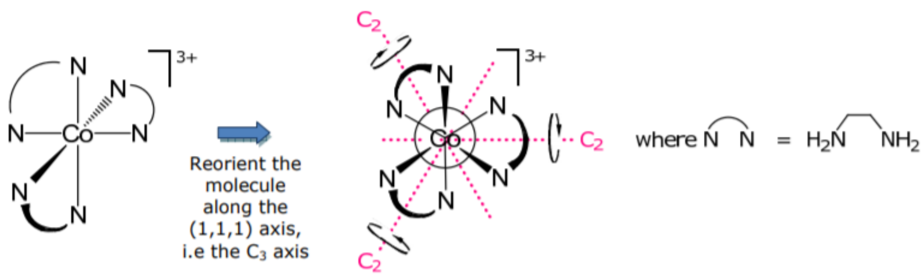
1.5: Molecular Point Groups 2

The D point groups are distiguished from C point groups by the presence of rotation axes that are perpindicular to the principal axis of rotation.

D_n : C_n and $n\perp C_2$ ($h = 2n$)

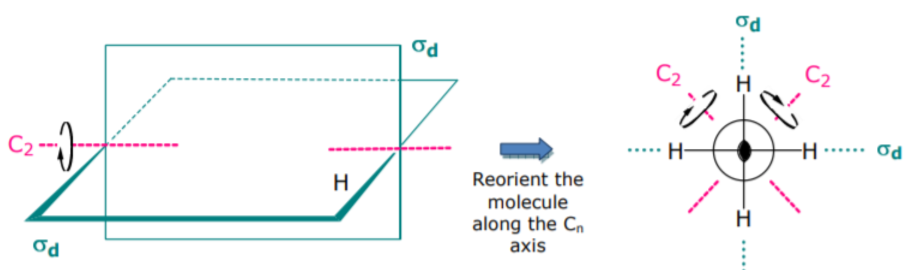
Example: $Co(en)_3{}^{3+}$ is in the D_3 point group,



In identifying molecules belonging to this point group, if a C_n is present and one $\perp C_2$ axis is identified, then there must necessarily be $(n–1)\perp C_2$s generated by rotation about C_n.

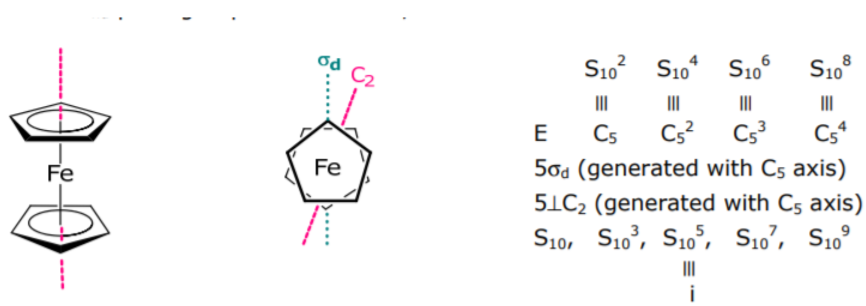
D_{nd} : C_n, $n\perp C_2$, $n\sigma_d$ (dihedral mirror planes bisect the $\perp C_2$s)

Example: allene is in the D_{2d} point group,

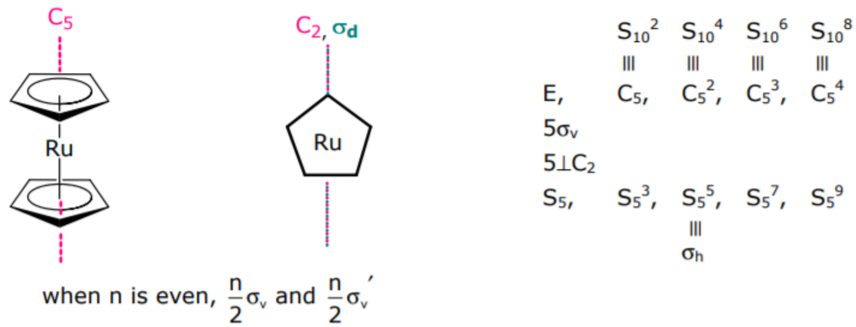


Two C_2s bisect σ_ds. The example on the bottom on pg 3 of the Lecture 4 notes was a harbinger of this point group. As indicated there, it is often easier to see these perpendicular C_2s by reorienting the molecule along the principal axis of rotation.

