

The full CSD database, maintained by the Cambridge Crystallographic Data Centre, contains over 850,000 real crystal structures. The full CSD software requires the purchase of an annual site licence, but individual structures may be viewed and manipulated free of charge using the "Access Structures" option on the CCDC website. It uses a JSMol viewer, thus enabling them to be viewed on both Windows and Apple devices in any common browser.

Getting Started

- To use the CSD "Access Structures" webpage you will require a computer or laptop or tablet with access to the internet.
- You will then need to find CSD "Access Structures" page using one of these two methods:
 - Type in the web address <https://www.ccdc.cam.ac.uk/structures>.
 - Type into a search engine, such as Google, "access structures" and click on the link that says "Search - Access Structures".

Basics

To view a particular structure, you need to type its CSD refcode (provided) into the 'Identifier(s)' box. For the purpose of this demo, type in the refcode 'CAFINE' for the crystal structure of caffeine.

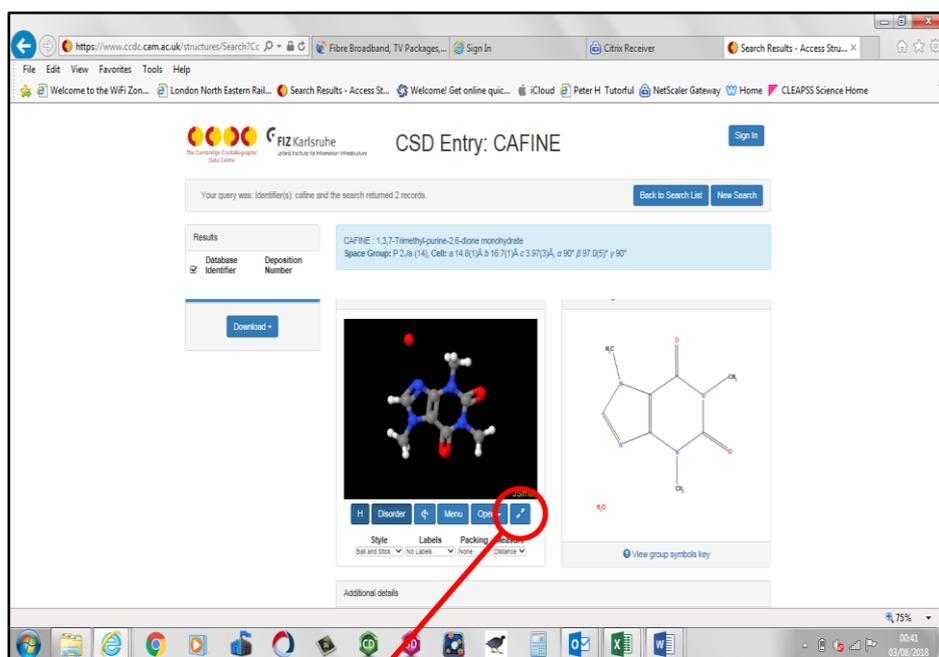
With the mouse you can hold left click to manually rotate the molecule and zoom using the middle button.

The drop-down headed 'Style' can be used to change the display.

The 'Labels' drop-down can be used to label different atoms in the molecule.

'Packing' options can be used to look at the larger crystal structure, e.g. the unit cell and the bulk structure of 3x3x3 unit cells.

NEW! The molecule viewer window can now be made almost full screen by clicking on this button below the viewer.



You will notice that caffeine also has an H₂O molecule incorporated to the crystal structure which appears to have no hydrogen atoms! Older X-ray experiments could not pick up the minimal electron density around the hydrogen atoms, so they weren't able to be resolved and therefore could not be included in the calculated crystal structure.

TOP TIP!

When looking at some crystal structures on the database there will be two species on a refcode, you may only need to look at one of them. The two species are ions; one is a positive ion and the other is a negative ion. It is of course not possible to have one ion without the opposite 'counter ion'.



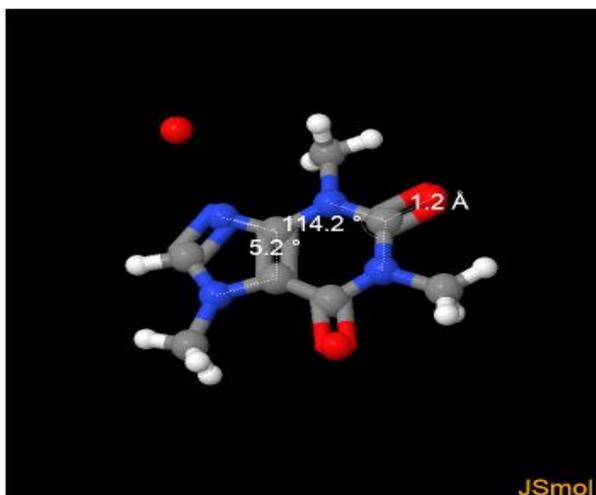
www.flickr.com/photos

Making Measurements

There are three fundamental measurements you can make in the JSMol viewer. Select the mode you require using the 'Measure' drop-down menu:

- 1. Bond Length** (select 'Distance'): Double click on the first atom and double click on the next atom to measure the bond length between them in Å ($1\text{Å} = 10^{-10}\text{m}$). You can change the units to nm or pm via the 'Menu' button.
Practice by measuring the length of the carbonyl (C=O) bond between the two nitrogens, which should be 1.2Å .
- 2. Bond Angle:** Double click on the first atom (not the central atom of the 3) then single click on the central atom then double click on the third atom.
Practice by measuring the bond angle of the carbonyl between the two nitrogens in caffeine, which should be 114.2° .
- 3. Torsion angle (how flat is it?):** You will require 4 adjacent atoms. Double click on the first, single click on the central two in sequence and then double click on the last. *Practice by measuring the torsion angle from the nitrogen next to the central C=C bond over the C=C double bond to the nitrogen on the same side, which should be 5.2° .*
4. To **delete all measurements** simply select 'none' from the 'Measure' drop-down menu.

Note: As you are viewing real crystal structures the lengths and angles measured may not be the same as the expected theoretical values. This is due to other interactions in the crystal structure.



3D Viewing

All of the structures can be viewed in 3D. For this you will need a pair of red and cyan 'anaglyph' glasses, like the ones used to see 3D images in old magazines, which can be purchased cheaply online.

Simply click the 'Menu' button and select 'Style', 'Stereographic' and 'Red+Cyan glasses'. Put on your glasses and view the structure in 3D!

There are lots of other functions that can be performed in the viewer, such as hydrogen bonding and Van der Waals radii. These additional functions will be explained as they are required when using specific worksheets of the resources.