

RULES FOR CLASSIFICATION INTO POINT GROUPS

1. If the molecule is linear, look for the highest rotational axis. This axis is infinite fold (C_∞) for a linear molecule.
 - If the molecule has a center of inversion (i) [or in other words, the two ends of the molecule are identical], then the point group is $D_{\infty h}$
 - Otherwise $C_{\infty v}$
2. If the molecule is non-linear and if the highest rotational axis is 3, 4 or 5 fold, look for other axes of the same order. There are 3 possibilities.
 - a) Several 5-fold axes (C_5):
The molecule belongs to I_h point group if it has a plane of symmetry. If not, the point group is I .
 - b) Three 4-fold (C_4) axes:
The molecule belongs to O_h point group if it has a plane of symmetry. If not, the point group is O .
 - c) Four 3-fold axis (C_3) but no C_4 or C_5 axis:
 - If there are no mirror planes or a center of inversion, the point group is T
 - If there is a center of inversion, the point group is T_h
 - If there are 6 mirror planes and three S_4 axes, the point group is T_d
3. If only one axis has $n \geq 2$ or if the axis of highest order is a C_2 axis, check for n more 2-fold axes (C_2) at right angles. If these exist and:
 - There are no mirror planes $\rightarrow D_n$ point group
 - Has a horizontal mirror plane $\rightarrow D_{nh}$ point group
 - No horizontal mirror planes, but has n vertical mirror planes $\rightarrow D_{nd}$ point group
4. If only one n-fold axis exists, check for S_{2n} axis. If this exists then the point group is S_{2n} . If not, the molecule belongs to:
 - C_n if it has no mirror planes
 - C_{nh} if it has a horizontal mirror plane
 - C_{nv} if it has n vertical mirror planes
5. If the molecule has no symmetry axes, but has a:
 - center of inversion \rightarrow point group is C_i
 - mirror plane \rightarrow point group is C_s
 - none of the above \rightarrow point group is C_1