

Instruction for using the Viewer.

Because the coordinates are based on experimental data, the structures are generally not 'perfect'; an allowance should be made for this when determining the point group. Note also that many structures are viewed more easily without their H atoms.

(a) Manipulating the molecule

- (i) Left-click and hold the button on the mouse to rotate the molecule on the screen.
- (ii) Two clicks then hold can be used to drag the molecule, alternatively alt key + right-click and hold the button.
- (iii) Use the wheel to magnify or diminish the image, or shift key + left-click and hold button.
- (iv) The screen axes are y vertical, x horizontal and z out of the screen towards you.
- (v) **spin**: this rotates the molecule continuously about the vertical screen axis.
- (vi) **labels**: these label the atoms and their position in the list of coordinates, thus C13 is a carbon, not the 13th carbon but atom 13 in the list.
- (vii) **H atoms on/off**: It is often easier to see the molecule without H atoms. If H atoms are not present initially, click a couple of times to see if they appear, however, not all molecules have H atoms associated with them in the model used.
- (viii) **perspective**: Sometimes the geometry is easier to see without perspective.
- (ix) **stereo**: You may need to reduce the size of the model slightly. Sit about arms length away from the screen and relax the eyes to see the stereo. It takes a little practice.
- (x) **Distances and angles**: An option is given in the main menu that shows some angles and distances. If you want others, right click on the image and a new menu is produced. Use the angle and distance measuring tool.
- (xi) **colours**: The colours menu gives you options. With the Rasmol colours it is sometimes easier distinguish different atoms than with the CPK colours.
- (xii) **style**: Choose whichever you find easier to use. The default is 'ball & stick'.
- (ix) **Orbitals**: You can view *p* and *d* orbitals set at the centre of the coordinates for molecules with a * after their name. This enables you to determine the Mulliken symbol for an orbital in that point group.

(b) Estimating the Point Group

The **rotate by 90, 120 and 180°** buttons move the molecule about the **screen** x, y and z-axes (see(iv)). You can use these to check on a possible rotation axis, C₂, C₃ etc by rotating the molecule to alight along one of these axes. If the axis is present then the structure will appear not to move, other than slight changes in atom positions due to minor imperfections in the x-ray coordinates. Any obvious changes in the geometry mean that such an axis is not present.

The remaining check boxes show axes and mirror planes for each molecule. In several examples, **not all the possible symmetry elements are included**, but by symmetry, you should be able to see what is missing.

If you use the '**view this pdf**' link at the top of the screen, the document that is opened gives examples of different point groups and a table of symmetry elements and operations for most

point groups. You can use the table to compare the axes and planes shown with those that must be present in a point group.

When you have worked out the point group use the table to check. You can of course also guess the point group from the table, eventually you will come across the correct one but then you will probably not understand why it has this point group.

Acknowledgements

The Jmol applet is used to manipulate molecules. The web address for this is

Jmol: an open-source viewer for chemical structures in 3D. <http://www.jmol.org/>.

The coordinates for many molecules are from the CSD database¹ <http://webcsd.ccdc.cam.ac.uk/>, other coordinates are taken from Jmol structure on Wikipedia. In many cases the coordinates have been modified, either to remove unwanted atoms or to make the molecule more 'perfect' for the purpose of teaching symmetry.

(1) WebCSD: the online portal to the Cambridge Structural Database
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