Chemistry and Group Theory: Symmetry of Molecules

Comps Part 2

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Abstract

My potential topic is on how group theory is used in chemistry to find the symmetries of molecules. The symmetry of molecules explains some properties of the molecule such as its polarity, dipole moment, vibrations, etc. There are 5 symmetry operations that can be performed on the molecule and each operation has to leave the molecule equivalent to its starting state. The operators are the identity, rotation, reflection, inversion and improper rotation. Each operation is performed on symmetry elements that can either be lines, points, or planes. The symmetry operations that act on the molecules have group structures or properties such as closure, identity, inverses, associativity, etc.

Symmetry Operations

1. Identity (E)
   - The identity does nothing to the molecule. Every molecule has the identity operation.
2. Rotation (C_n)
   - This is a Rotation of $\frac{2\pi}{n}$ around some axis, known as the n-fold axis of symmetry (C_n), that rotates it to an equivalent state.
   - The axis with the biggest n is known as the principal axis.
3. Reflection (σ)
   - This is a reflection of a molecule on a plane. There are three types of reflection planes.
   - The first type is called the vertical plane (σ_v) which is a plane on the principal axis. The second one is called a horizontal plane (σ_h) which is a plane that is perpendicular to the principal axis. The third plane is called the dihedral (σ_d) which is a plane that bisects an angle between 2, 2-fold rotation (C_2) axes.
4. Inversion (i)
   - If there exists a point where all atoms are reflected through that point, that point is the inversion center. If a straight line is drawn through the inversion center from one atom, it would hit the same atom on the other side.
5. Improper Rotation (S_n)
   - This is a combination of two operations. First, there is a rotation of $\frac{2\pi}{n}$. Then a reflection on a plane perpendicular to the axis of symmetry.

References

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3. http://chemwiki.ucdavis.edu/Core/Theoretical_Chemistry/Symmetry/Group_Theory%3A_Theory