# Mercury[1]

Mercury is part of the CCDC (Cambridge Crystallographic Data Centre) Software package and is used for visualising crystal structures and investigating some of their properties. Features include bond lengths and angles, atomic distances, inter-and intra-molecular interactions, similarity of molecules and packing in the solid state. Multiple structures can be displayed at once and overlaid to assess similarity/differences.

Mercury is availabe on all university computers and also as a free download from http://www.ccdc.cam.ac.uk/Solutions/CSDSystem/Pages/Mercury.aspx

Use this tab to generate powder patterns or expand the molecular shell to see more molecules

Search for structures via the refcode (as found through Conquest searches)
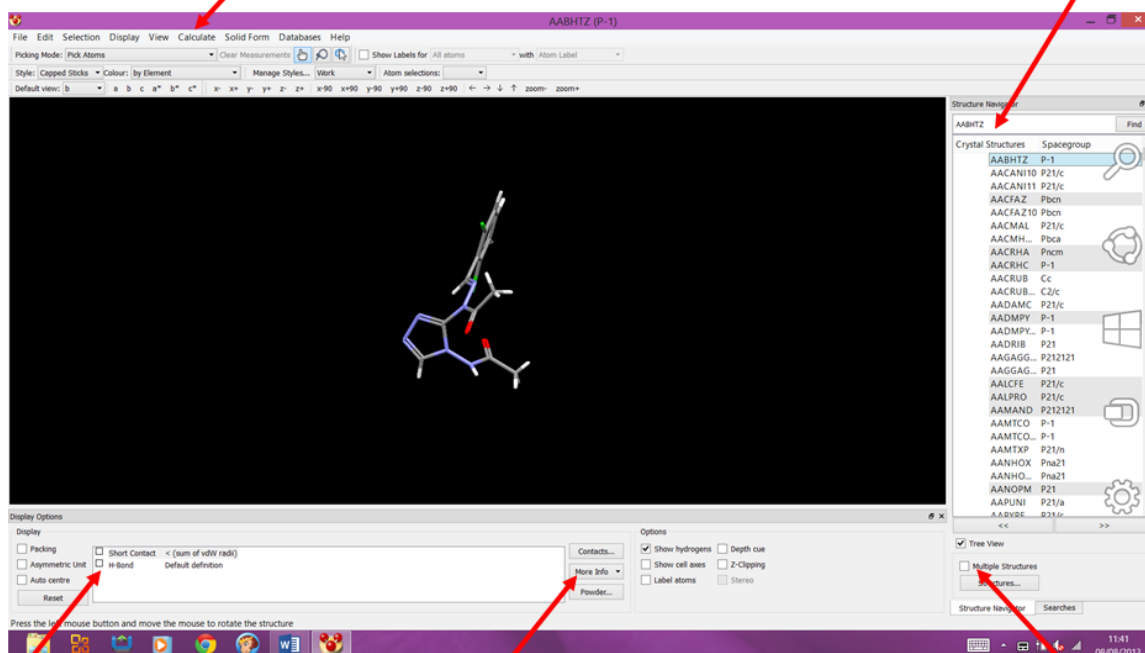
Select this box to view hydrogen bonds and the expand contacts to view more interacting molecules

For more information (as found in the CSD entry)

Select this box to view multiple structures on the same screen

To measure bond lengths or angles, change the option in 'Picking mode' (top left drop down menu) where you will be able to measure distances (between any atoms, not just those bonded to one another). There are a variety of other options in this menu which allow further analysis of the crystal structure. For analysing and comparing structures use the options at the bottom of the display (eg short contacts, packing etc).

