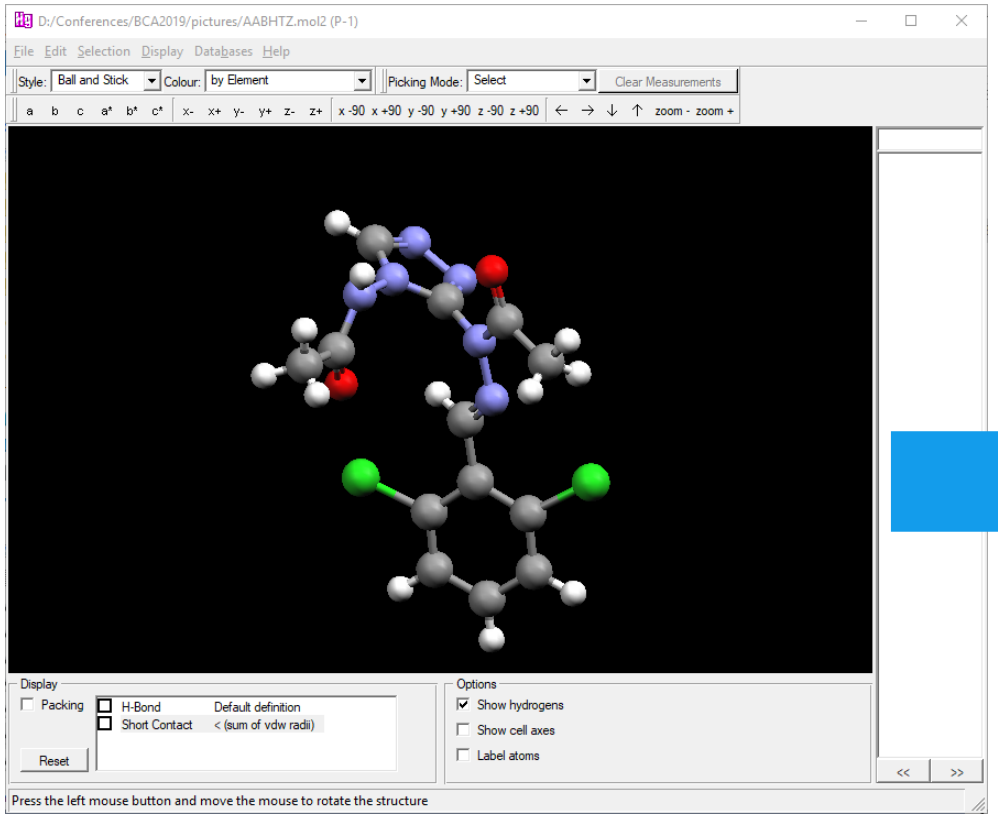
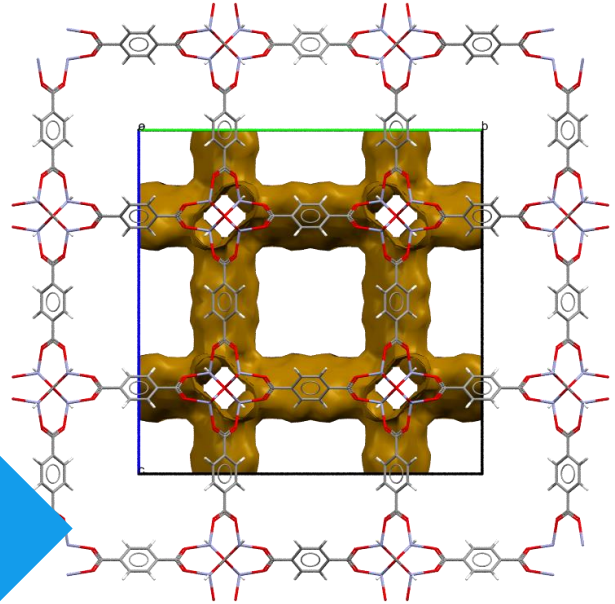
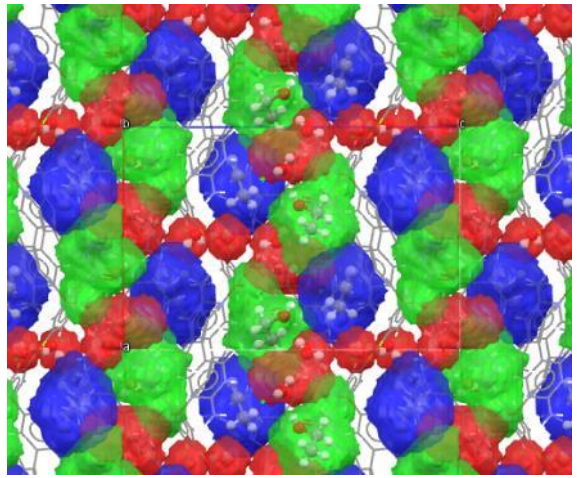
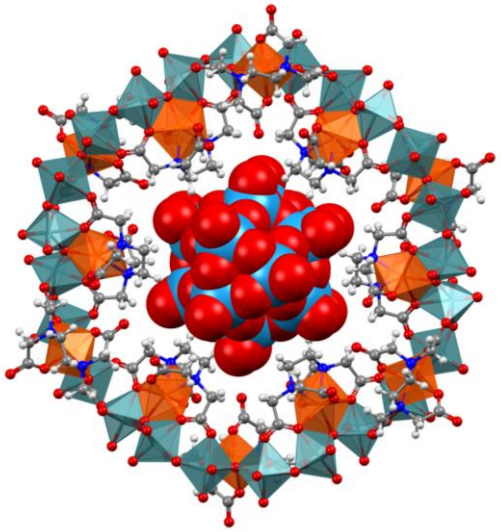
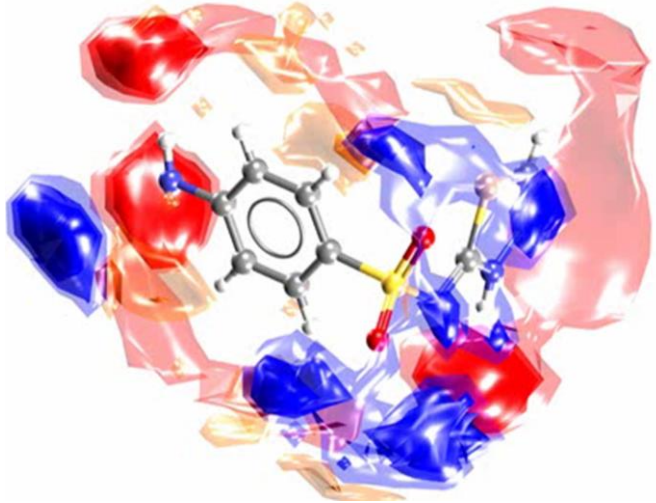
Mercury – first launched in 2001





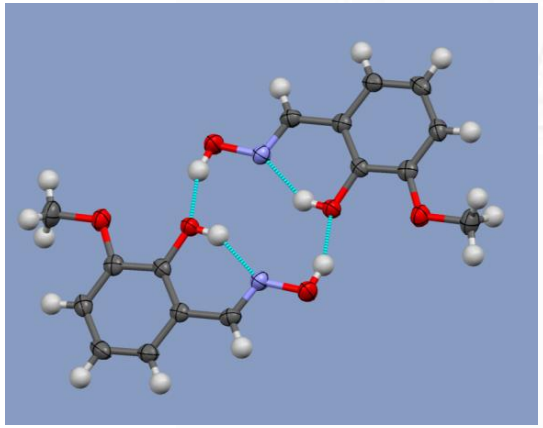


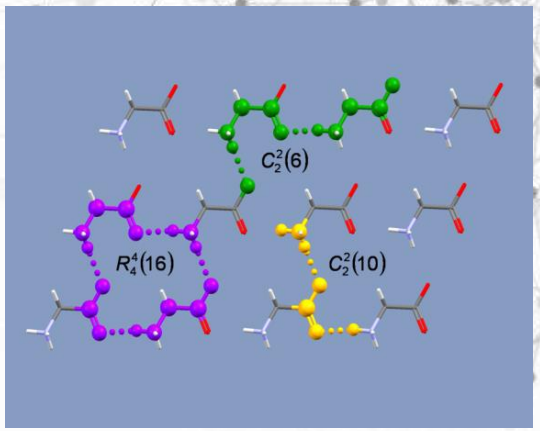


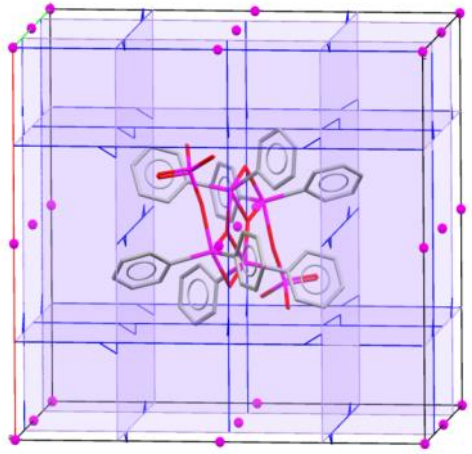


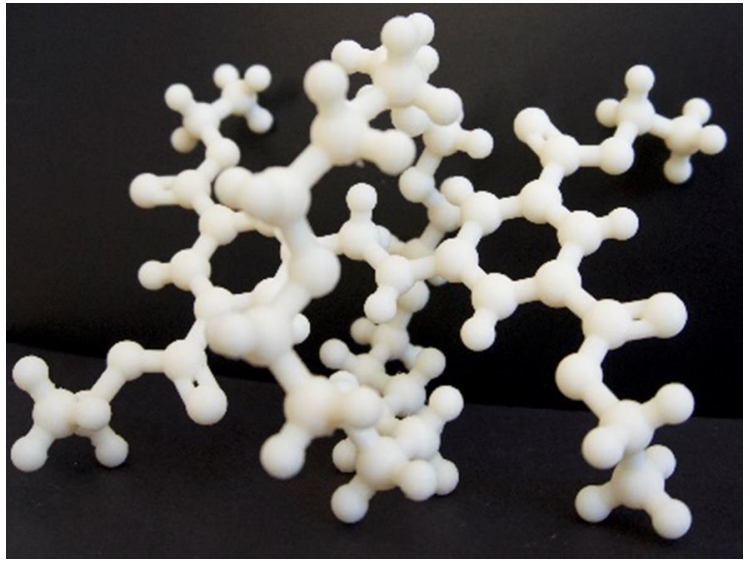
Structure visualisation

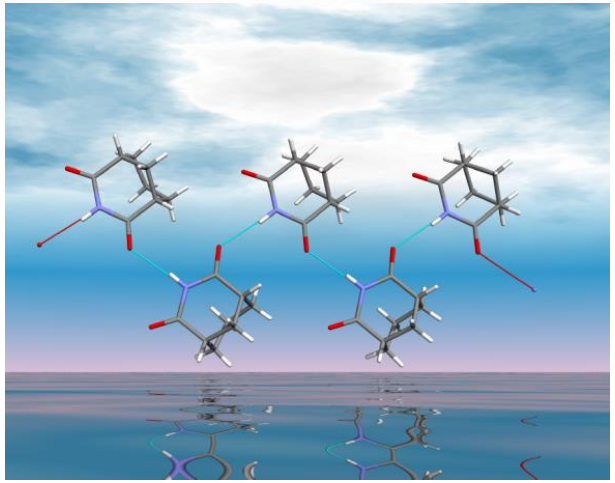
- Symmetry elements
- Displacement ellipsoids etc.
- POV-Ray
- 3D printing
- Graph sets
- Movies











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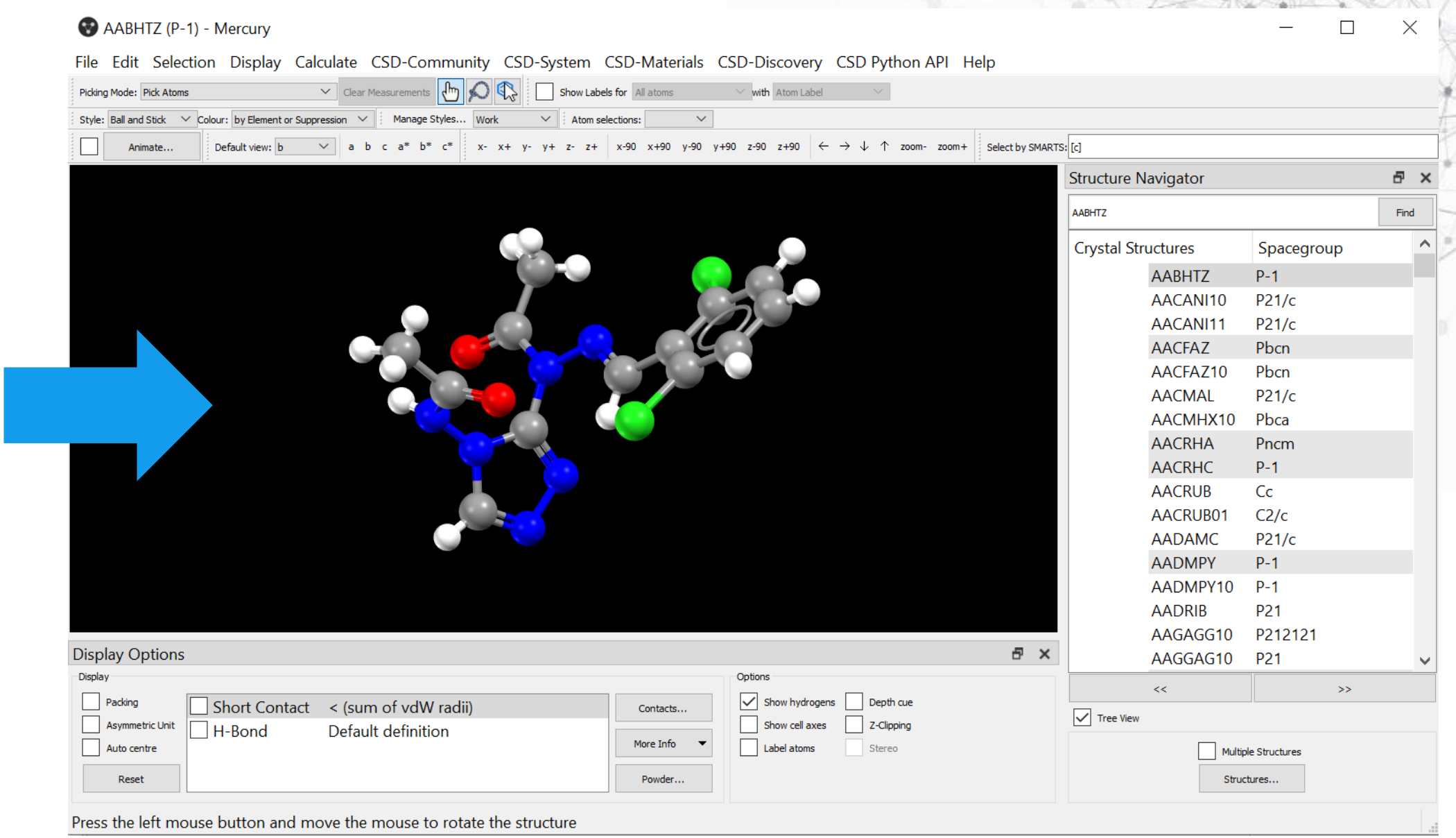
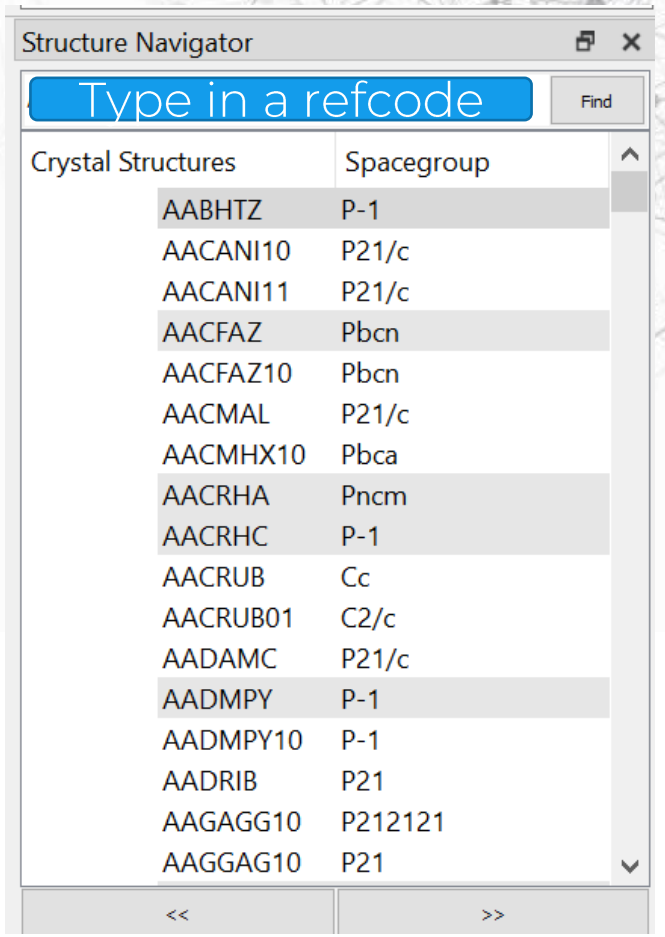
Show One: Mercury Demo



