Predicting the point group of molecules using Jmol application

M.Nivetha[1],P.Sivaranjana[2]
[1]Department of Chemistry, Kaliswari college of arts and science, Sivakasi- 626123
[2]Department of Chemistry, Kalasalingam Academy of Research and Education- 626126

Abstract

The knowledge of symmetry and point group of molecules play a key role in understanding the physical and chemical characteristics of the molecules relevant to its applications. The details of point groups of any molecules provide a systematic technique to define the symmetry of molecules. This knowledge aids in predicting a variety of physical and chemical features, including molecule polarity, spectroscopic behaviour, and reaction process. For example, it helps to determine a molecule's vibrational modes and optical activity, which are important in fields such as materials science, drug design, and catalysis. A point group defines all of the symmetry operations that can be performed on a molecule to get a conformation that is indistinguishable from its original. A point group in chemistry and crystallography is a set of symmetry operations that leave at least one point fixed in space. These procedures include rotation and inversion. Point groups are used to categorize molecules and crystals according to their symmetry features. The 3D viewing of the molecules offers a better platform for understanding the concept of symmetry and point group of various molecules. The Jmol application- an open source software is user friendly and provides the learners a complete guide to predict the point group of the wide variety of molecules. The level of learning improves drastically using the 3D viewer like Jmol compared to the traditional methods. It enables better visualization of how molecules or crystals behave under various symmetry operations. In this report we have discussed how to predict the point group of various molecules using Jmol, by taking one molecules as example for each point group.

Keywords

Jmol, Point group, symmetry, rotation, axis of rotation.