Point groups are used to describe molecular symmetries and are a condensed representation of the symmetry elements a molecule may possess. This includes both bond and orbital symmetry. Knowing molecular symmetry allows for a greater understanding of molecular structure and can help to predict many molecular properties.

**Introduction**

Point groups are a quick and easy way to gain knowledge of a molecule. They not only contain a molecule's symmetry elements, but also give rise to a character table, which is a complete set of irreducible representations for a point group. A molecule's point group can be determined by either elucidating each symmetry element contained in a molecule or by properly using the Schreiber chart (see below).

Point groups usually consist of (but are not limited to) the following elements:

- **E** - The identity operator. This operation leaves a molecule completely unchanged and exists for mathematical purposes.
- **C_n** - The C_n proper axis of rotation is a 360/n° rotation that when performed leaves a molecule the same. A proper rotation with the highest value of n is known as the major axis of rotation.
- **σ** - The mirror plane. The mirror plane can be described as a plane which produces a reflection of part of a molecule that is unnoticeable and can be labeled as either σ_h, σ_v, σ_d.
- **i** - The inversion center. A molecule has a center of inversion if, when inverted, the molecule is unchanged.

See the section on symmetry elements for a more thorough explanation of each.

**Each point group is associated with a specific combination of symmetry elements**

Each point group has its own combination of symmetry elements. Listed below are some of the many point groups and their respective symmetry elements, according to category, followed by a representative example.

**Non axial groups**

- C₁: E
- C₂: E, i

**C_n groups**

- C₂: E, C₂ (notice the major axis of rotation is the point group)
- C₃: E, C₃, C₃²
$\text{H}_2\text{O}_2 \text{ C}_2$

$D_n$ groups

$D_2$: E $C_2(z)$, $C_2(y)$, $C_2(x)$ $D_3$: E, 2$C_3$, 3$C_2$

$C_{nv}$ groups

$C_{2v}$: E, C2, $\sigma_v(xz)$, $\sigma_v'(yz)$ $C_{3v}$: E, 2$C_3$, 3$\sigma_v$

\[ \text{H}_2\text{O} \text{ C}_2v \]

$C_{nh}$ groups

$C_{2h}$: E, C2, i, $\sigma_h$ $C_{3h}$: E, C3, $C_3^2$, $\sigma_h$, S3, S3$^3$

\[ \text{B(OH)}_3 \]

$D_{nh}$ groups

$D_{2h}$: E

\[ \text{C}_2\text{H}_4 \text{ D}_{2h} \]
How to determine a molecule's point group

A molecule's point group can be determined by calculating all the symmetry elements of a molecule and matching them to a respective point group. This process, however, is greatly simplified when the Schreiber chart is used:

References


Outside Links

• Point groups in 3-D

Problems

1. Determine the point group of BH$_3$ by calculating all its symmetry elements then use the chart and determine which method is faster.
2. Determine the point groups of BH$_3$ and NH$_3$. Why is there a difference?
3. What is the point group of PPh$_3$?
4. Determine the point groups of CO$_2$ and H$_2$O and then compare them.
5. Propose a molecule with no symmetry. What is its point group?

Contributors