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



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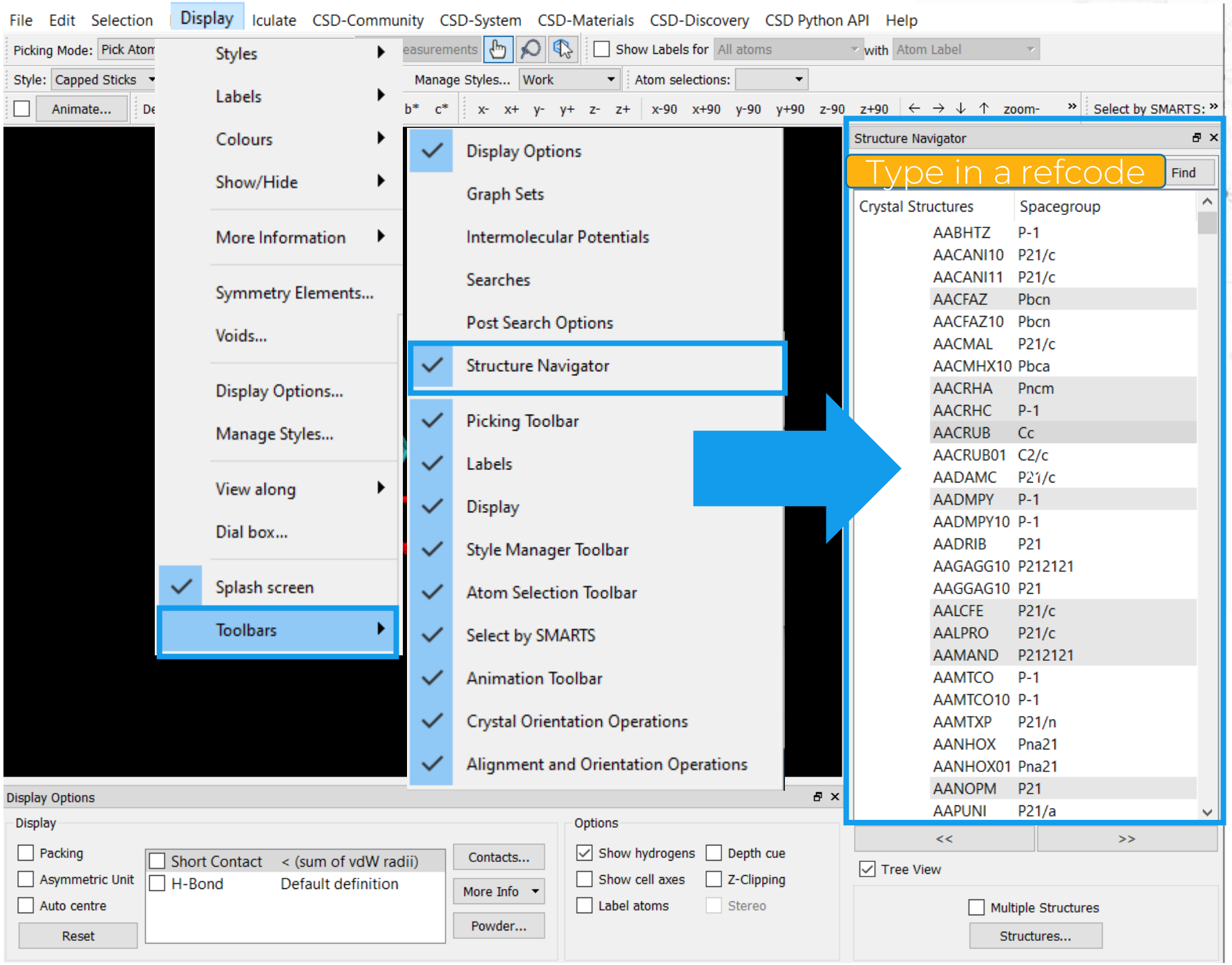
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More Information
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Manage Styles...
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Graph Sets
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AACANI10 P21/c
AACANI11 P21/c
AACFAZ Pbcn
AACFAZ10 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
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AAMTXP P21/n
AANHOX Pna21
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Tree View
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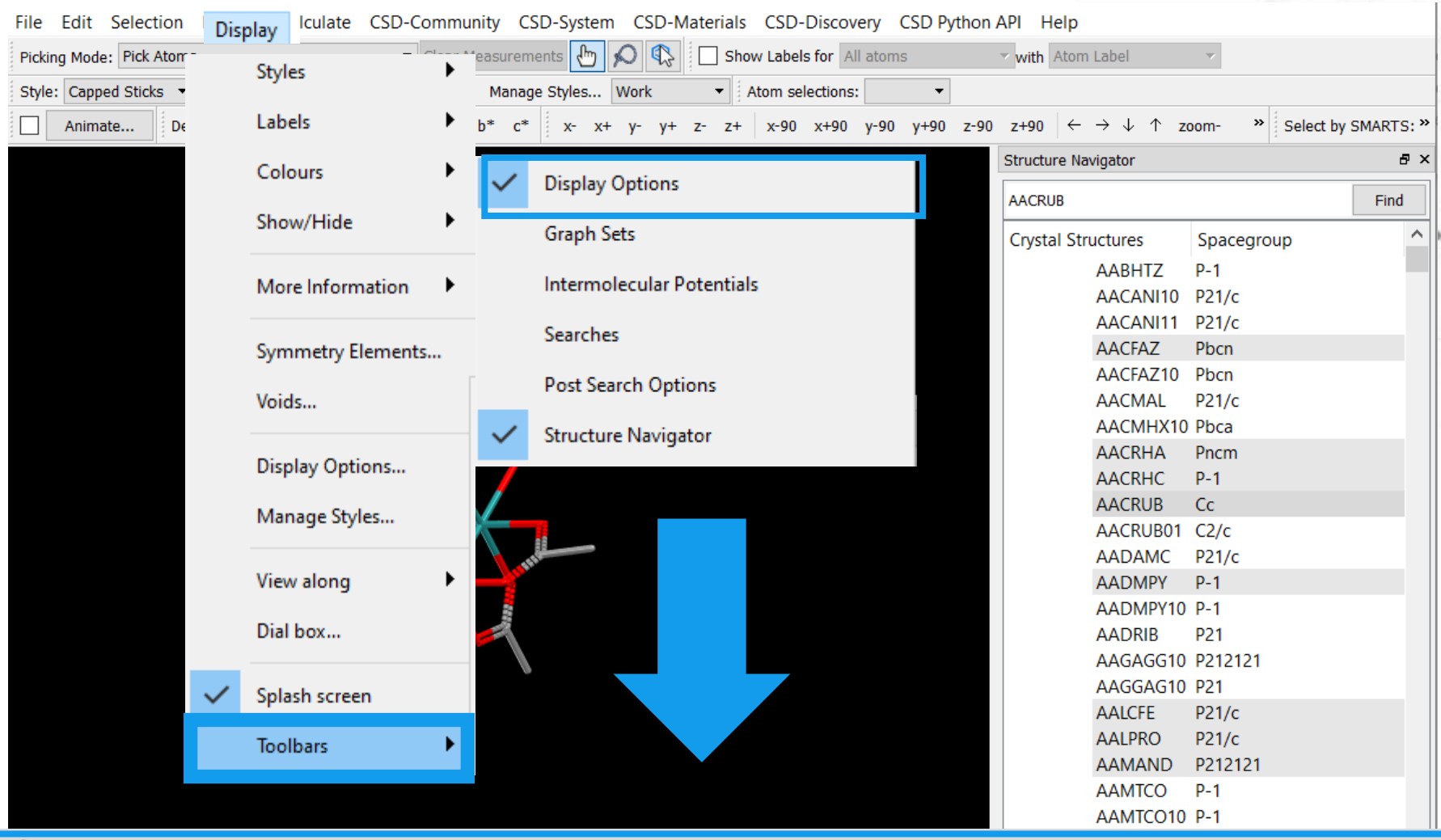
Show cell axes
Z-Clipping
Label atoms
Stereo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View along
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Splash screen
Toolbars
Display Options
Graph Sets
Intermolecular Potentials
Searches
Post Search Options
Structure Navigator
Structure Navigator
AACRUB
Find
Crystal Structures
Spacegroup
AABHTZ P-1
AACANI10 P21/c
AACANI11 P21/c
AACFAZ Pbcn
AACFAZ10 Pbcn
AACMAL P21/c
AACMHX10 Pbca
AACRHA Pncm
AACRHC P-1
AACRUB Cc
AACRUB01 C2/c
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AADRIB P21
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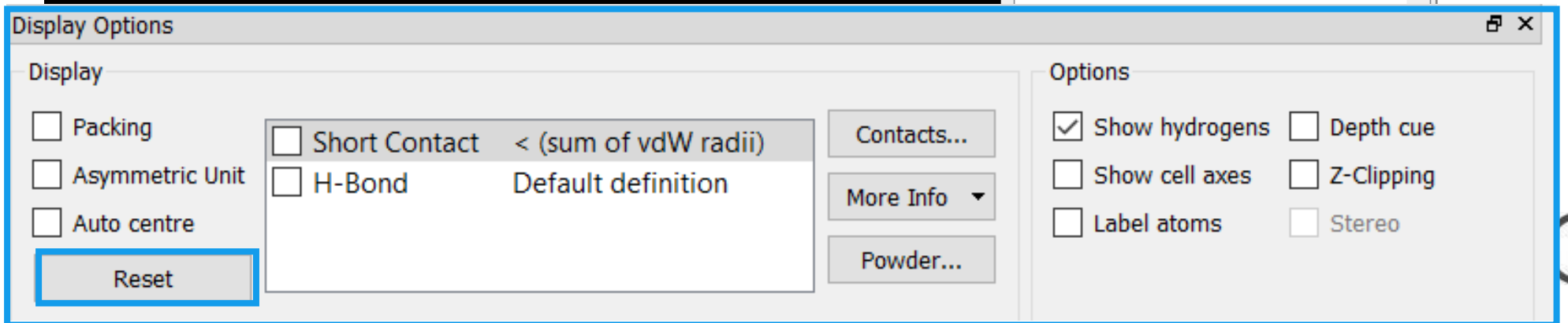
Display Options
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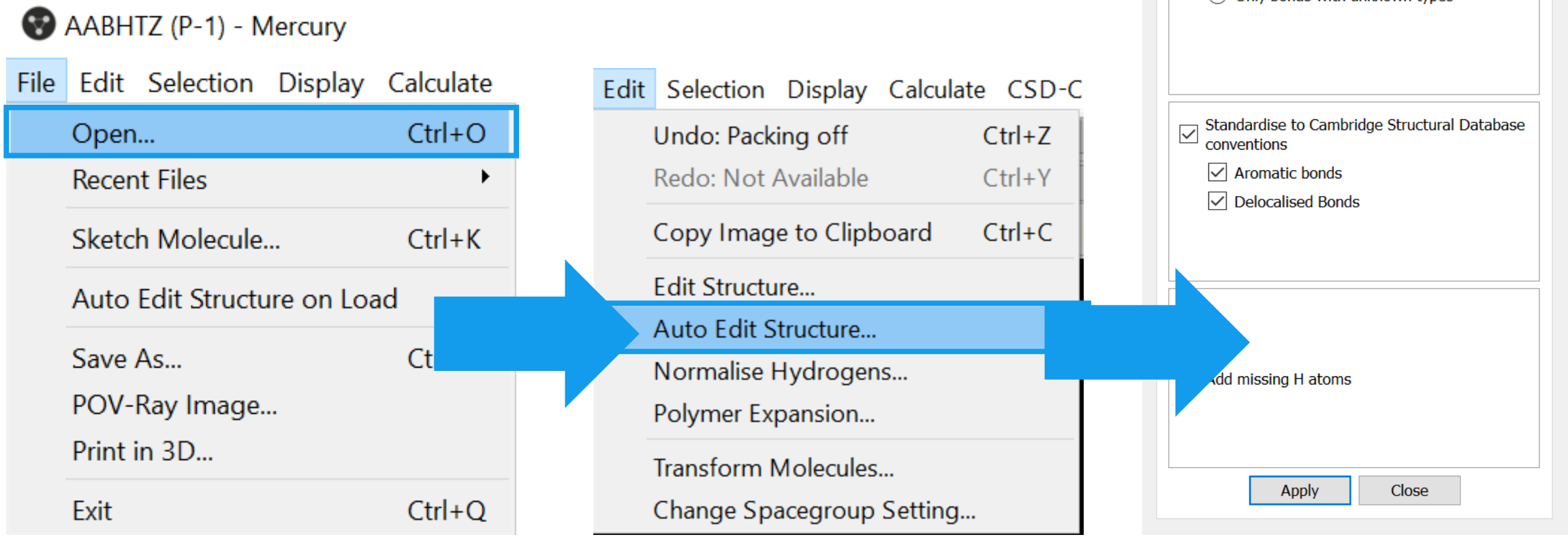
H-Bond Default definition
Contacts...
More Info
Powder...
Options
Show hydrogens
Depth cue
Show cell axes
Z-Clipping
Label atoms
Stereo

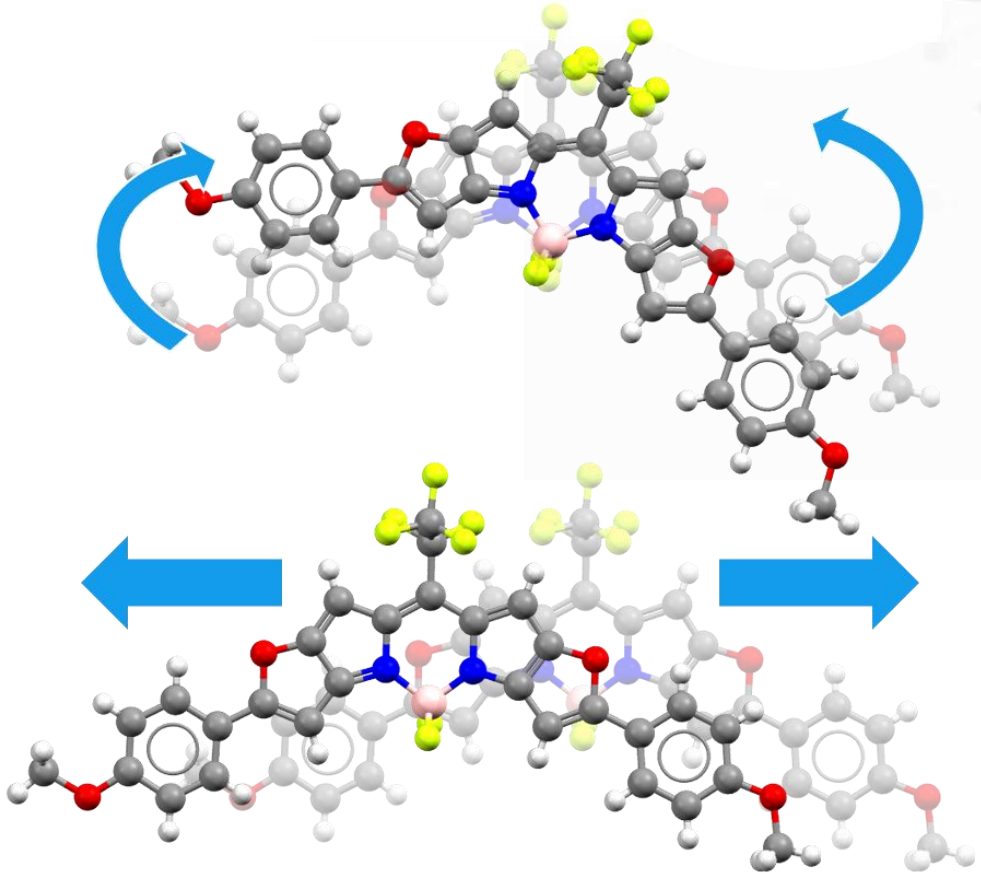
Using your own file

- 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



Moving and rotating on the plane

With the keyboard:



CSD Refcode: GIMXUY

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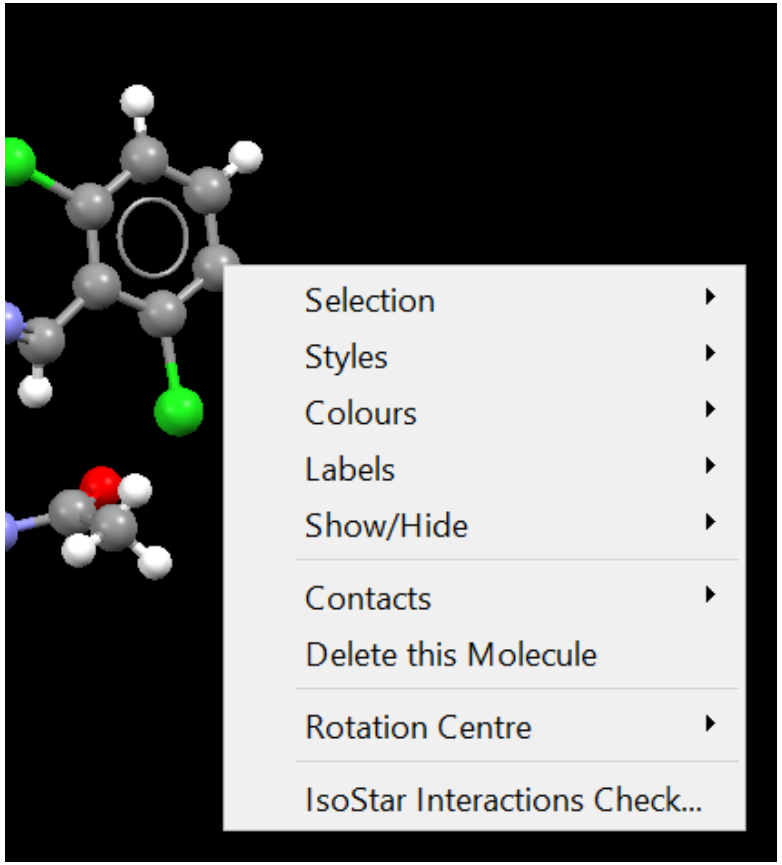
Right mouse click