Note: D_{nd} point groups will contain i, when n is odd

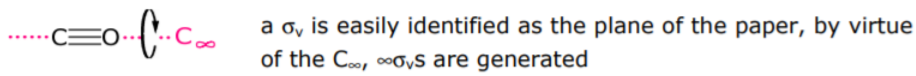


D_{nh} : C_n, $n\perp C_2$, $n\sigma_v$, σ_h ($h = 4n$)



$\mathbf{C_{\infty v}}$: C_∞ and $\infty\sigma_v$ (h = ∞)

linear molecules without an inversion center

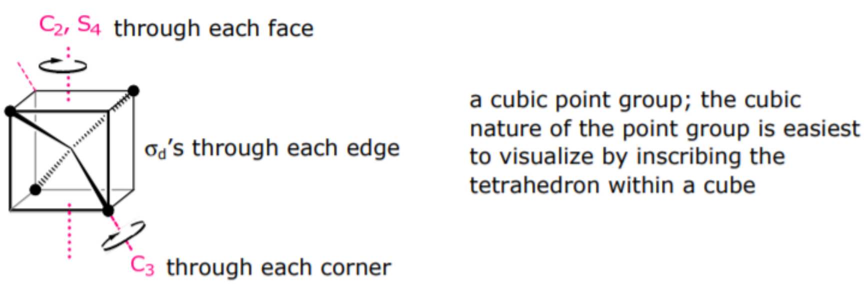


$\mathbf{D_{\infty h}}$: C_∞, $\infty\perp C_2$, $\infty\sigma_v$, σ_h, i (h = ∞)

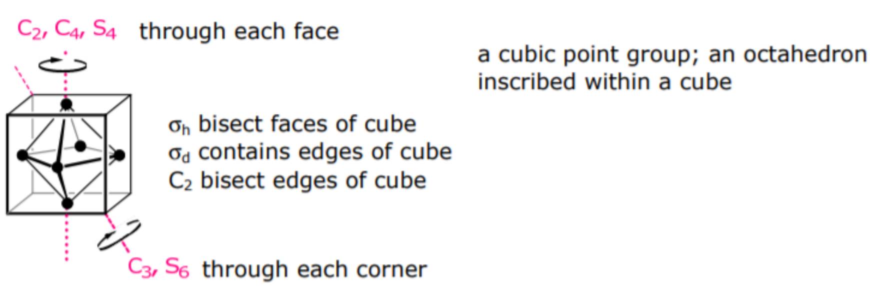
linear molecules with an inversion center

when working with this point group, it is often convenient to drop to D_{2h} and then correlate up to $D_{\infty h}$

$\mathbf{T_d}$: E, $8C_3$, $3C_2$, $6S_4$, $6\sigma_d$ (h = 24)



$\mathbf{O_h}$: E, $8C_3$, $6C_2$, $6C_4$, $3C_2$ (=$C_4{}^2$), i, $6S_4$, $8S_6$, $3\sigma_h$, $6\sigma_d$ (h = 48)



O : E, $8C_3$, $6C_2$, $6C_4$, $3C_2$ (=$C_4{}^2$) A pure rotational subgroup of O_h, contains only the C_n's of O_h point group **T** : E, $8C_3$, $3C_2$ A pure rotational subgroup of T_d, contains only the C_n's of T_d point group	O and T are rare point groups; whereas few molecules possess this symmetry, they are mathematically useful for molecules of O_h and T_d, respectively

$\mathbf{I_h}$: generators are C_3, C_5, i (h = 120) $\Longrightarrow$ the icosahedral point group

$\mathbf{K_h}$: generators are C_φ, C_φ', i (h = ∞) $\Longrightarrow$ the spherical point group

Flow chart for assigning molecular point groups: