Symmetry of molecular systems

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

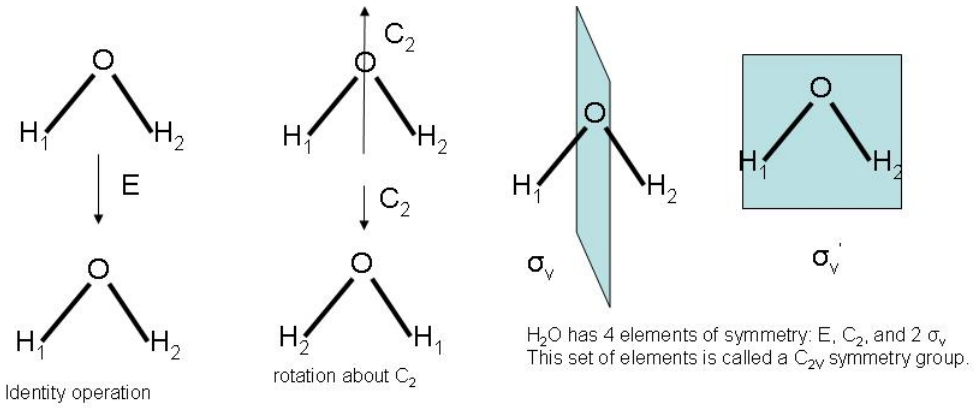
Symmetry operations:

1. rotation about a proper axis. For example, $\mathbf{C}_2$ means rotation about $360^0/2$ (180^0), $\mathbf{C_3}$ – rotation about $360^0/3$ (120^0), where n is an *order* of the axis.
2. reflection in a plane of symmetry, $\boldsymbol{\sigma}$. there are 3 types of planes. $\boldsymbol{\sigma_h}$ is perpendicular to $\mathbf{C_n}$ (main axis); $\boldsymbol{\sigma_v}$ contains the main axis, $\boldsymbol{\sigma_d}$ divides in half the angle between the two $\mathbf{C_2}$ which are perpendicular to $\mathbf{C_n}$.
3. inversion of all atoms through a center of symmetry, (center of inversion) denoted as $\boldsymbol{i}$.
4. identity operation $\mathbf{E}$- position of atoms do not change- corresponds to the rotation about 360^0.

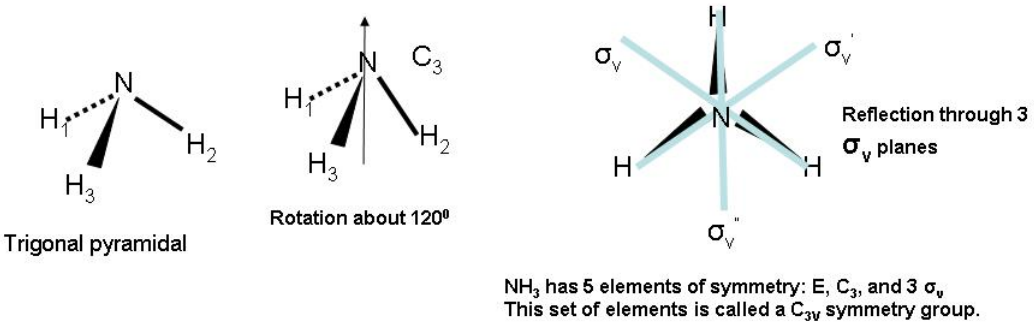
All other operations is just a combination of the symmetry operations described above. Of particular importance is rotation about an axis, $\mathbf{C_n}$, followed by reflection through the plane perpendicular to the axis, $\boldsymbol{\sigma_h}$. This operation is called a rotation about an **improper axis**, denoted as $\mathbf{S_n}$.

Examples:

Symmetry elements of H_2O

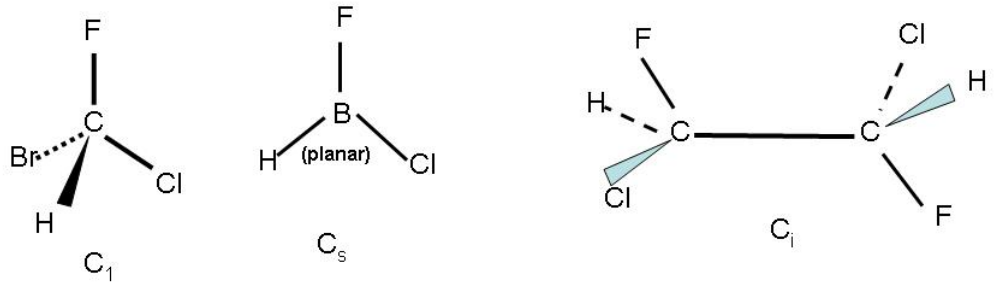


Symmetry elements of NH_3:

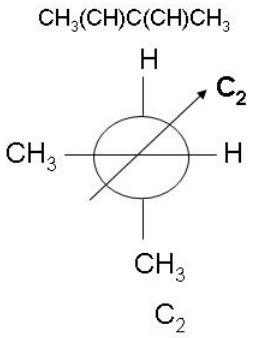


Symmetry groups:

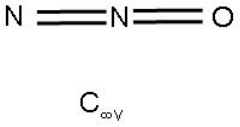
1. No axis other than C_1 : C_1 (no symmetry), C_s, C_i



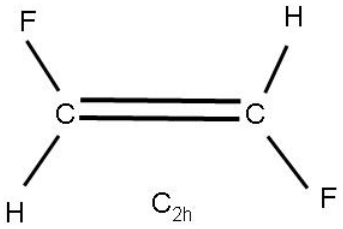
2. Only one axis with n>1: C_n, S_n, C_{nv}, C_{nh}



C_2



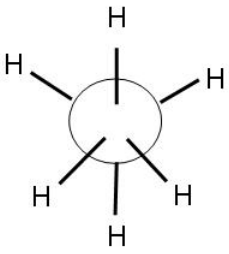
$C_{\infty v}$



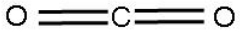
C_{2h}

2. dihedral groups, D: contain C_n and n C_2 perpendicular to C_n.

D_n, D_{nh}, D_{nd}



D_{3d}



$D_{\infty h}$

D_{2d}