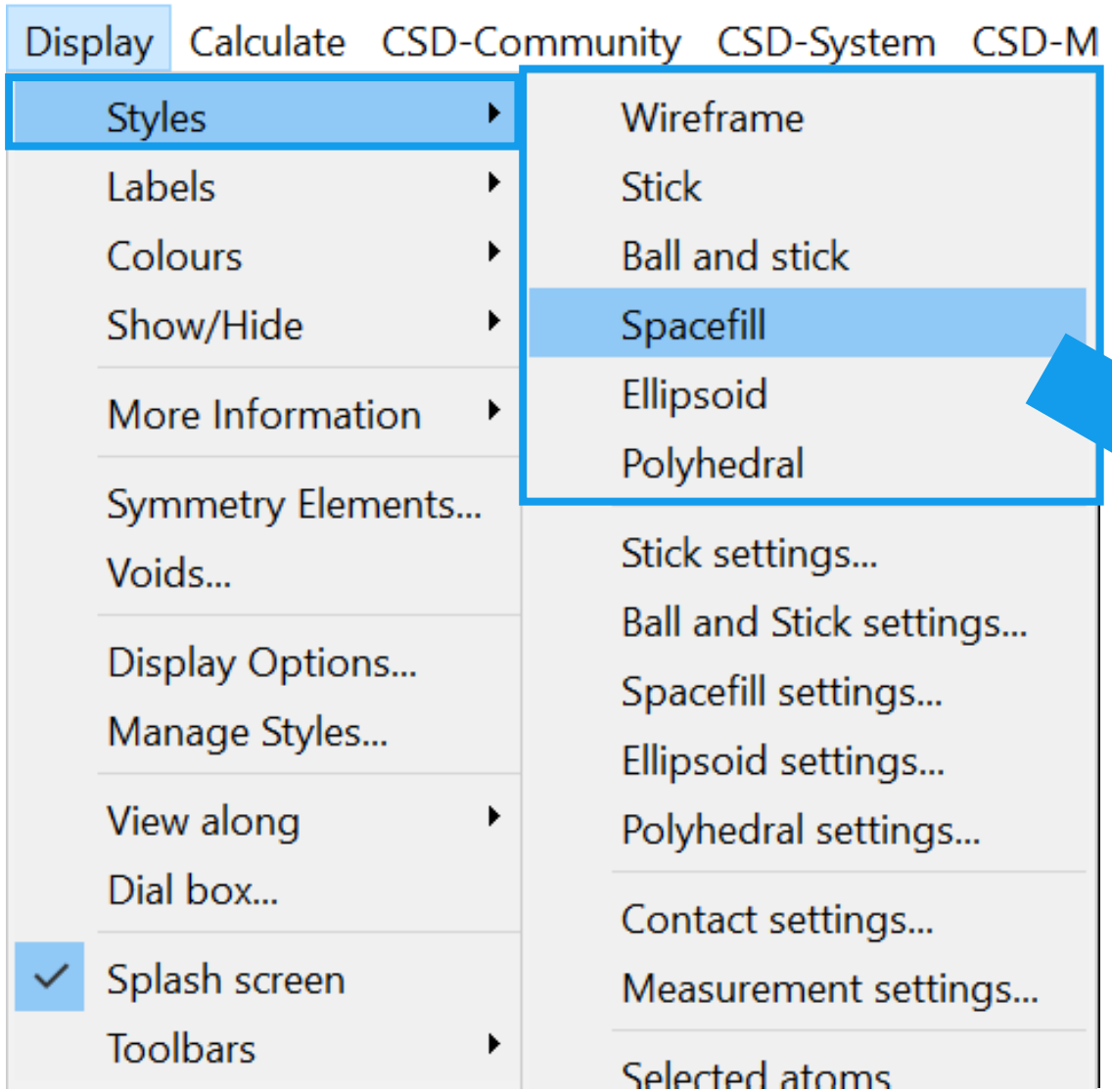
Near a molecule

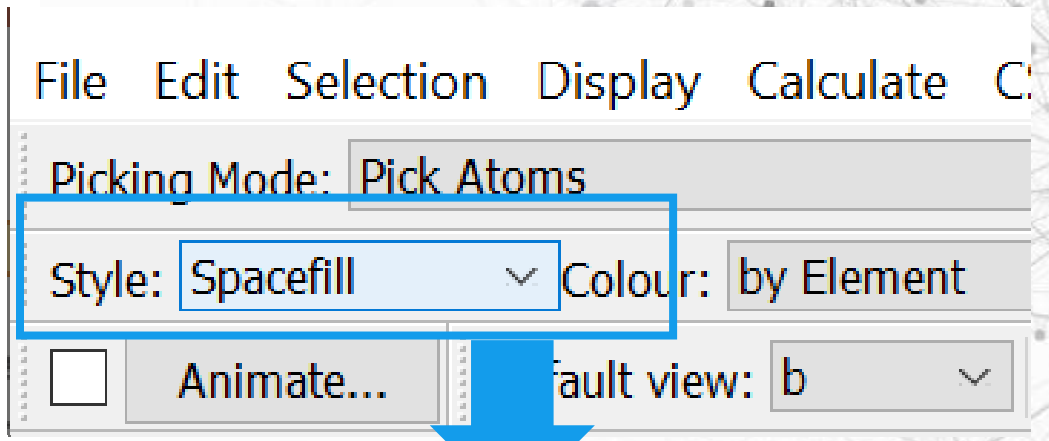


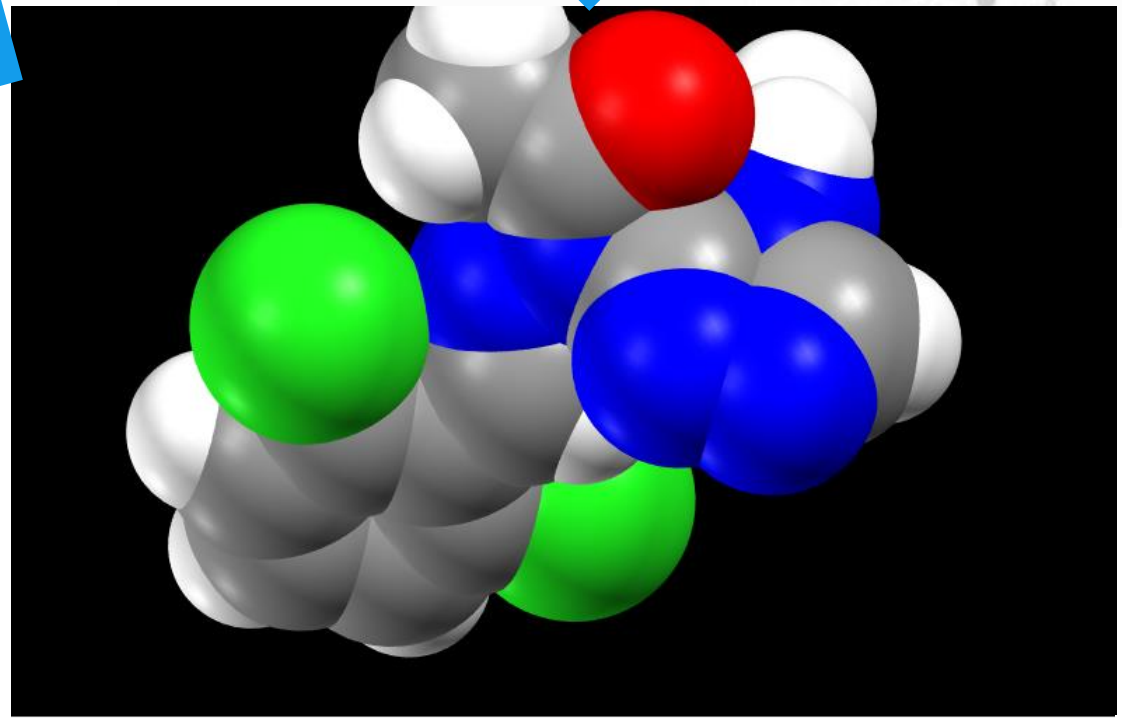
Away from a molecule

CCDC

Changing display - Style

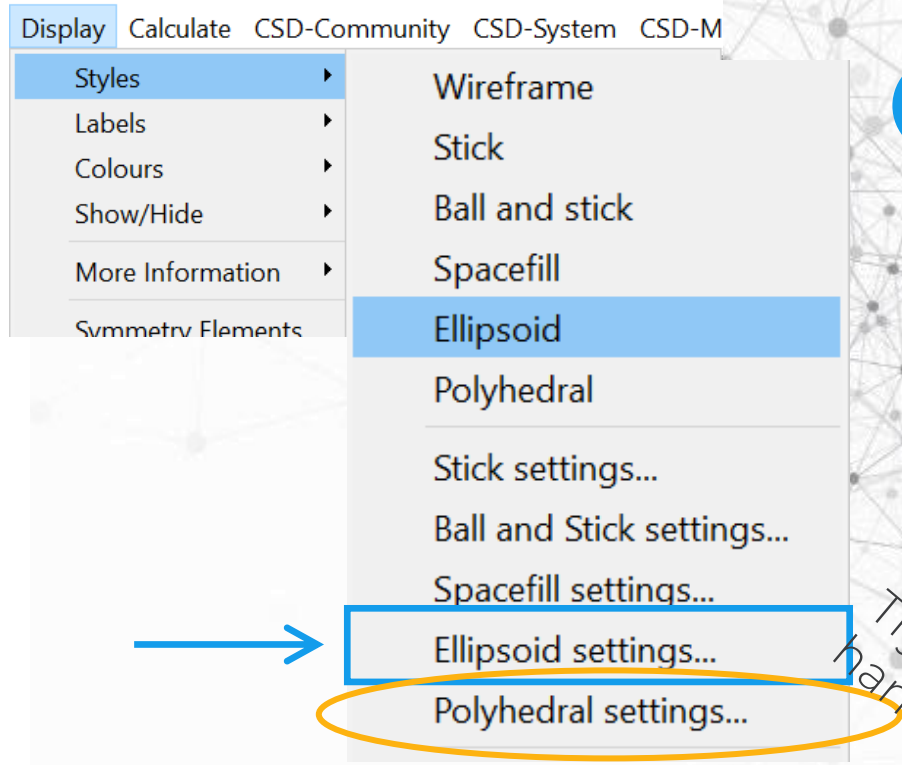




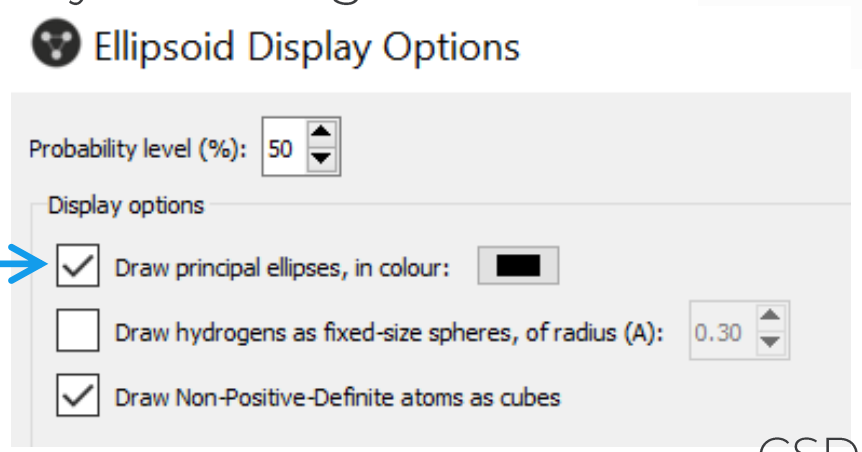


Thermal Ellipsoids

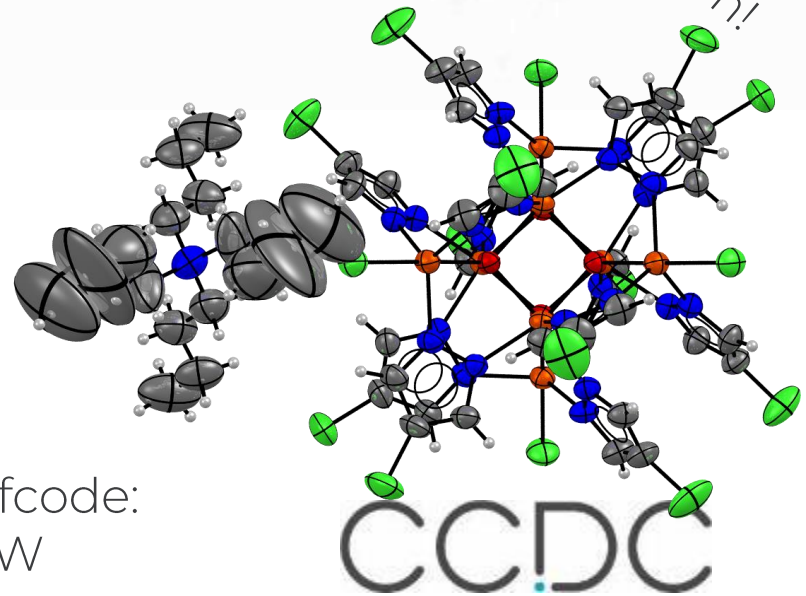
- Anisotropic Displacement Parameters
- Only available for CSD structures with ADPs
- Indicate thermal vibrations of atoms
- Size of ellipsoid is scaled
  - Usually to probability of finding 50% of electron density



Try it in the hands-on!



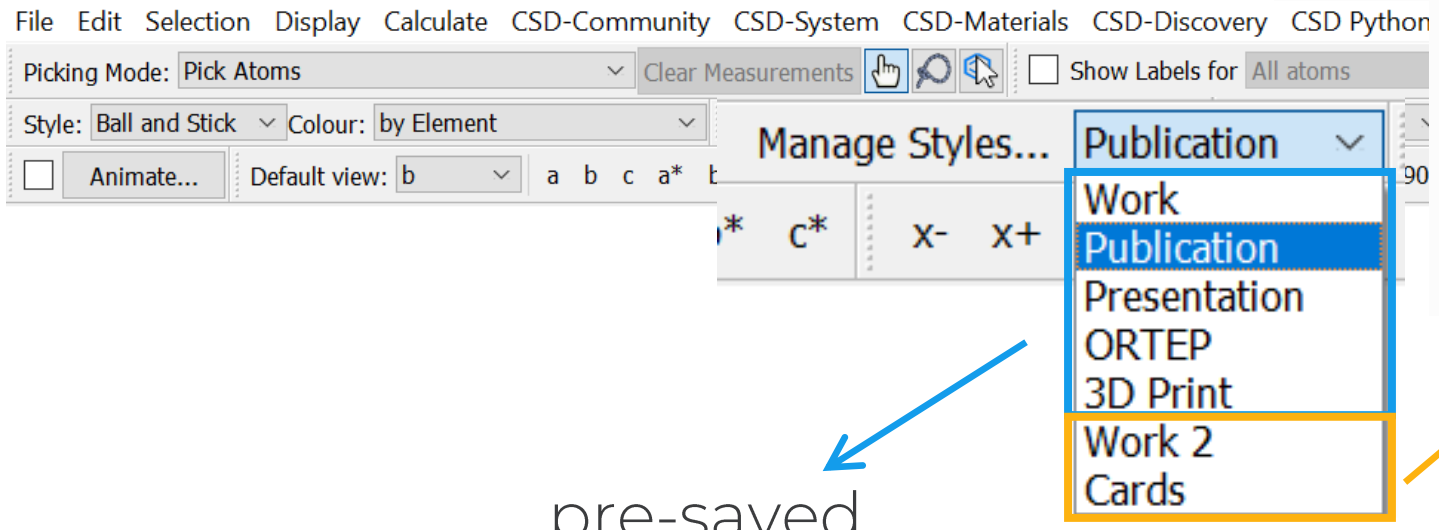
Read more about ADPs and Thermal Ellipsoids in the *Dictionary* on the handout.



CSD Refcode: LORBAW

Manage Styles

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

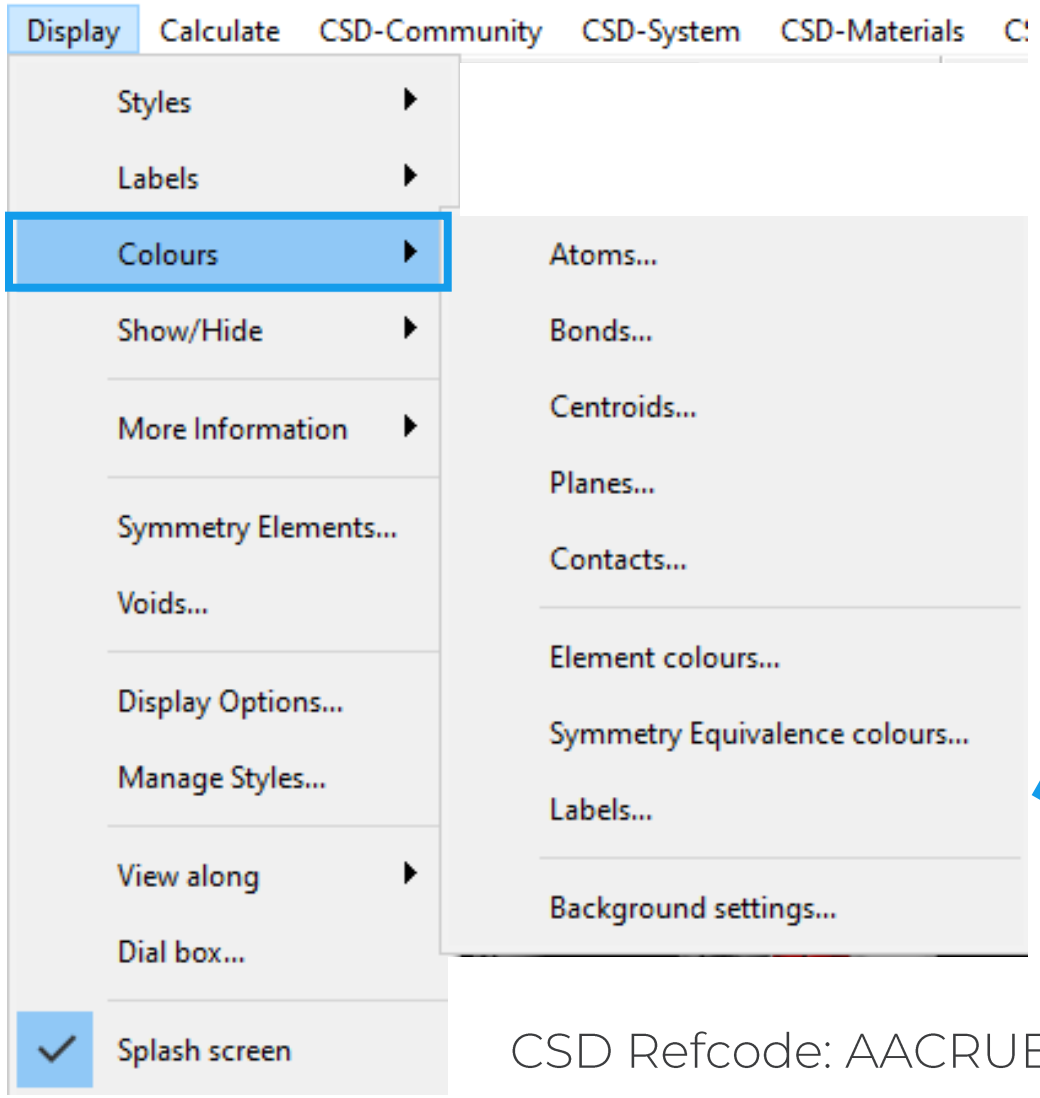


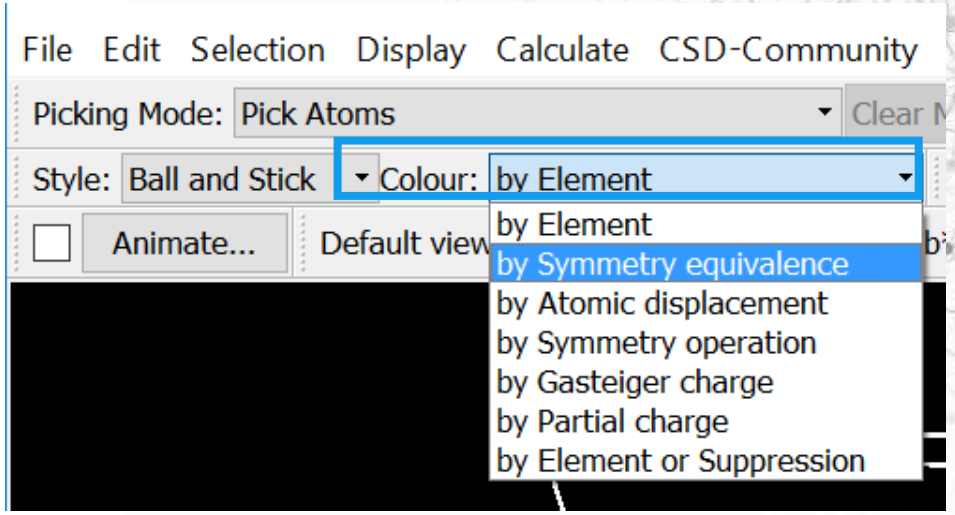
pre-saved options

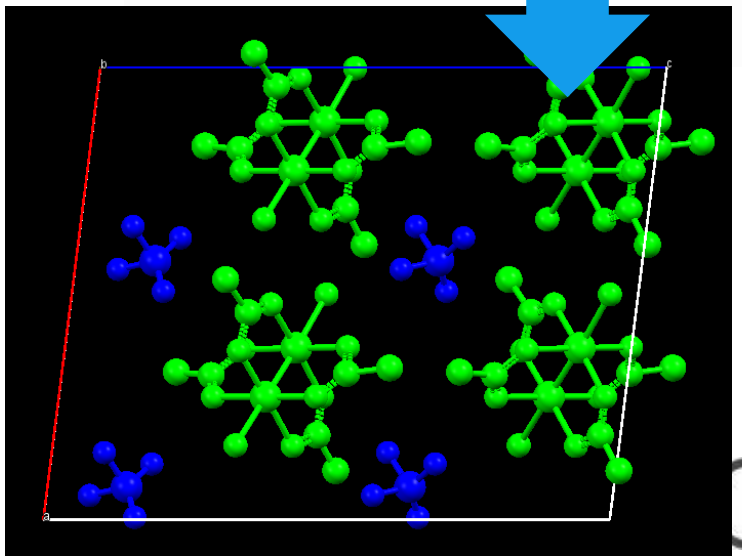
personalised options

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

Changing display - colours

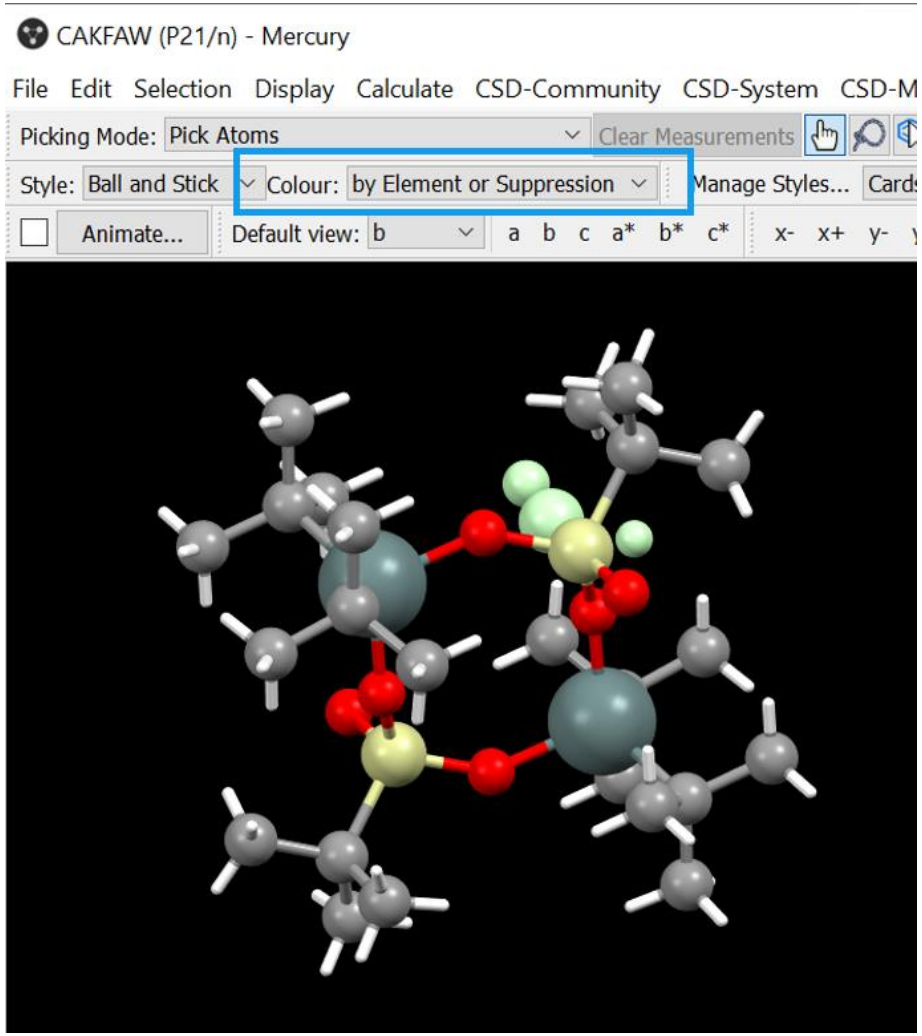


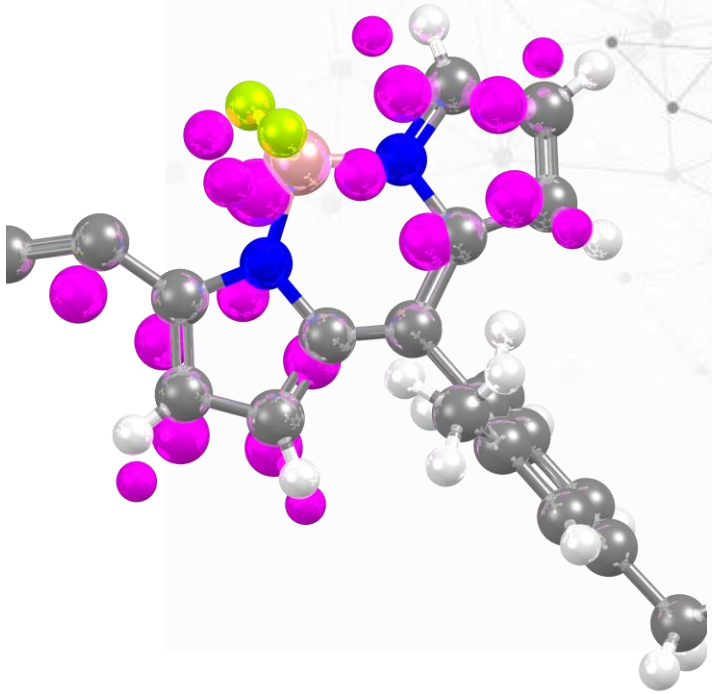




CSD Refcode: AACRUB

Changing display - colours



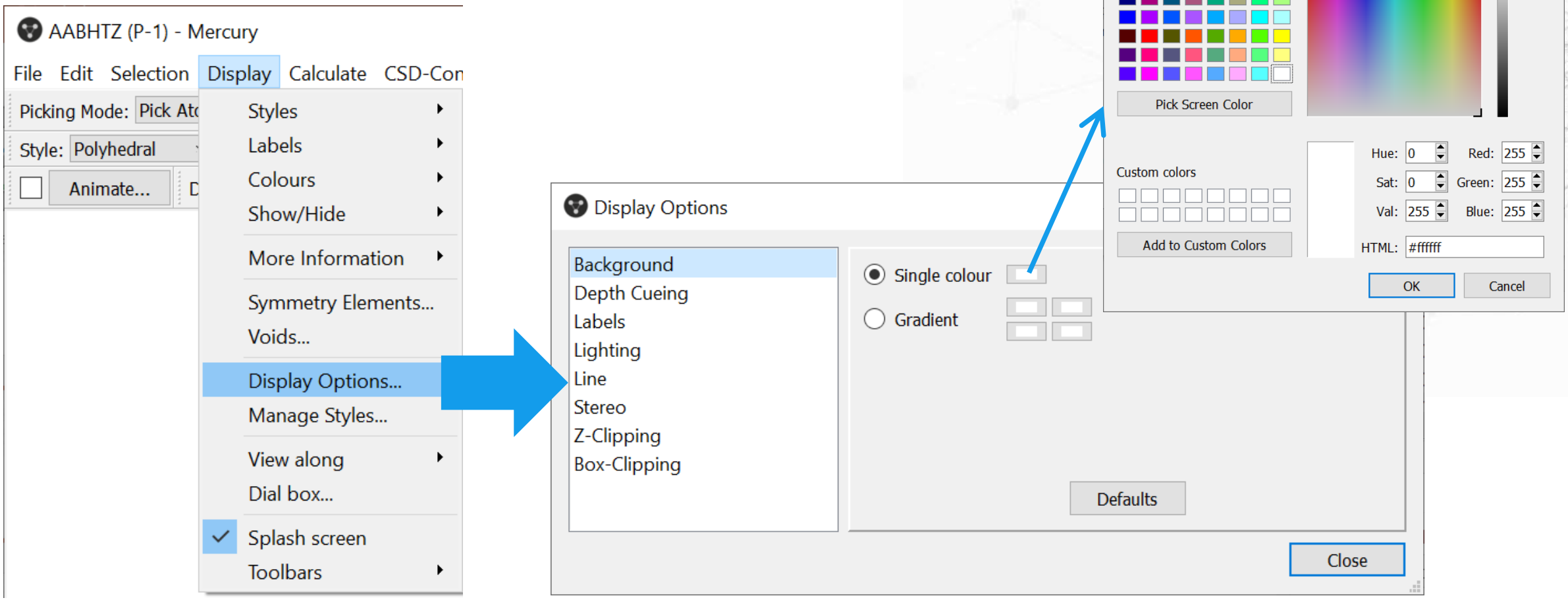


Disordered structures report two sets of atomic coordinates: major and minor sites. In most cases the atoms of the minor site will be suppressed.

Learn more in the *Dictionary* on the handout.

CSD Refcodes: CAKFAW and PIYDEI

Changing background colour



File Edit Selection Display Calculate CSD-Communit SD-Materials CSD-Discovery CSD Python API Help

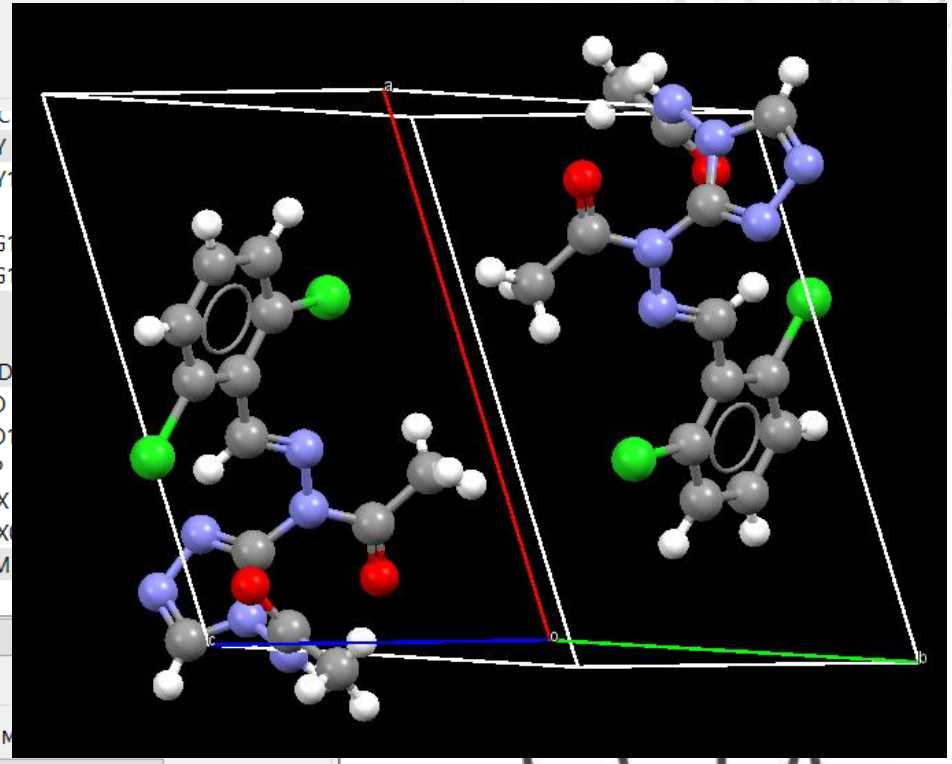
Centroids...
Planes...
Packing/Slicing...
Contacts...
Molecular Shell...
Graph Sets...
Powder Pattern...
Structure Overlay...
Molecule Overlay...

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
Reset 3x3x3

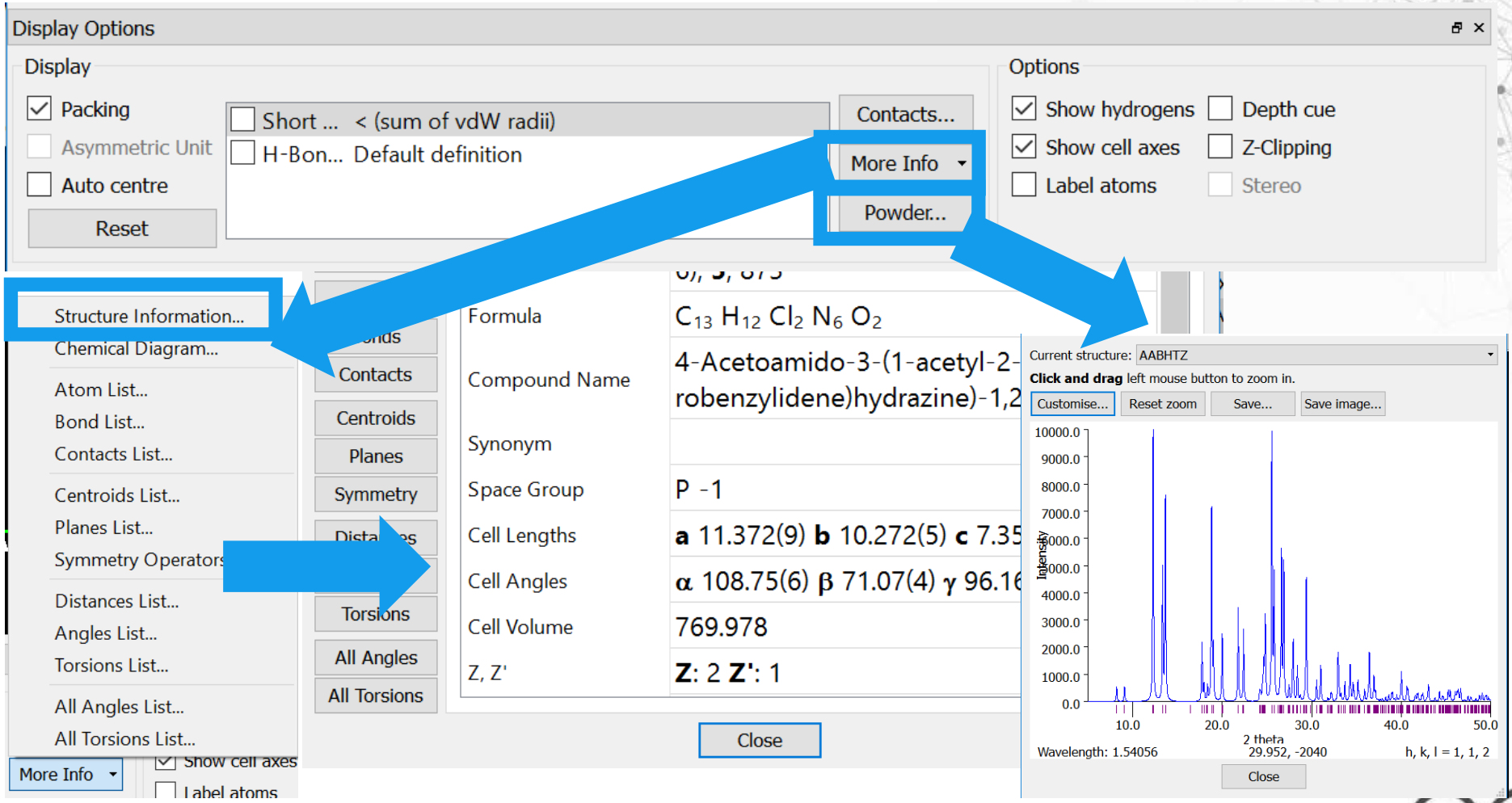
Include atoms
... that Fit
... in molecules whose Centroids fit
... in molecules where Any atom fits
... in molecules where All atoms fit

Reset button:
a friend!

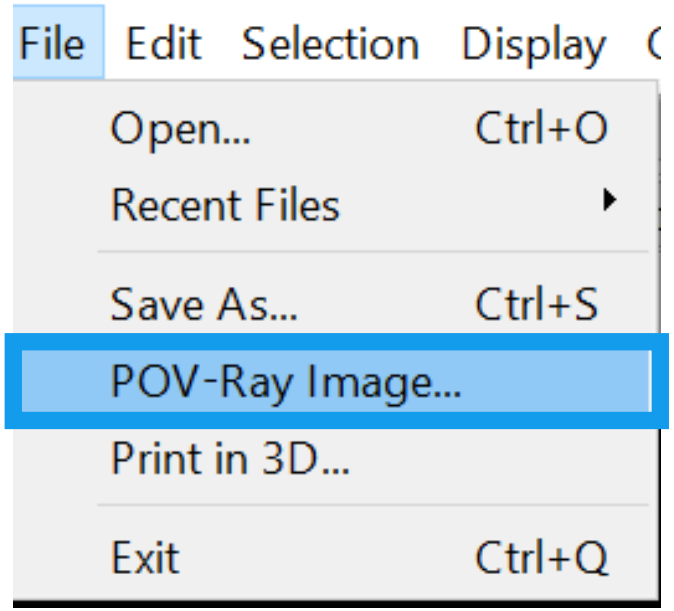
Display Options
Display
Packing
Asymmetric Unit
Short Contact < (sum of vdW radii)
H-Bond Default definition
Contacts...
More Info
Powder...
Reset
Options
Show hydrogens Depth
Show cell axes Z-Clipp
Label atoms Stereo
Structures...

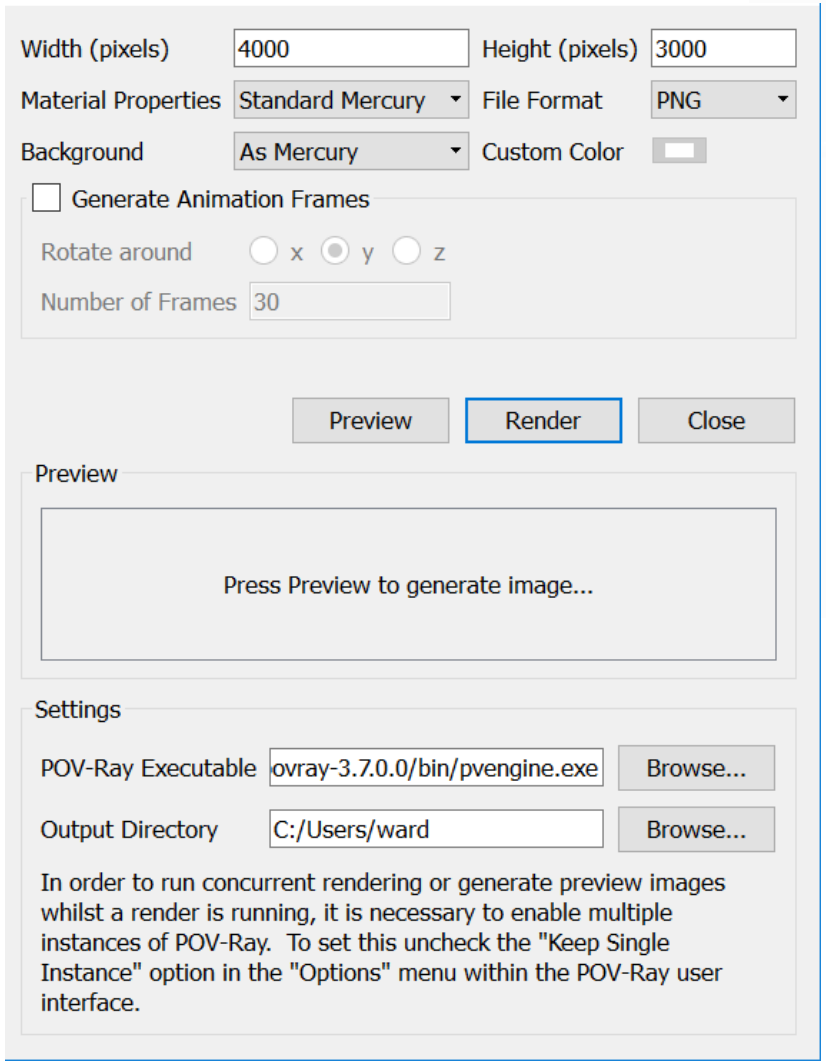


Other display options



Generating high quality images





File > POV-Ray Image

Change Resolution

- Width = 4000
- Height = 3000

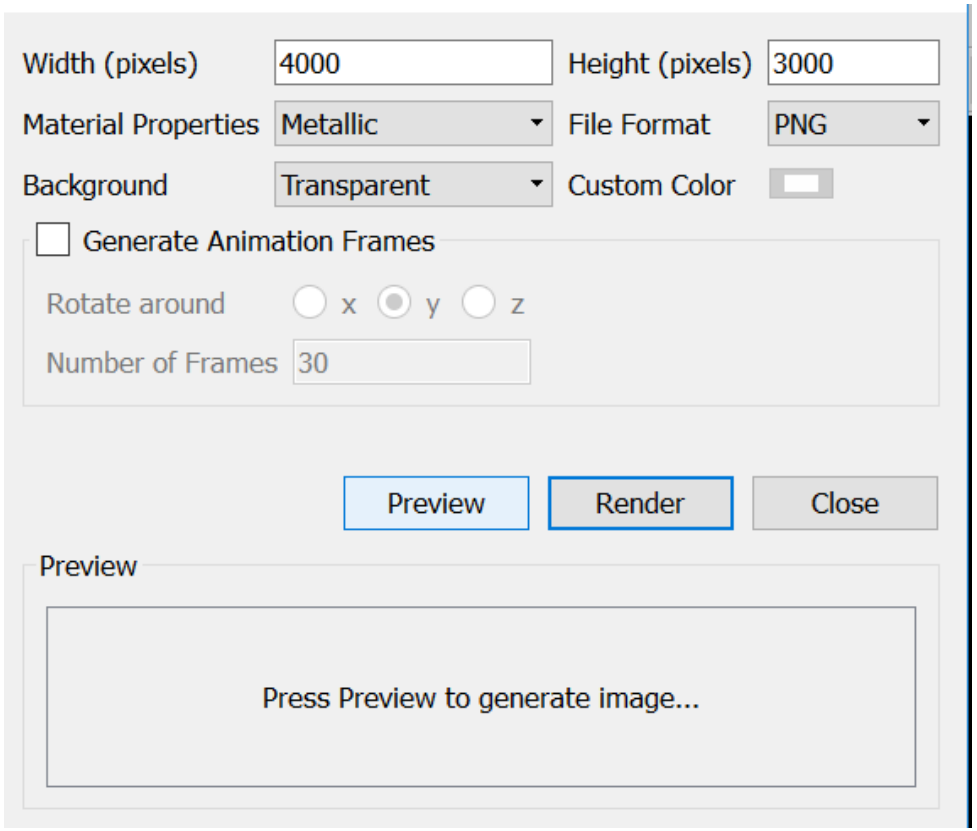
Change ‘Material Properties’ to ‘Metallic’

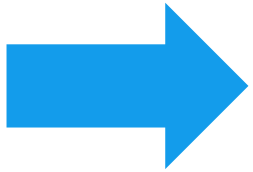
Set ‘Background’ to ‘Transparent’

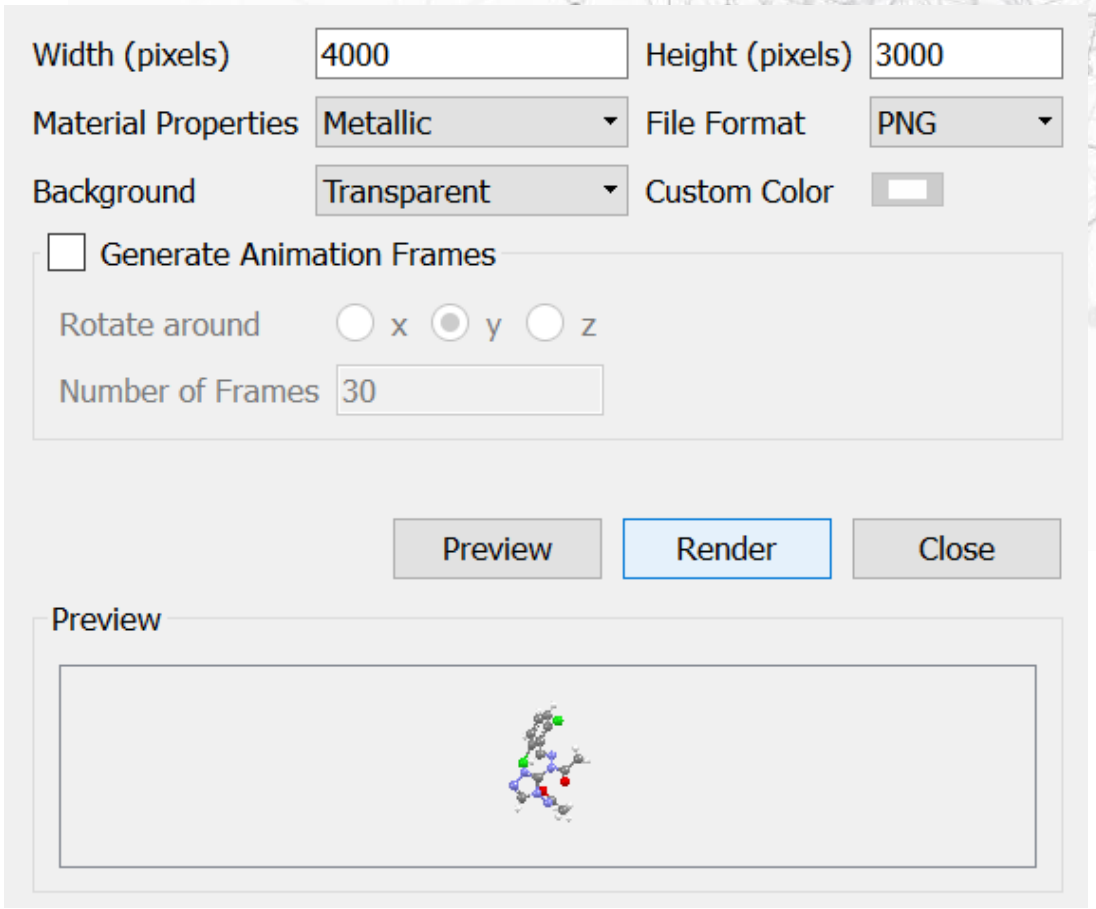
Press ‘Preview’

