Symmetry of molecular systems

Symmetry elements: plane, axis and point (center of inversion)

Symmetry operations:

1. rotation about a proper axis. For example, $C_2$ means rotation about $360^\circ/2$ (180°),

   $C_3$ – rotation about $360^\circ/3$ (120°), where $n$ is an order of the axis.

2. reflection in a plane of symmetry, $\sigma$. there are 3 types of planes. $\sigma_h$ is

   perpendicular to $C_n$ (main axis); $\sigma_v$ contains the main axis, $\sigma_d$ divides in half

   the angle between the two $C_2$ which are perpendicular to $C_n$.

3. inversion of all atoms through a center of symmetry, (center of inversion) denoted

   as $i$.

4. identity operation $E$- position of atoms do not change- corresponds to the rotation

   about $360^\circ$.

All other operations is just a combination of the symmetry operations described above.

Of particular importance is rotation about an axis, $C_n$, followed by reflection through the

plane perpendicular to the axis, $\sigma_h$. This operation is called a rotation about an

improper axis, denoted as $S_n$. 

Examples:

Symmetry elements of $\text{H}_2\text{O}$

1. $\text{H}_2\text{O}$ has 4 elements of symmetry: $E$, $C_2$, and 2 $\sigma_v$.
   This set of elements is called a $C_{2v}$ symmetry group.

Symmetry elements of $\text{NH}_3$:

1. $\text{NH}_3$ has 5 elements of symmetry: $E$, $C_3$, and 3 $\sigma_v$.
   This set of elements is called a $C_{3v}$ symmetry group.

Symmetry groups:

1. No axis other than $C_1$ : $C_1$ (no symmetry), $C_s$, $C_i$
2. Only one axis with \( n > 1 \): \( C_n, S_n, C_{nv}, C_{nh} \)

2. Dihedral groups, \( D \): contain \( C_n \) and \( n \) \( C_2 \) perpendicular to \( C_n \).

\[ D_n, D_{nh}, D_{nd} \]