Overlaying structures

Use the 'Calculate' tab and select molecule or atom overlay as appropriate. The related pop up box will appear and follow the commands to view the overlaid structures in the viewing window.
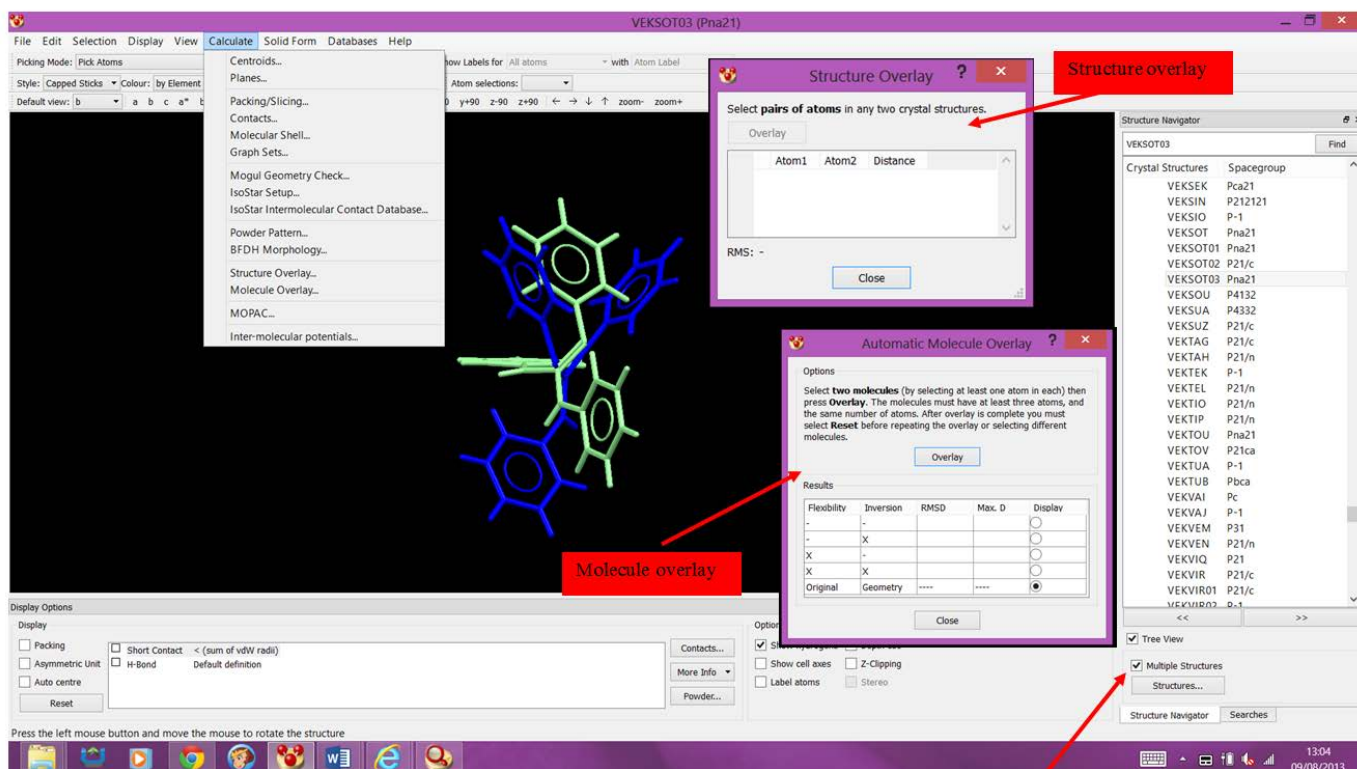
Ensure multiple structures is selected

Calculated XRPDs

A powder pattern can be calculated from a crystal structure and then can be saved in a variety of formats depending what you wish to do with the pattern. Select the powder button (below more info) or use Calculate→ Powder pattern

Saving it as an ASCII file allows the data to be opened in Excel and plotted on a chart so that comparisons can be made.
Note, check the wavelength of the radiation used for the calculation as there are different x-ray sources available and used experimentally (in the customise section in calculate pattern). XRPD typically uses Cu radiation (such as the MiniFlex600), 1.54Å) whereas for SCXRD (XtaLAB mini) we use Mo (0.71Å).

When opening in Excel, select delimited (rather than fixed width) then select the delimiter as space (tick the box next to space and uncheck any others). This should give three columns in the preview at the bottom and each data value contained within the appropriate column. Click finish and you will be presented with a set of data in an Excel sheet.
This can be converted into a powder pattern (as seen in Mercury) by plotting a scatter chart with a smooth line connecting the data points (2θ against intensity). By modifying the chart options a clear powder pattern can be achieved and multiple patterns plotted on the same chart to give an overlay for comparisons of structures.

1.	C. F. Macrae, I. J. Bruno, J. A. Chisholm, P. R. Edgington, P. McCabe, E. Pidcock, L. Rodriguez-Monge, R. Taylor, J. van de Streek and P. A. Wood, *J. Appl. Crystallogr.*, 2008, **41**, 466-470.