CCDC

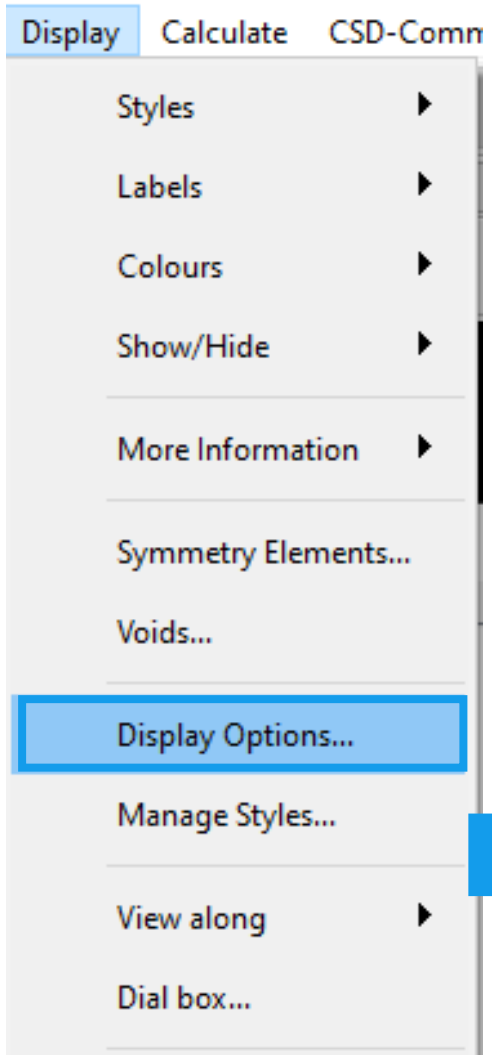
Previewing and rendering an image

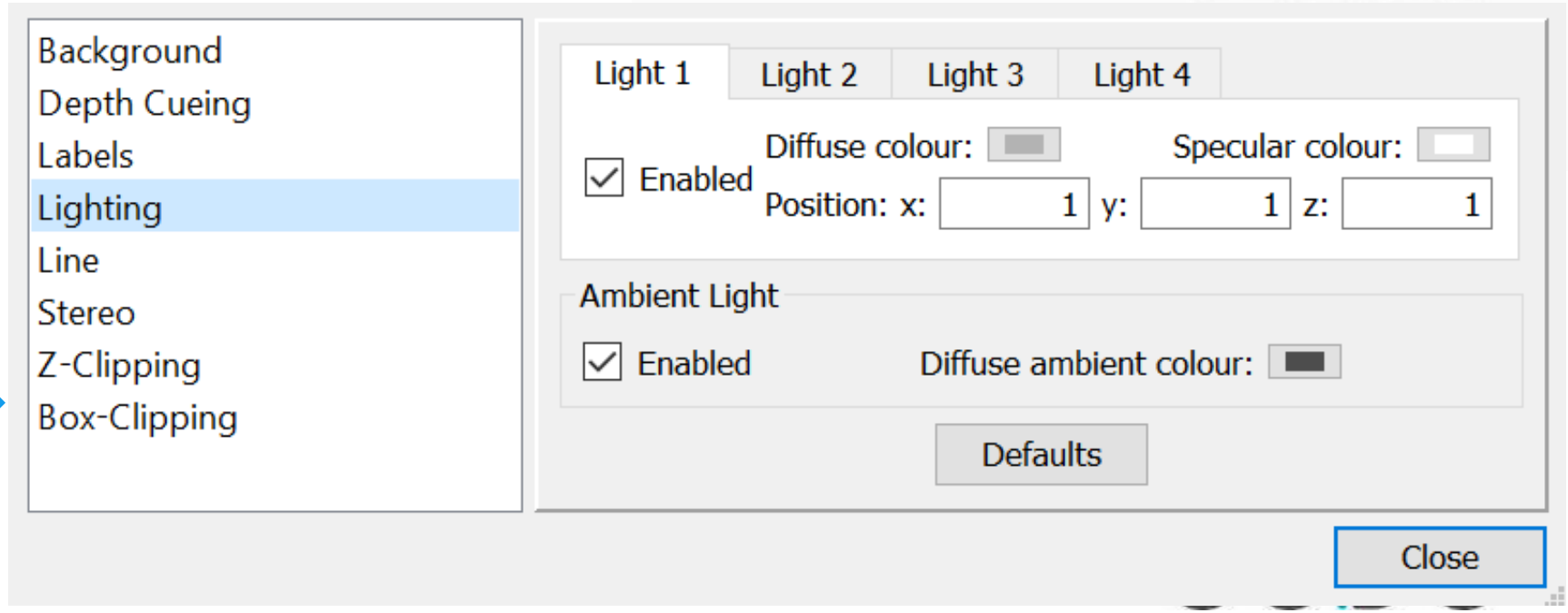


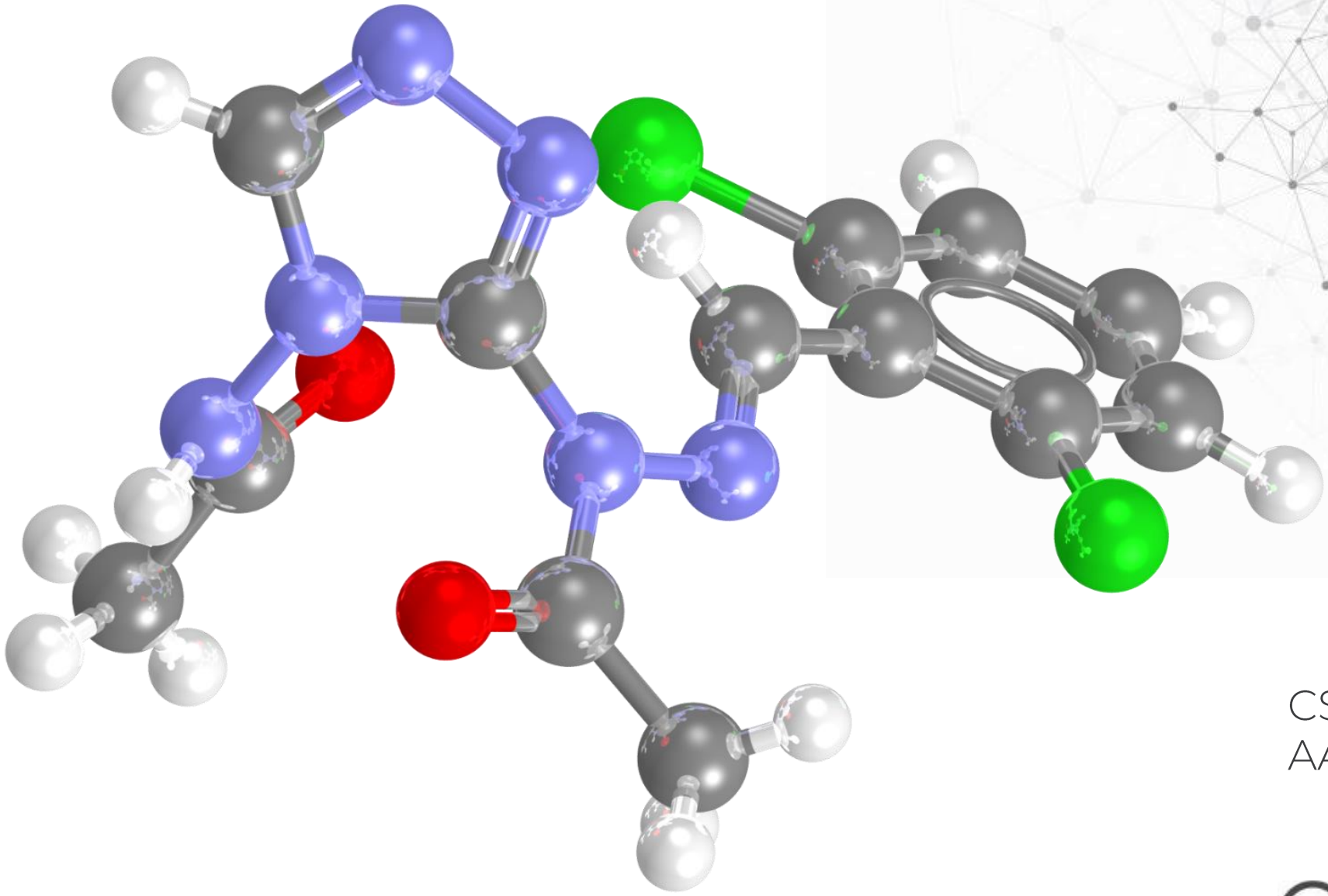




Display - Options







CSD Refcode:
AABHTZ

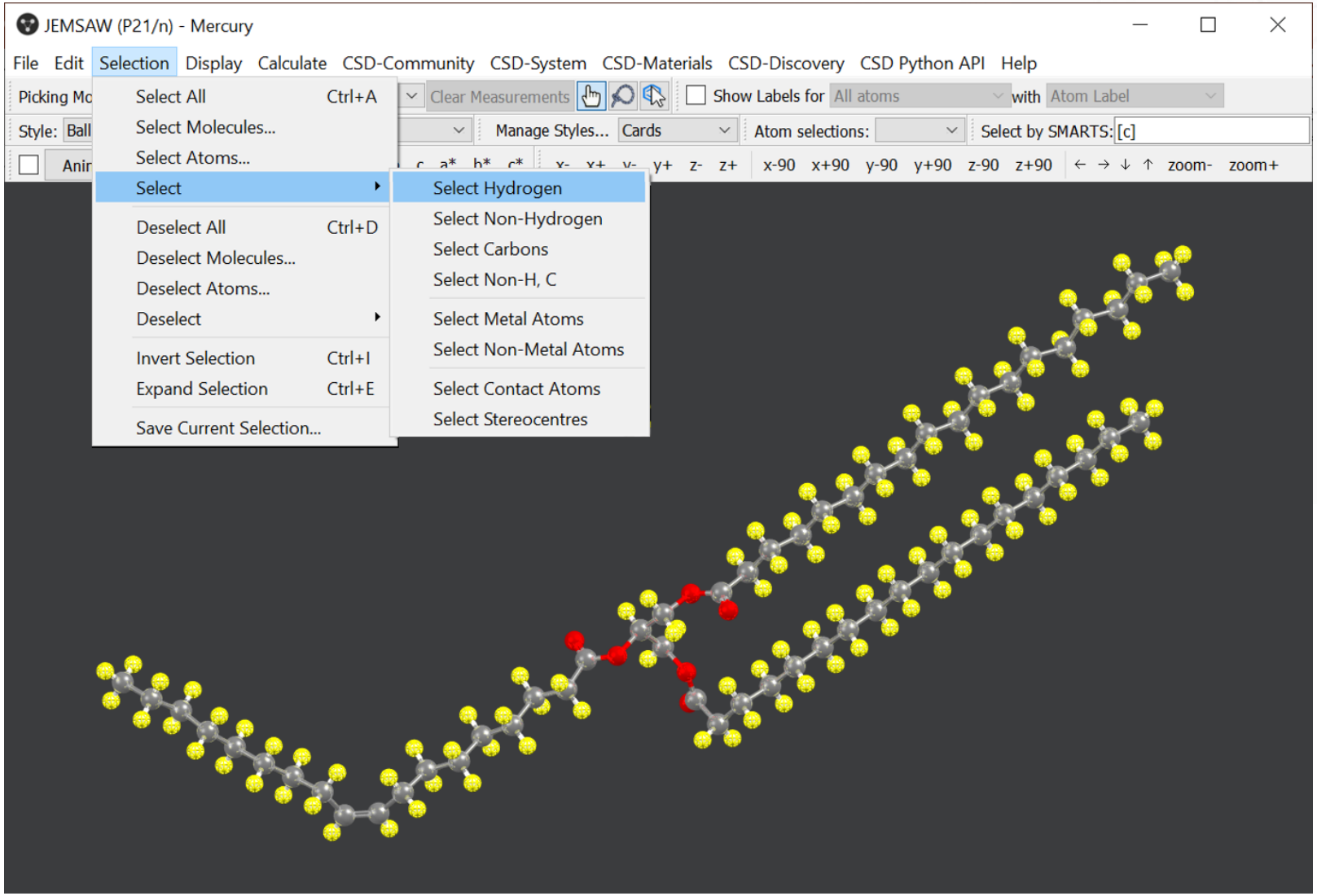
CCDC

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

CCDC

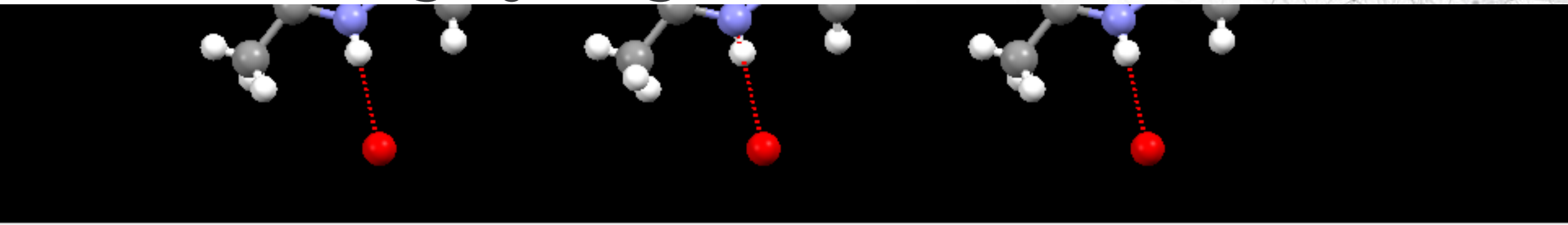
Selection



CSD Refcode:
JEMSAW

CCDC

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...

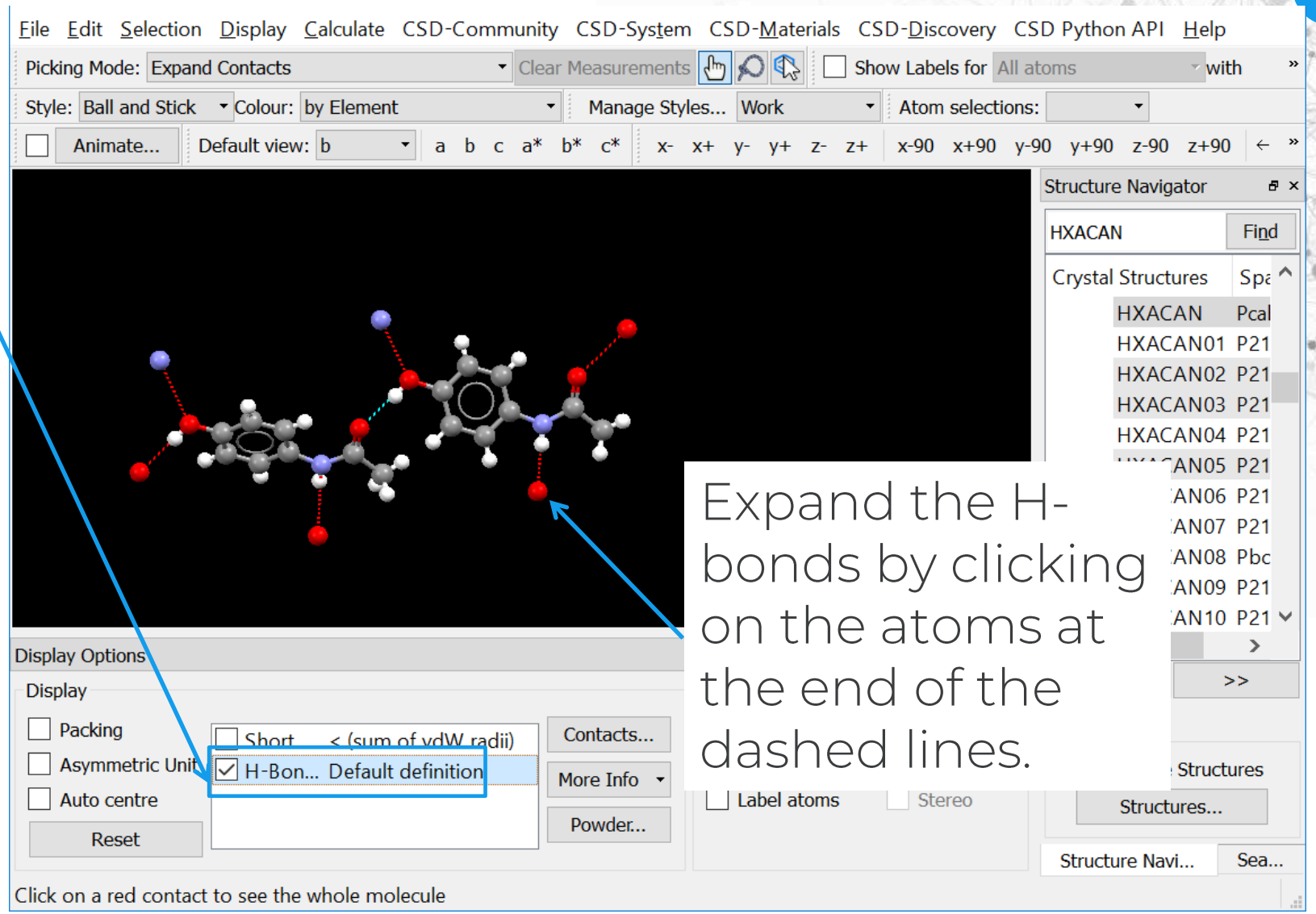
Options

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

Click on a red contact to see the whole molecule

CCDC

Turn on H-bond interactions using the tick box

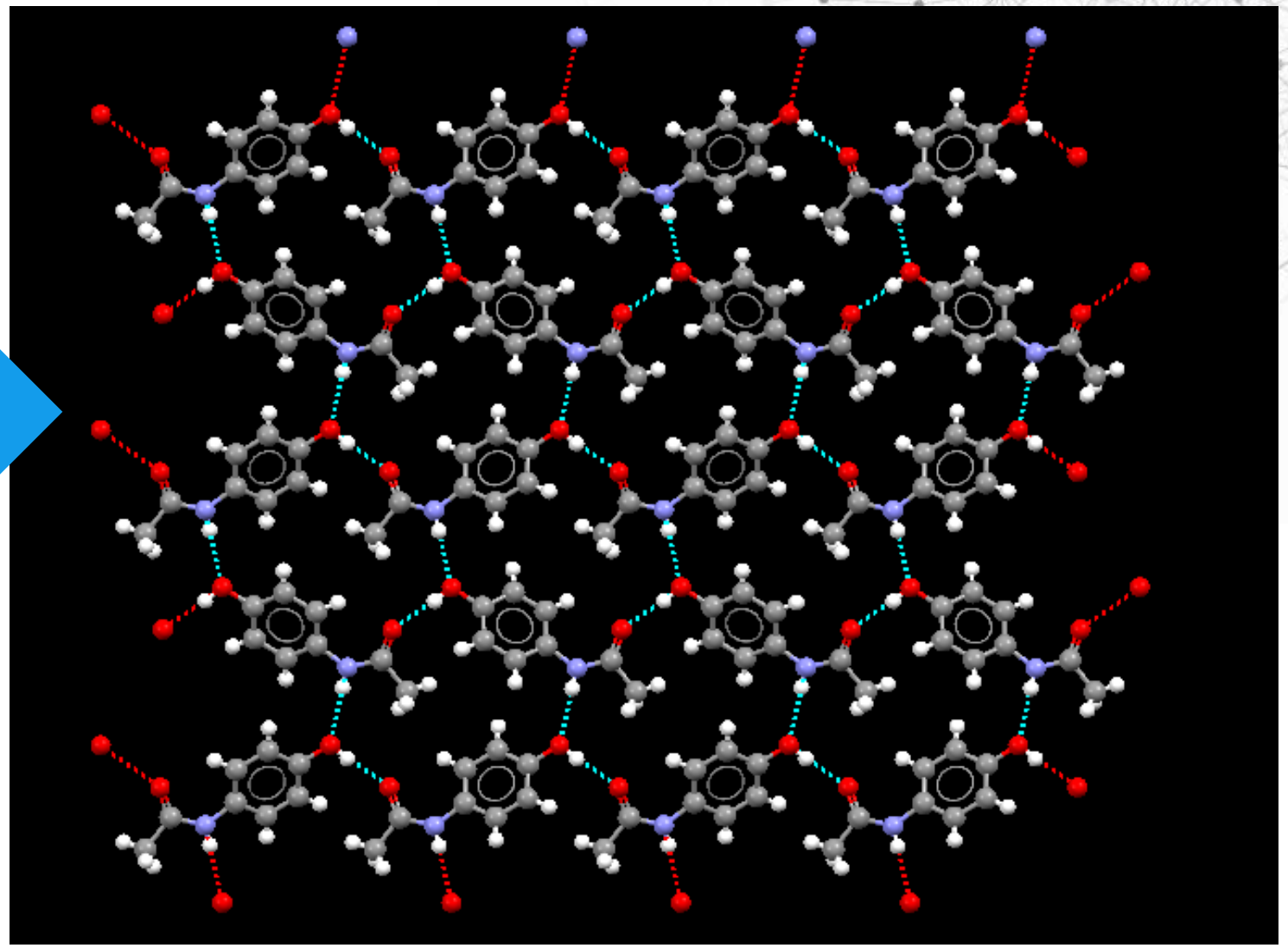


Expand the H-bonds by clicking on the atoms at the end of the dashed lines.

