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 $\mathbf{D_{\infty h}}$
    - Otherwise $\mathbf{C_{\infty v}}$

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 $\mathbf{I_h}$ 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 $\mathbf{O_h}$ 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 $\mathbf{T_h}$
    - If there are 6 mirror planes and three S_4 axes, the point group is $\mathbf{T_d}$

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 <u>right angles</u>. If these exist and:

    - There are no mirror planes $\rightarrow \mathbf{D_n}$ point group
    - Has a horizontal mirror plane $\rightarrow \mathbf{D_{nh}}$ point group
    - No horizontal mirror planes, but has n vertical mirror planes $\rightarrow \mathbf{D_{nd}}$ 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:

    - $\mathbf{C_n}$ if it has no mirror planes
    - $\mathbf{C_{nh}}$ if it has a horizontal mirror plane
    - $\mathbf{C_{nv}}$ 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 $\mathbf{C_i}$
    - mirror plane $\rightarrow$ point group is $\mathbf{C_s}$
    - none of the above $\rightarrow$ point group is $\mathbf{C_1}$