## Group H: Symmetry

To understand bonding in molecular orbital (MO) theory one must describe a chemical species mathematically. The first step in this mathematical description is to describe the symmetry of ions and molecules. While a full description of MO theory is well beyond the scope of this course, we can begin to appreciate symmetry as it relates to chemical species.

Mathematically symmetry is described by what physical operations can be performed on an object such that it is brought to a new position that is indistinguishable from the original. These operations are rotation about a line (a rotation axis), reflection through a plane (a mirror plane), inversion through a point and the improper rotation (a rotation followed by a reflection in a plane perpendicular to the rotation axis). The geometric features of a point, a line and a plane are called symmetry elements, about which a symmetry operation (reflection, rotation, inversion, or improper rotation) is performed. For example, a triangle has rotational and mirror symmetry, but not inversion symmetry. Inverting the triangle through the center does not give us the same configuration. Note that a triangle has only one rotation axis, but we can do two rotations about it ( $120^{\circ}$ and $240^{\circ}$, which is the same as a $120^{\circ}$ rotation done twice). We can not do a $90^{\circ}$ rotation of a triangle and get a configuration that is the same as the original. Objects that have more symmetry elements are more symmetrical and are said to have higher symmetry.


For the molecules listed in the table, determine what symmetry elements, and how many of each, are present. Differentiate the rotations by how many degrees you must rotate about the axis to obtain a configuration that is identical to the original. Be as descriptive as possible in describing the location of the different symmetry elements.

| Rotations |  |  |  |  |  | Mirror Planes | Inversion |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Species | $30^{\circ}$ | $60^{\circ}$ | $90^{\circ}$ | $120^{\circ}$ | $180^{\circ}$ |  |  |
| $\mathrm{F}_{2}$ |  |  |  |  |  |  |  |
| HF |  |  |  |  |  |  |  |
| $\mathrm{NH}_{3}$ |  |  |  |  |  |  |  |
| $\mathrm{H}_{2} \mathrm{O}$ |  |  |  |  |  |  |  |
| $\mathrm{BH}_{3}$ |  |  |  |  |  |  |  |
| $\mathrm{CH}_{4}$ |  |  |  |  |  |  |  |
| $\mathrm{SF}_{4}$ |  |  |  |  |  |  |  |
| $\mathrm{XeF}_{4}$ |  |  |  |  |  |  |  |
| $\mathrm{PCl}_{5}$ |  |  |  |  |  |  |  |
| $\mathrm{SF}_{6}$ |  |  |  |  |  |  |  |