CSD Refcode: HXACAN

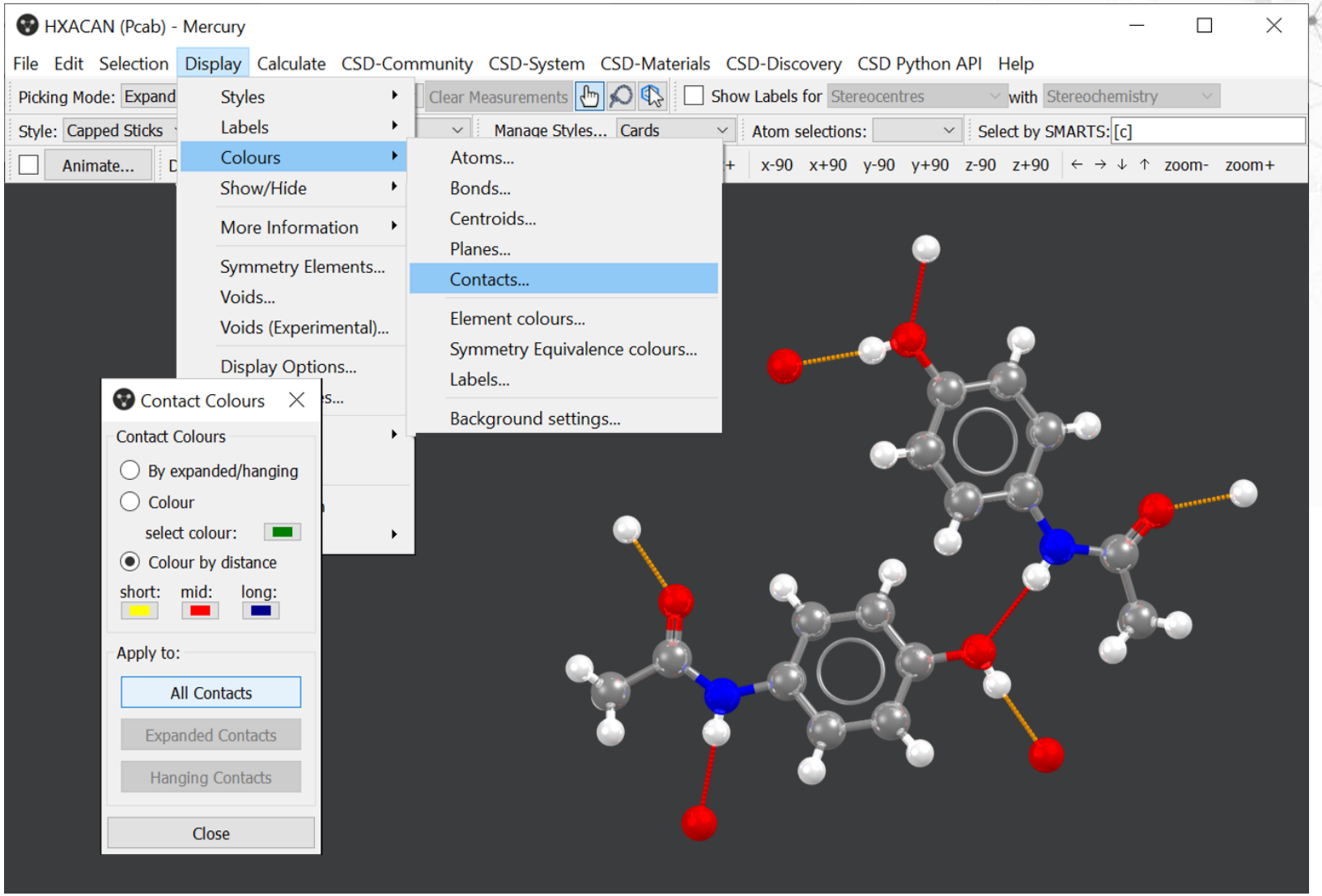
Building the H-bond network

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



CSD Refcode: HXACAN

Colour H-bonds by distance

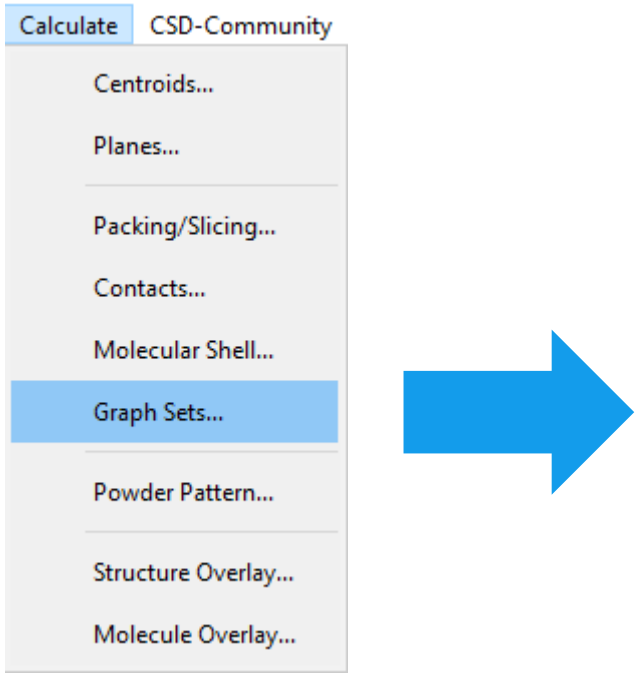


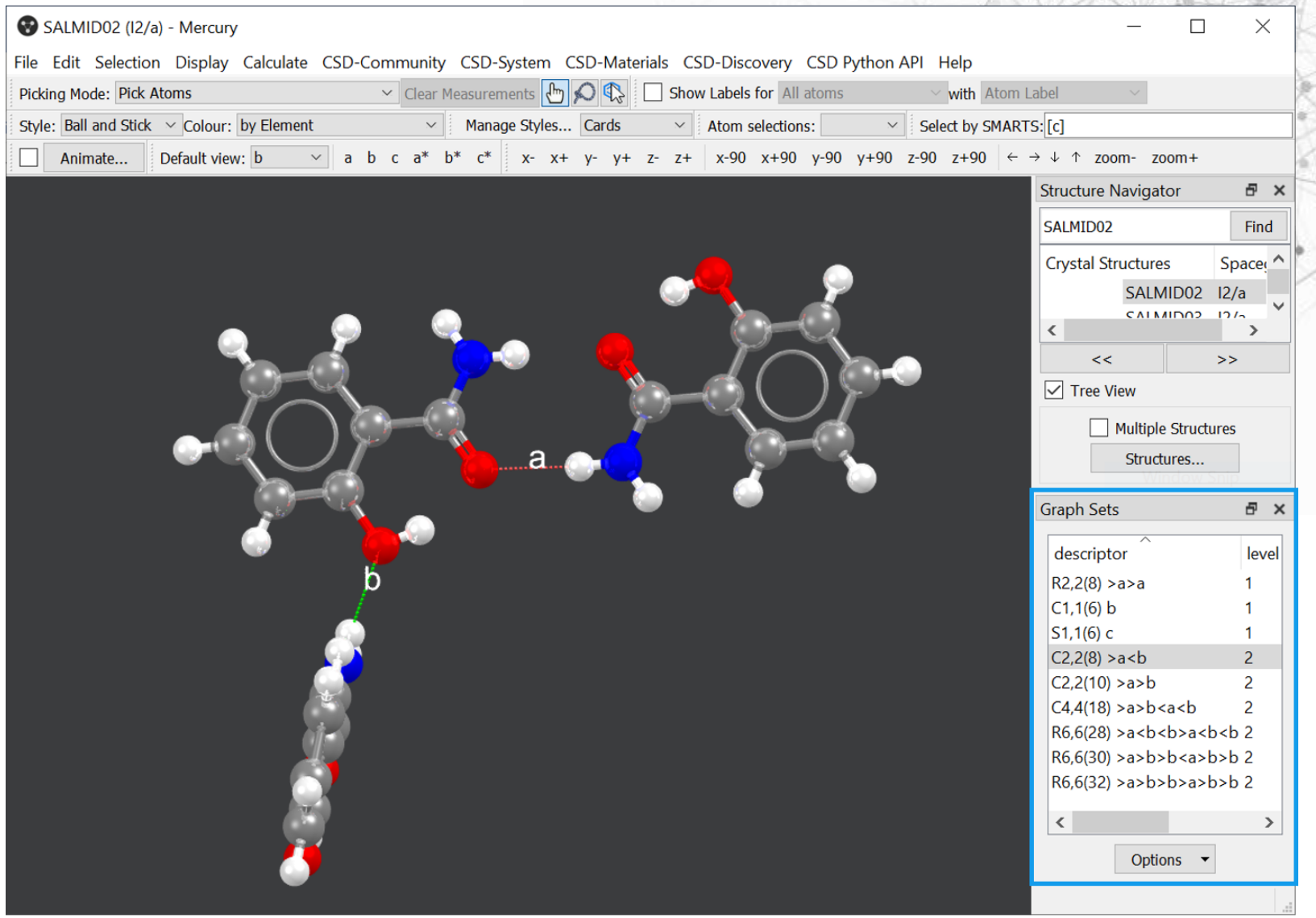
CSD Refcode: HXACAN

CCDC

Bonus: Graph Sets

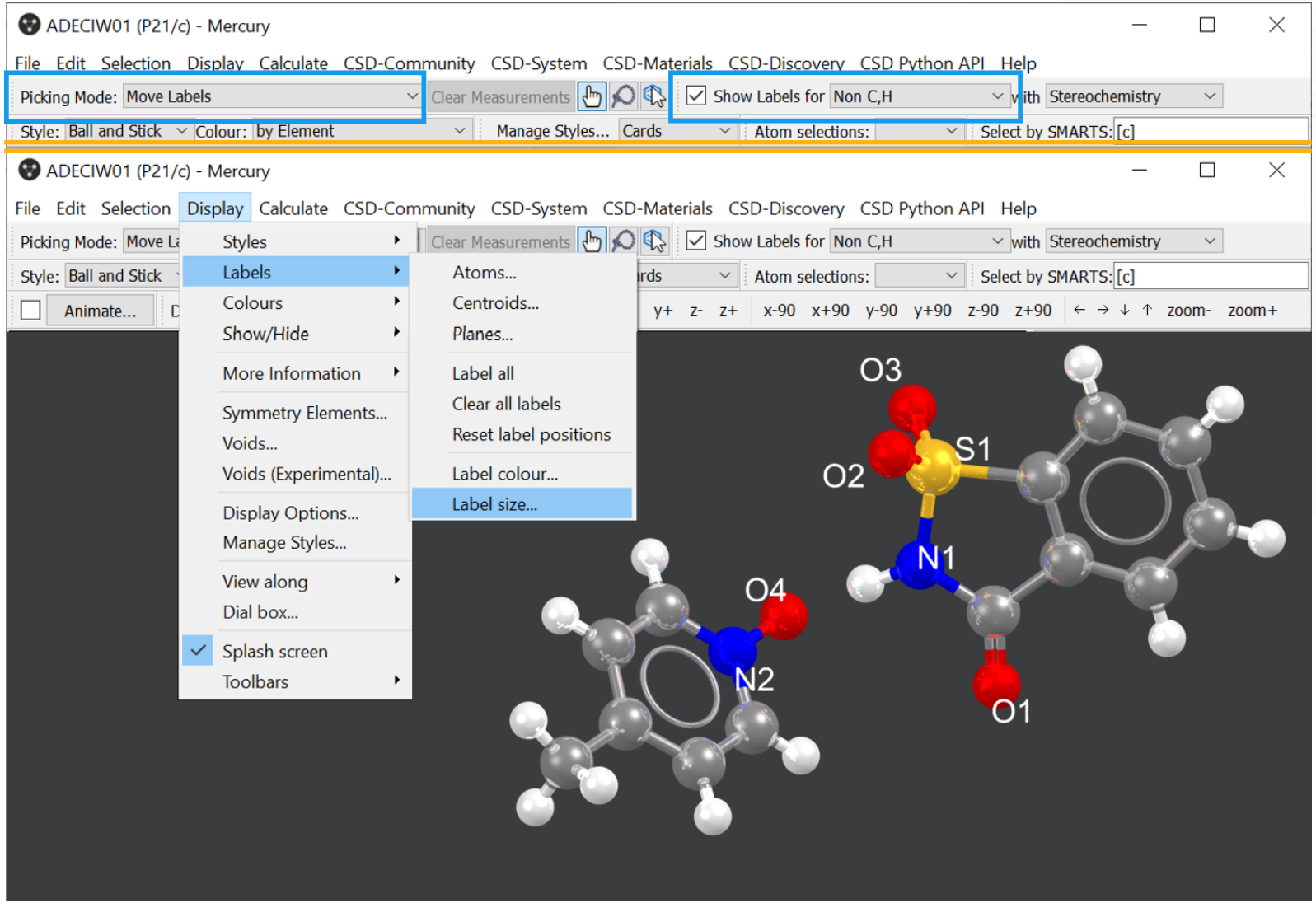
CSD Refcode: SALMID02





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

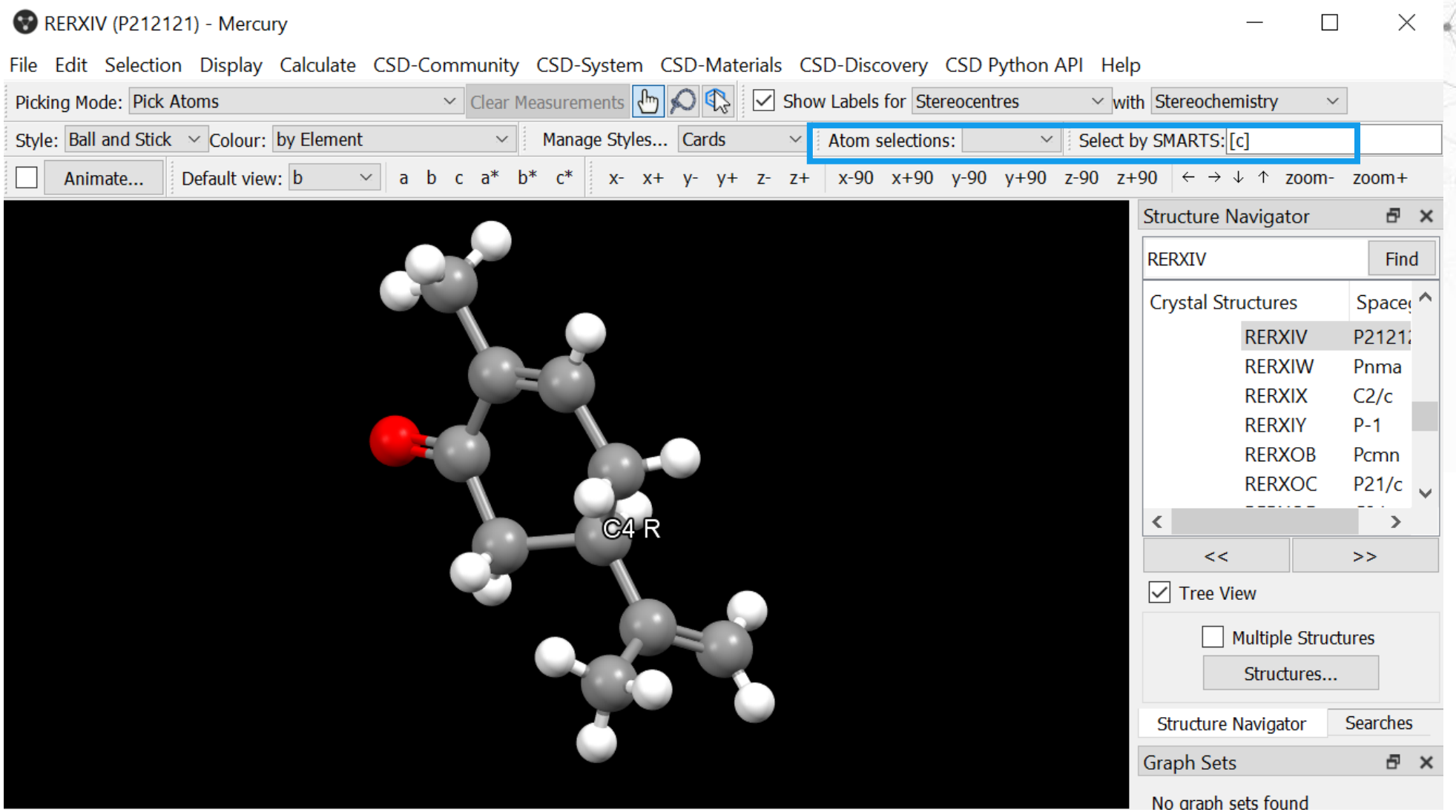
Adding, moving and sizing labels



CSD Refcode: ADECIW01

CCDC

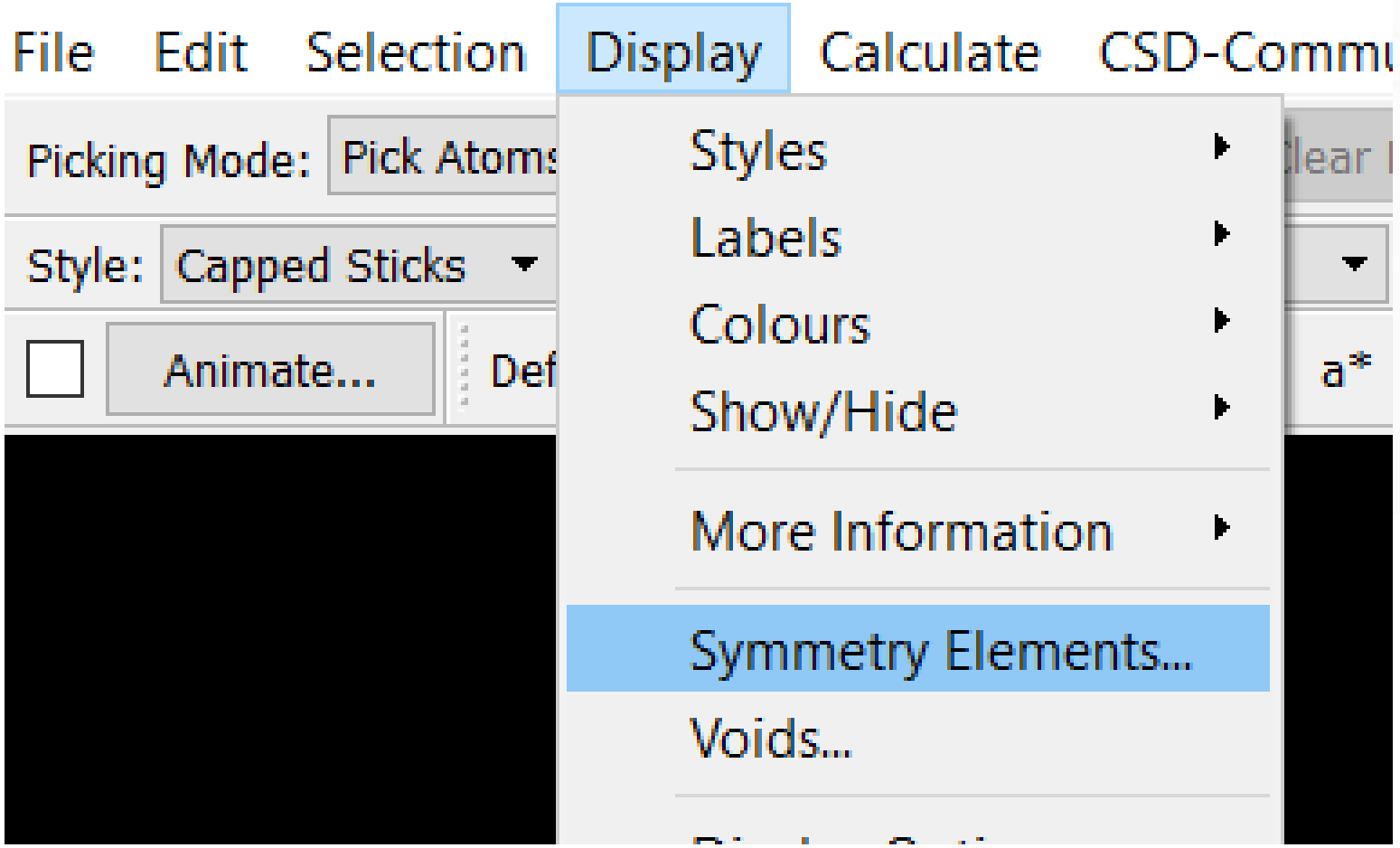
Labelling chiral molecules



CSD Refcode: RERXIV

CCDC

Symmetry


File
Edit
Selection
Display
Calculate
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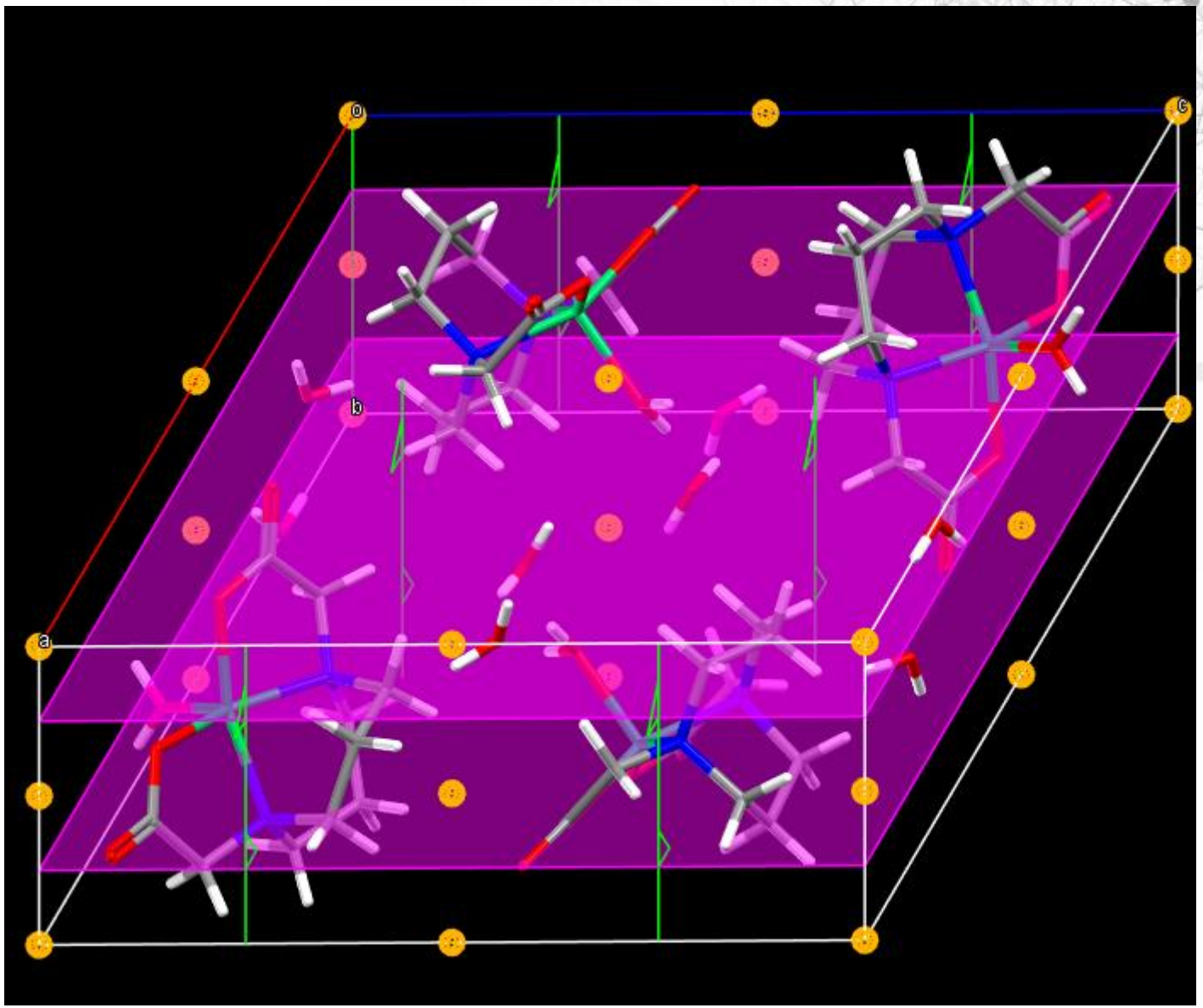
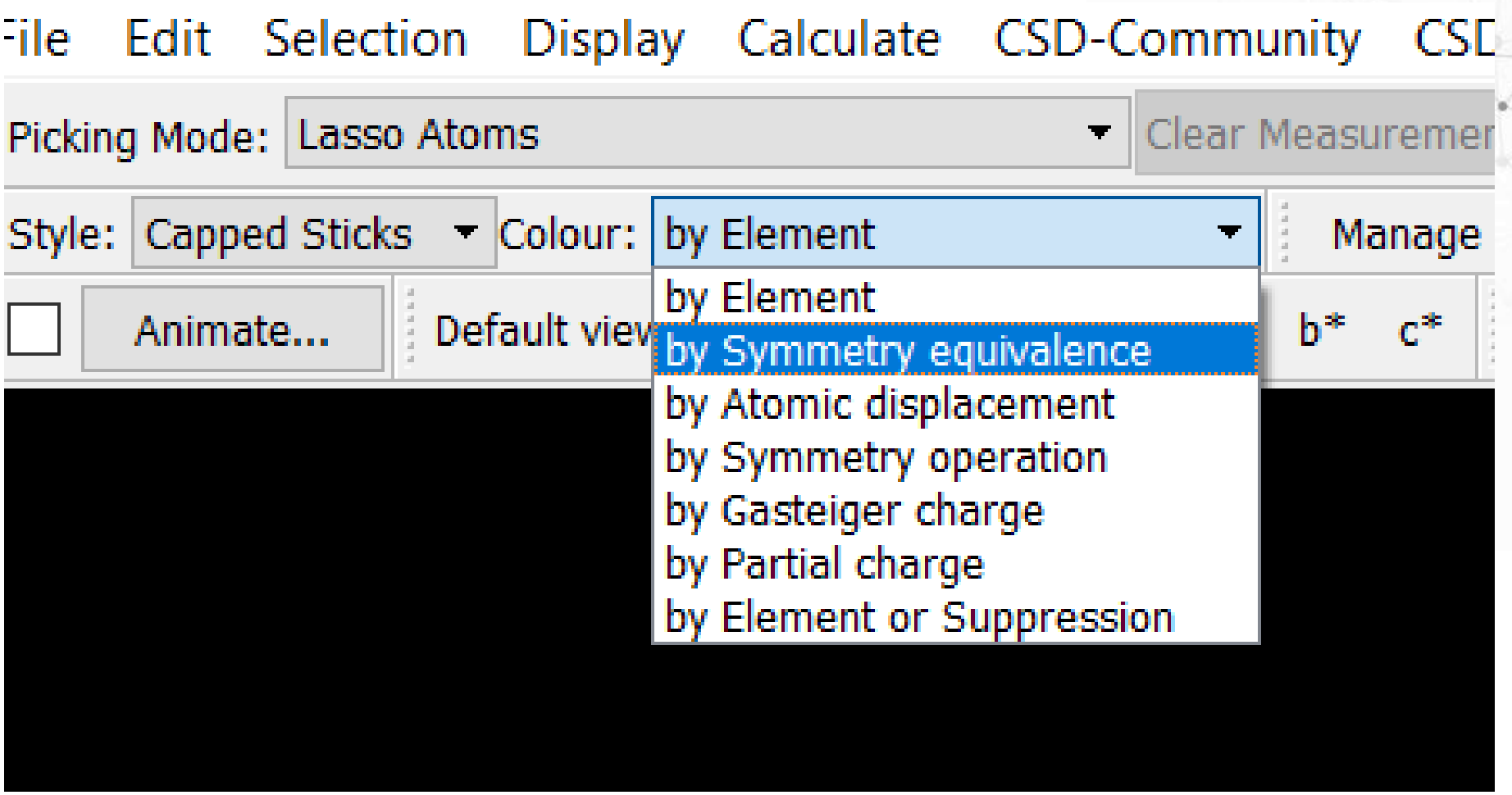
Picking Mode:
Pick Atoms
Style:
Capped Sticks
Animate...
Styles
Labels
Colours
Show/Hide
More Information
Symmetry Elements...
Voids...

