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Chemistry by Interactive 3D

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Chemistry is a visual, even tactile, science but is based upon fundamental concepts, such as complex molecular and crystal structures as well as mathematical descriptors, which are often difficult to appreciate. Interactive three-dimensional (3D) visualisation provides a tool by which such concepts are more readily grasped, by user manipulation of images in various ways (such as rotation, expansion to focus in certain areas, projection onto one of the three planes, measurement, colouring, labelling, etc.).

Jmol is Java-based open-source software, run by most Web browsers, initially for displaying molecular structures. However, in recent years, Jmol has been greatly expanded to manage data in 3-coordinate space, among other features. We demonstrate the use of Jmol in display and manipulation of images of various kinds: molecular and crystal structures, phase diagrams, mathematical functions, etc. These features and images are readily and freely available to add interest, immediacy and depth of understanding to teaching (and not only of chemistry) at all levels.

