

## **Rules for assigning x, y, and z axes to molecules**

1. If the molecule contains only one axis of rotation, that axis is the z axis.
2. If there are more than one axes of rotation, then the one of highest order is taken to be the z axis.
3. If there are several axes of the highest order, then the one that passes through the maximum number of atoms is the z axis.

### **Once the z axis is selected, then use the following rules to select the x axis.**

1. If the molecule is planar and the z axis is on the plane of the molecule, the x axis is chosen to be out of the plane.
2. If the molecule is planar and the z axis is perpendicular to the plane, then x axis lies on the plane and passes through the largest number of atoms.
3. If a non-planar molecule has one plane containing a large number of atoms than any other plane, then they are treated as if they were planar and as if this preferred plane is the plane of the molecule. If a decision cannot be made on this basis, it does not matter how the axes are picked.