CSD Refcode: AACANI11




File Edit Selection Display Calculate CSD-Community CSD
Picking Mode: Lasso Atoms
Clear Measuremer
Style: Capped Sticks
Colour: by Element
Manage
Animate...
Default view
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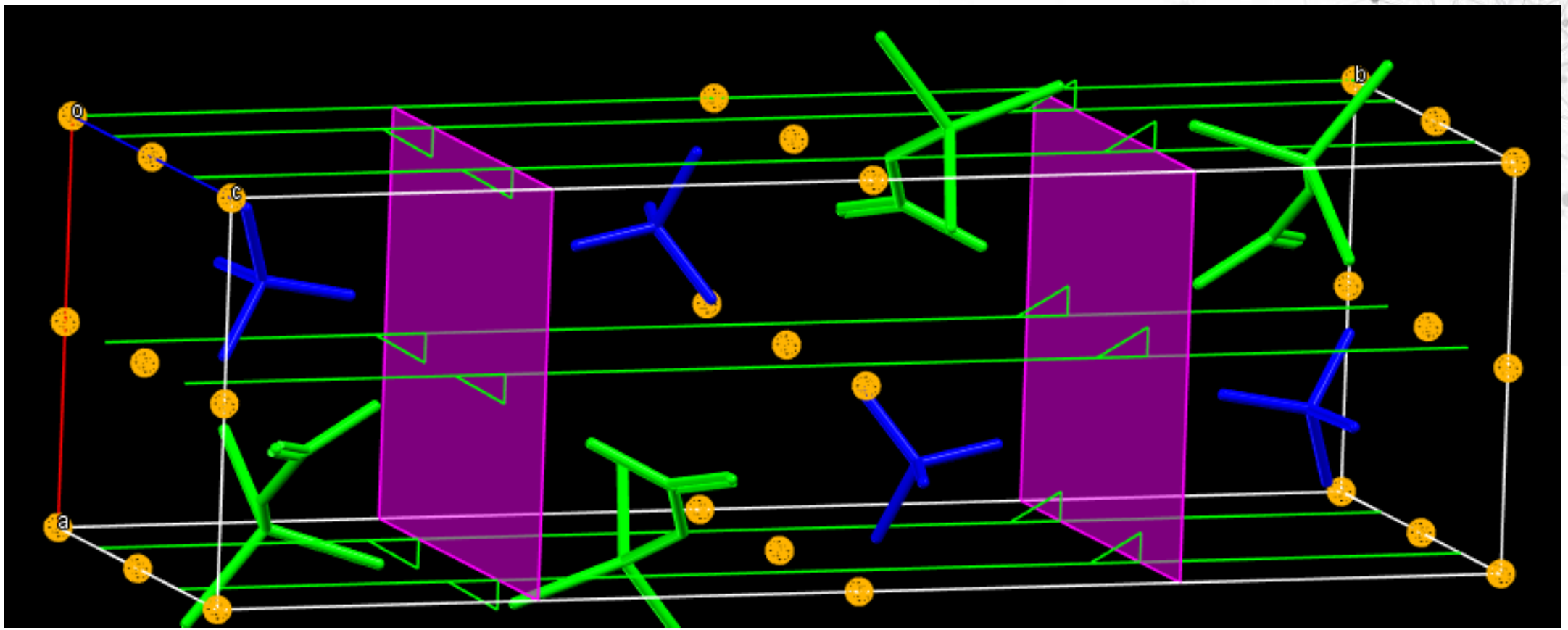
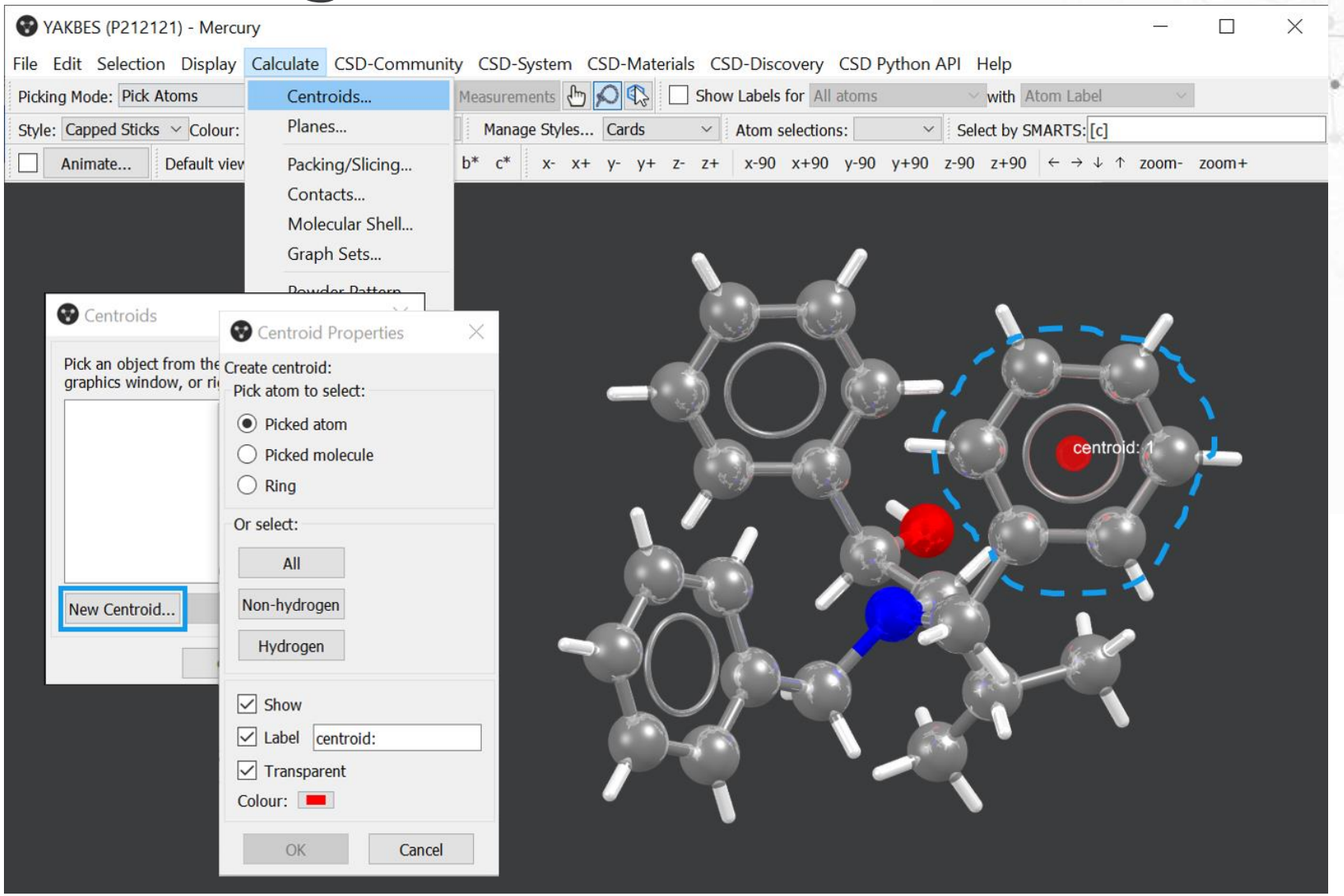
by Element
by Symmetry equivalence
by Atomic displacement
by Symmetry operation
by Gasteiger charge
by Partial charge
by Element or Suppression

CSD Refcode: AACMAL



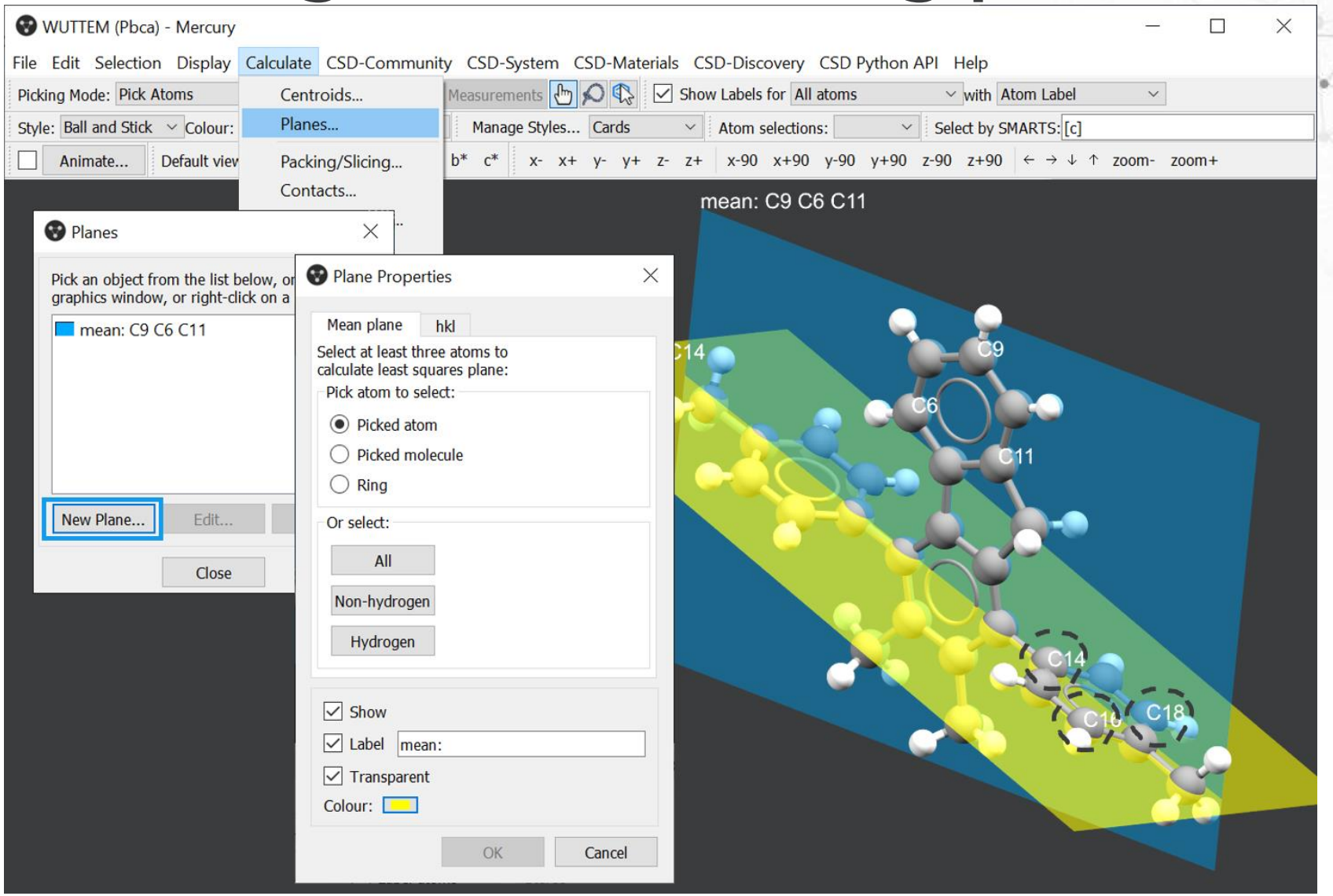
Calculating centroids



CSD Refcode:
YAKBES

CCDC

Calculating and visualising planes

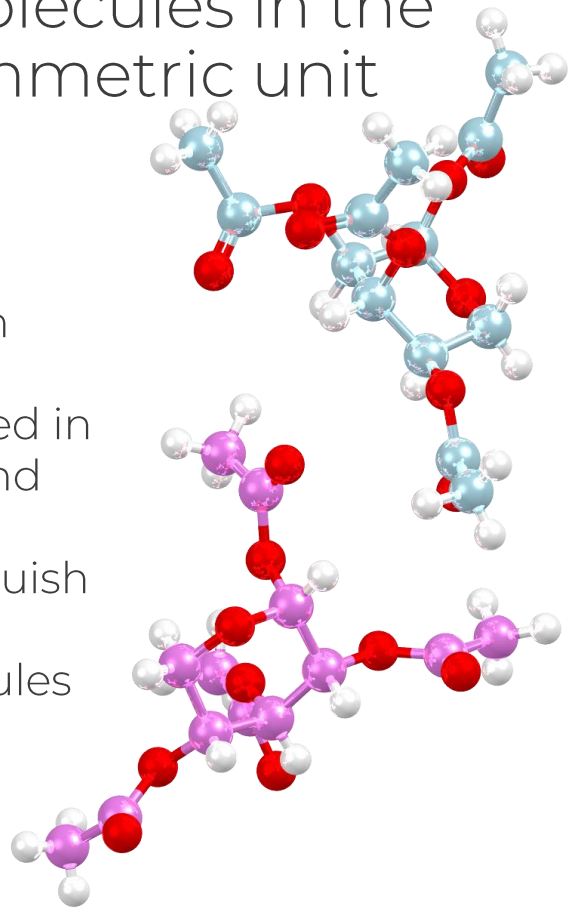


CSD Refcode:
WUTTEM

CCDC

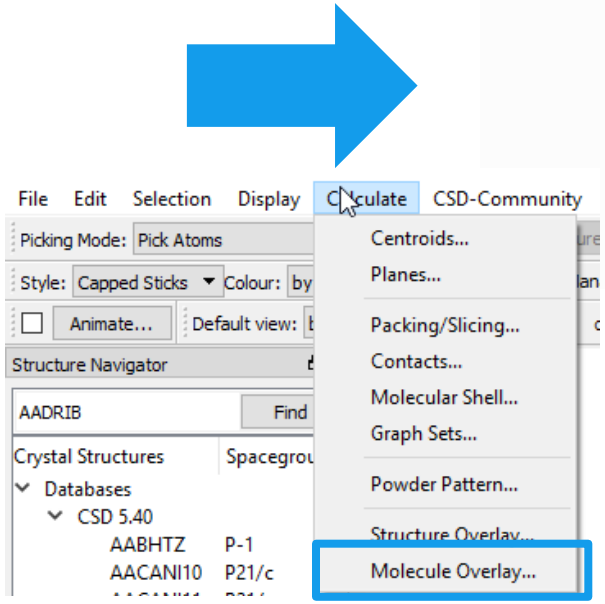
Molecule overlay

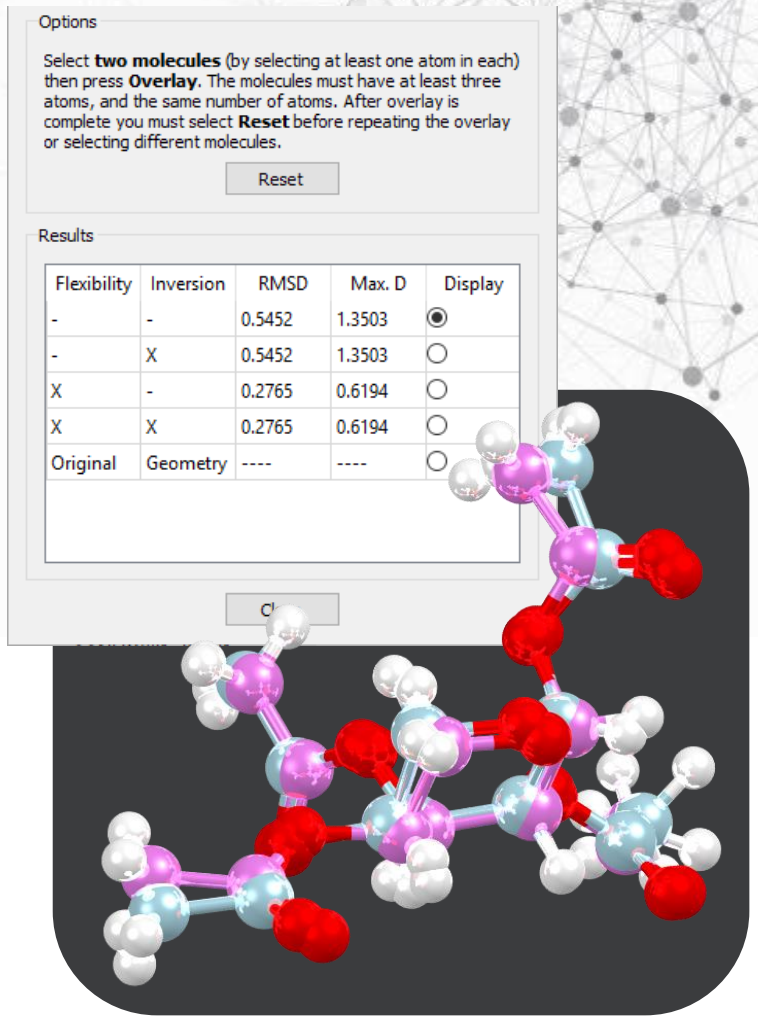
2 molecules in the asymmetric unit



Carbon atoms coloured in blue and pink to distinguish the molecules

compare their conformation overlapping them

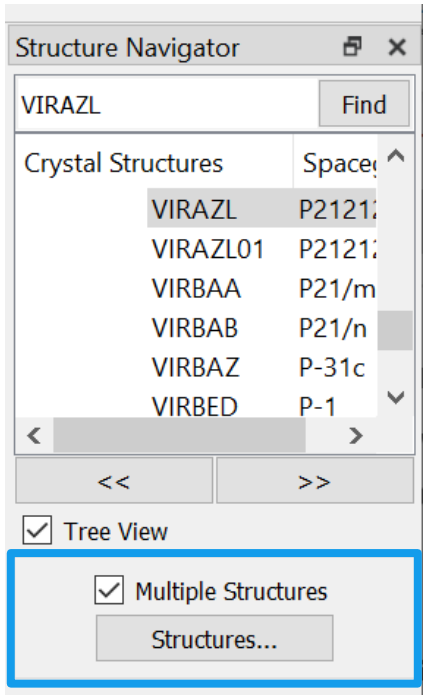


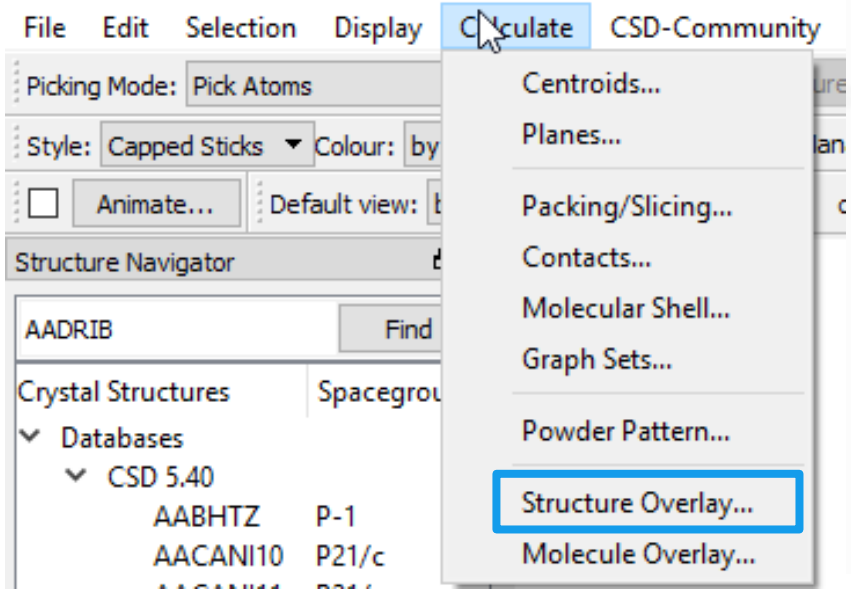


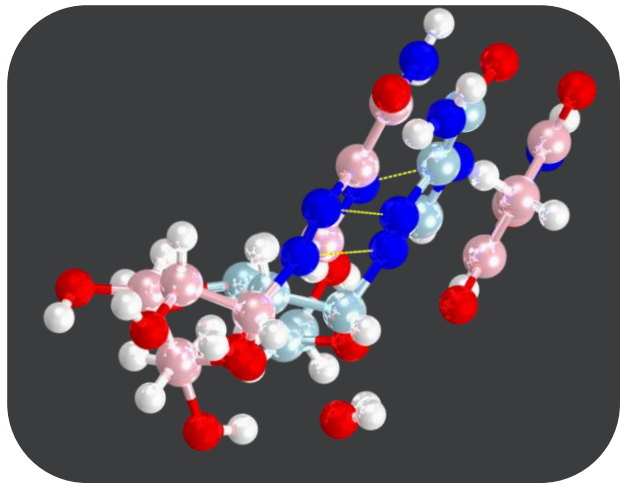
Structure overlay

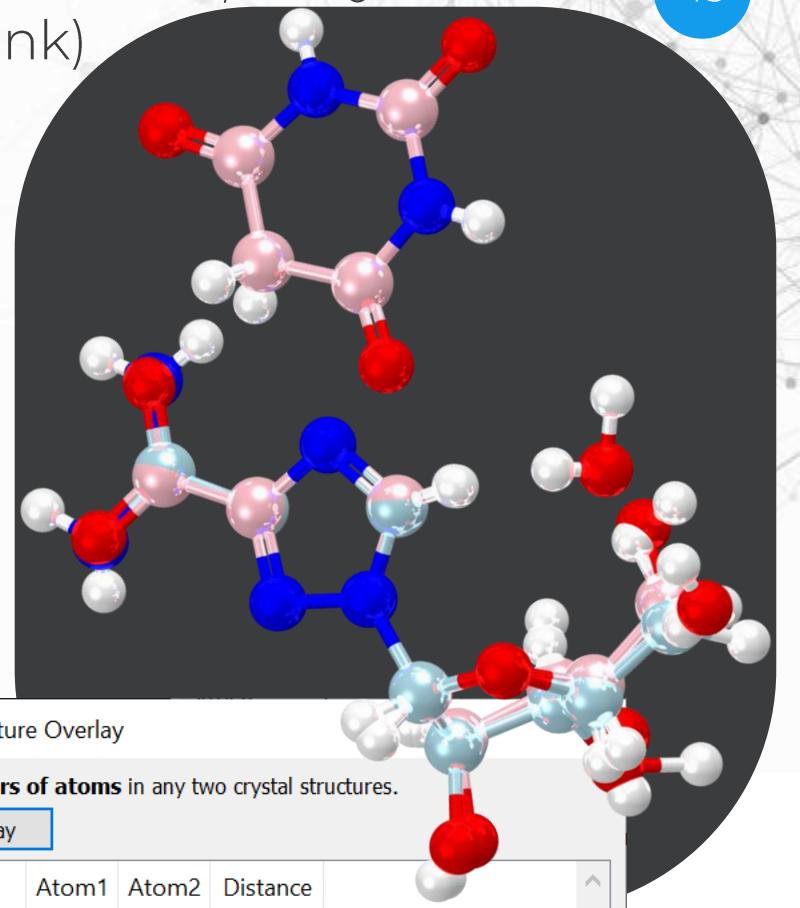
CSD Refcodes: VIRAZL, FOQROU (light blue – pink)

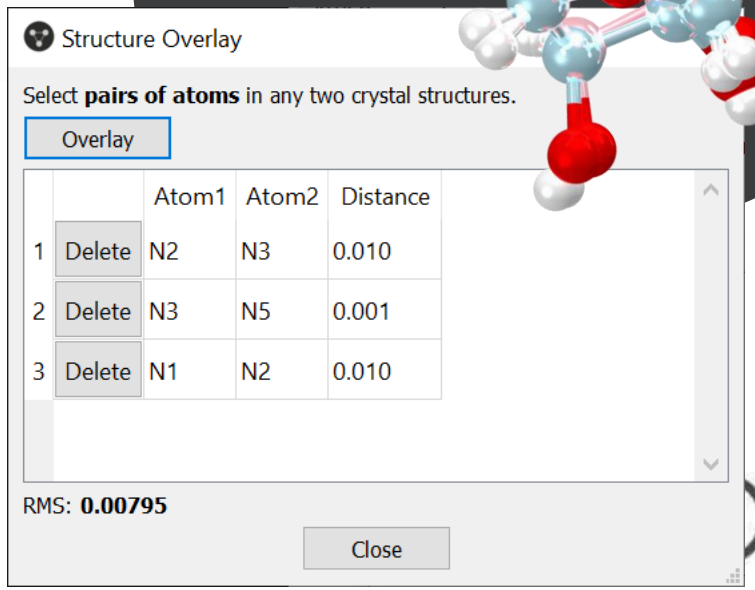
Tick Multiple structures to load more than one structure



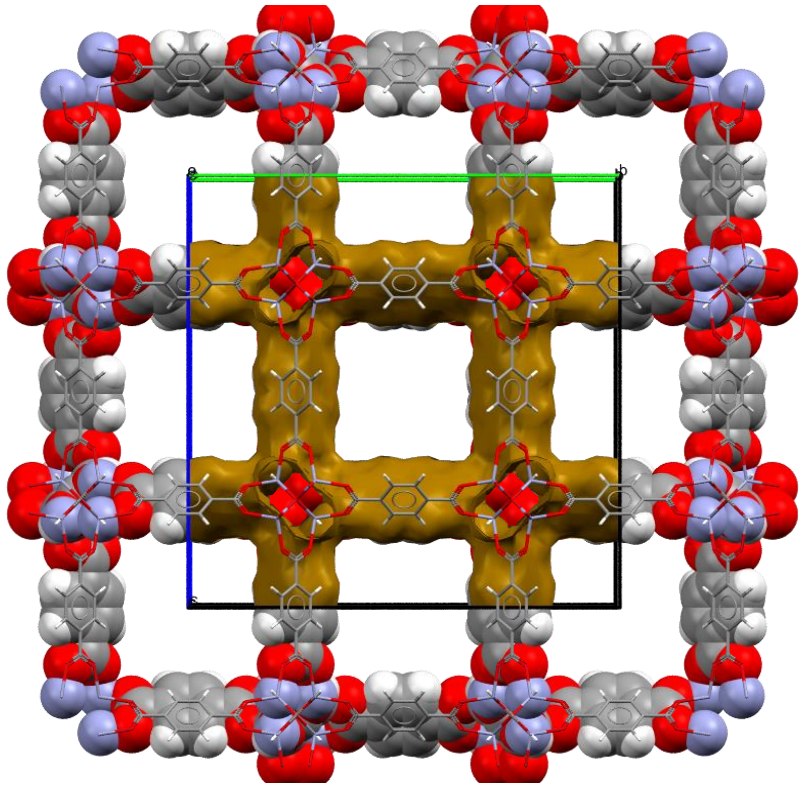




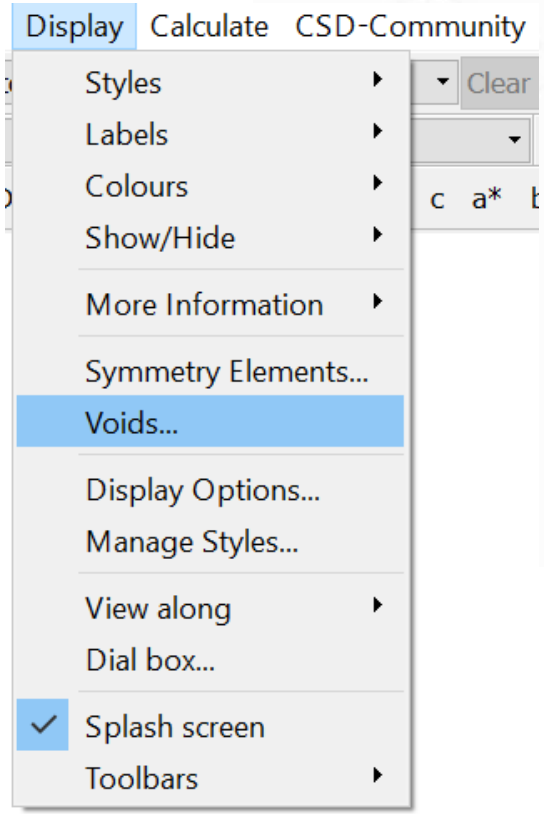


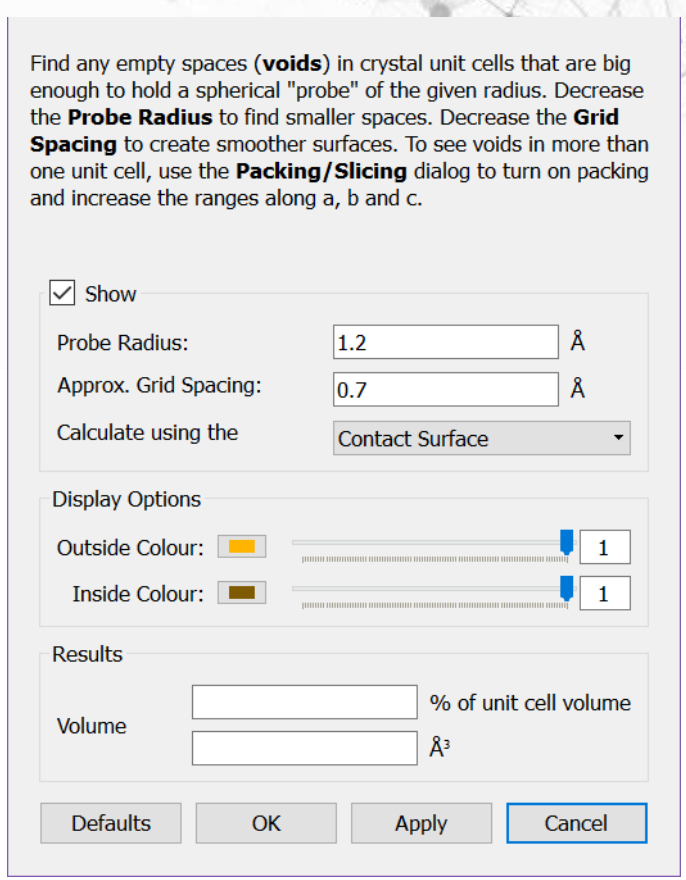


Empty space visualisation

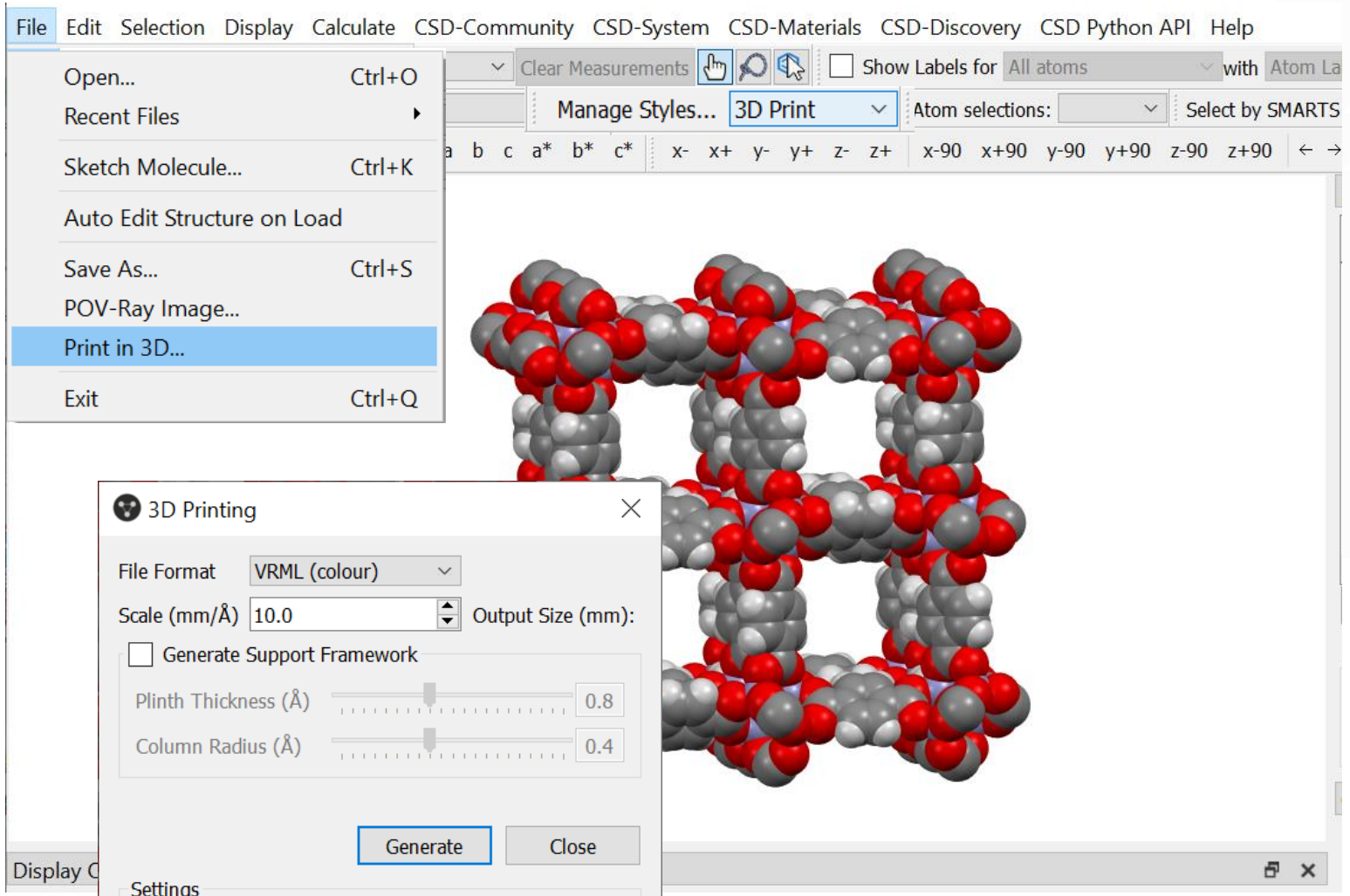


CSD Refcode: SAHYIK
(MOF5)

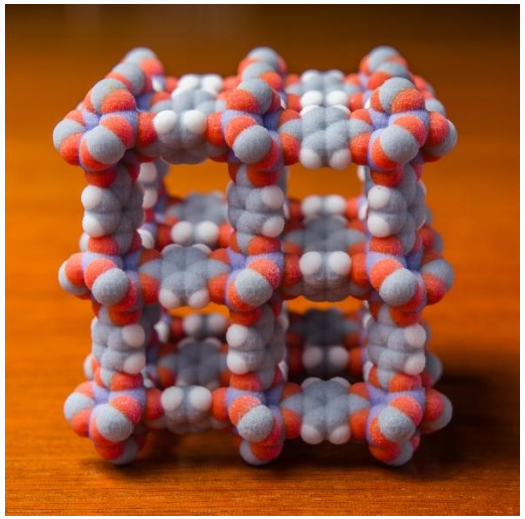




3D printing



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



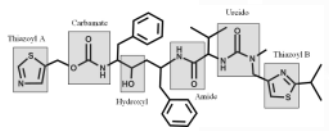
P. A. Wood, A. A. Sarjeant, et al., *CrystEngComm*, 2017, **19**, 690-698

CCDC

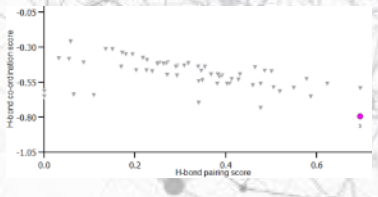
What else can you explore in Mercury?

CSD Python API functionalities

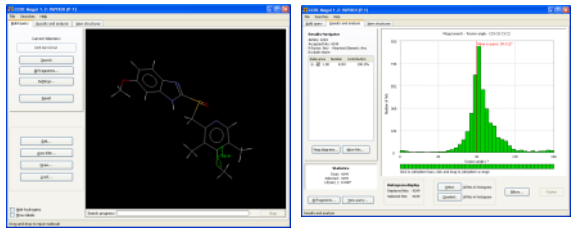
Hydrogen bond propensity



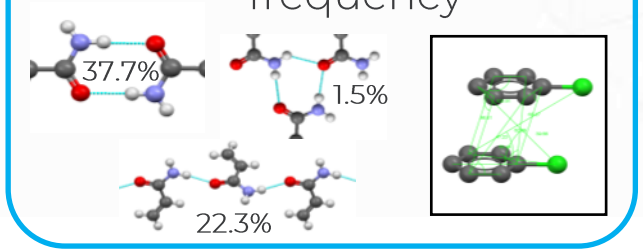
Donor group	Acceptor Group	π	+/− [σ]	Form I	Form II
amide	carbamate	0.618	0.094	✗	✗
amide	hydroxyl	0.551	0.052	✗	✓
carbamate	carbamate	0.538	0.090	✓	✗
amide	amide	0.501	0.055	✓	✗
carbamate	amide	0.420	0.083	✗	✓
hydroxyl	ureido	0.417	0.058	✗	✓
ureido	carbamate	0.319	0.086	✗	✓
ureido	ureido	0.224	0.044	✓	✗
hydroxyl	thiazoyl a	0.114	0.039	✓	✗



Mogul geometry library

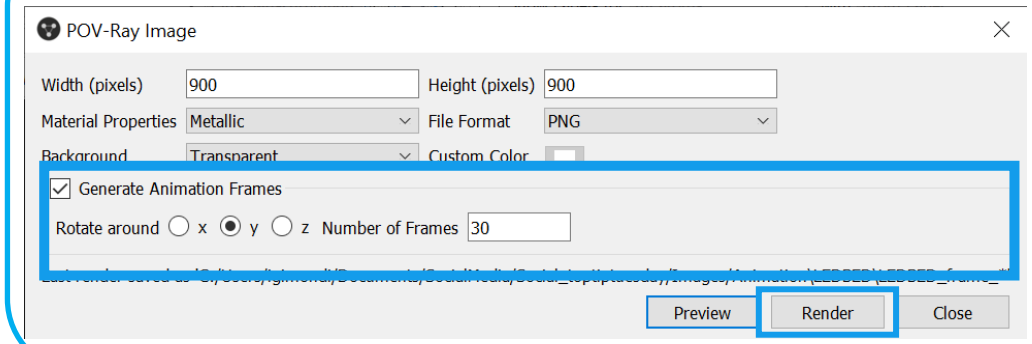


Motif & packing feature frequency

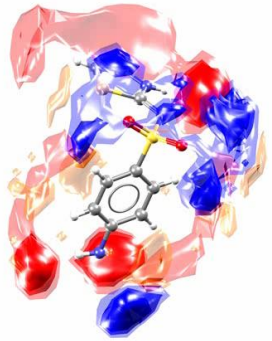


CSD Materials

Videos



Full Interaction Maps

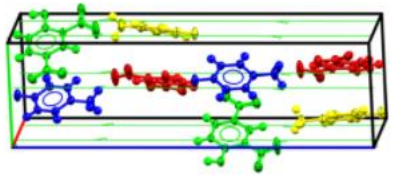


CSD Materials & CSD Discovery

...and more!

CCDC

Want to explore more?



CSD-System

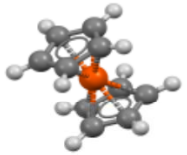
Essential crystallographic and structural chemistry capabilities.

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.

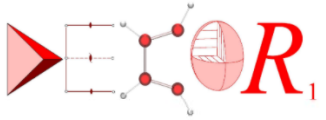
The CCDC and our colleagues continually produce educational materials for use in classroom and computer lab settings, or as independent study modules. Many of these materials make use of the Teaching Subset - a freely available set of over 750 structures that can be investigated with the free version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



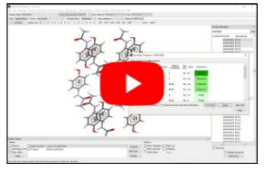
Information on the Teaching Subset

Access a series of teaching modules for use in the classroom

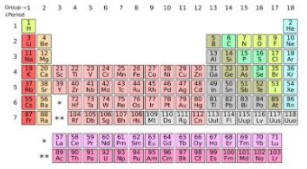


DECOR: Educational Resources for Teaching Crystallography

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/