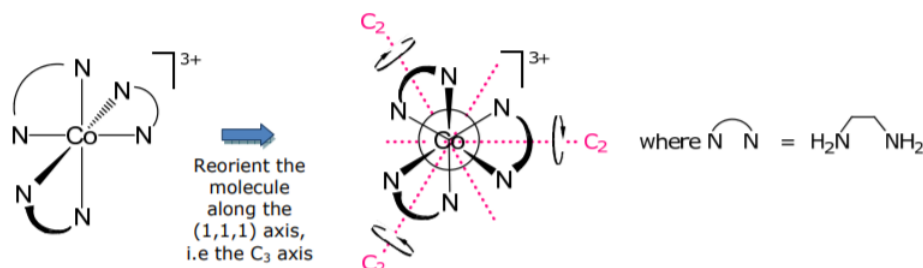


## 1.5: Molecular Point Groups 2

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

**D<sub>n</sub>** : C<sub>n</sub> and n ⊥ C<sub>2</sub> (h = 2n)

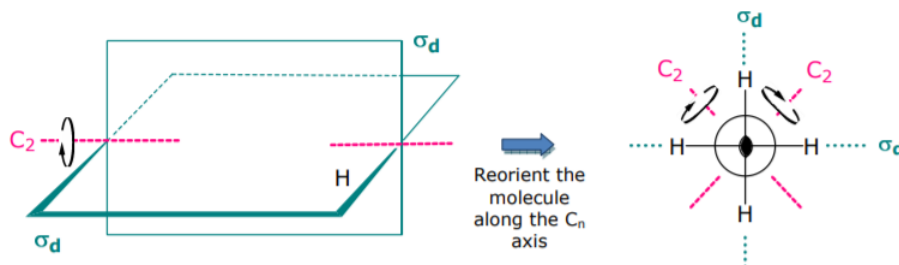
Example: Co(en)<sub>3</sub><sup>3+</sup> is in the D<sub>3</sub> point group,



In identifying molecules belonging to this point group, if a C<sub>n</sub> is present and one ⊥ C<sub>2</sub> axis is identified, then there must necessarily be (n-1) ⊥ C<sub>2</sub>s generated by rotation about C<sub>n</sub>.

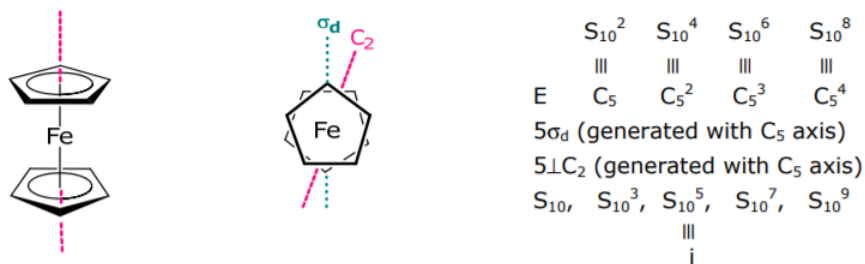
**D<sub>nd</sub>** : C<sub>n</sub>, n ⊥ C<sub>2</sub>, n σ<sub>d</sub> (dihedral mirror planes bisect the ⊥ C<sub>2</sub>s)

Example: allene is in the D<sub>2d</sub> point group,

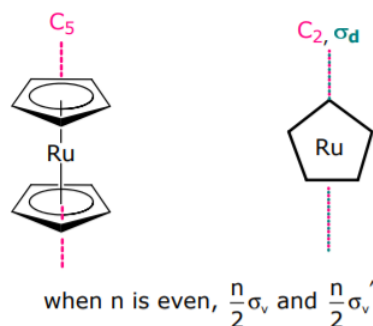


Two C<sub>2</sub>s bisect σ<sub>d</sub>s. The example on the bottom on pg 3 of the Lecture 4 notes was a harbinger of this point group. As indicated there, it is often easier to see these perpendicular C<sub>2</sub>s by reorienting the molecule along the principal axis of rotation.

Note: D<sub>nd</sub> point groups will contain i, when n is odd



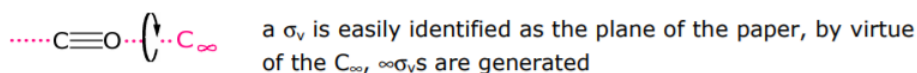
**D<sub>nh</sub>** : C<sub>n</sub>, n ⊥ C<sub>2</sub>, n σ<sub>v</sub>, σ<sub>h</sub> (h = 4n)



	$S_{10}^2$	$S_{10}^4$	$S_{10}^6$	$S_{10}^8$
	III	III	III	III
$E,$	$C_5,$	$C_5^2,$	$C_5^3,$	$C_5^4$
$5\sigma_v$				
$5\perp C_2$				
$S_5,$	$S_5^3,$	$S_5^5,$	$S_5^7,$	$S_5^9$
		III		
		$\sigma_h$		

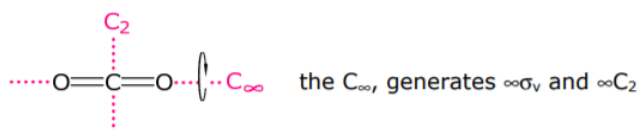
$C_{\infty v}$  :  $C_{\infty}$  and  $\infty\sigma_v$  ( $h = \infty$ )

linear molecules without an inversion center



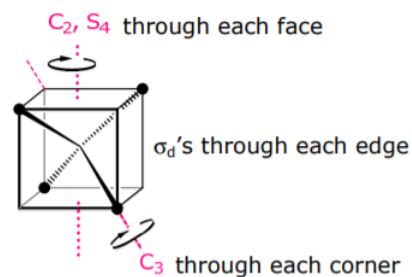
$D_{\infty h}$  :  $C_{\infty}$ ,  $\infty\perp C_2$ ,  $\infty\sigma_v$ ,  $\sigma_h$ ,  $i$  ( $h = \infty$ )

linear molecules with an inversion center



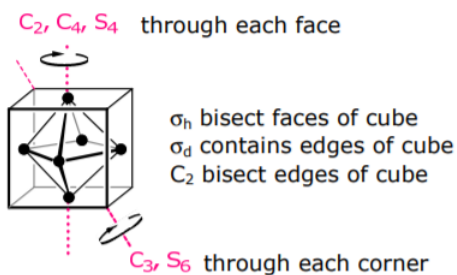
when working with this point group, it is often convenient to drop to  $D_{2h}$  and then correlate up to  $D_{\infty h}$

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



a cubic point group; the cubic nature of the point group is easiest to visualize by inscribing the tetrahedron within a cube

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



a cubic point group; an octahedron inscribed within a cube

**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,  $8C_3$ ,  $3C_2$

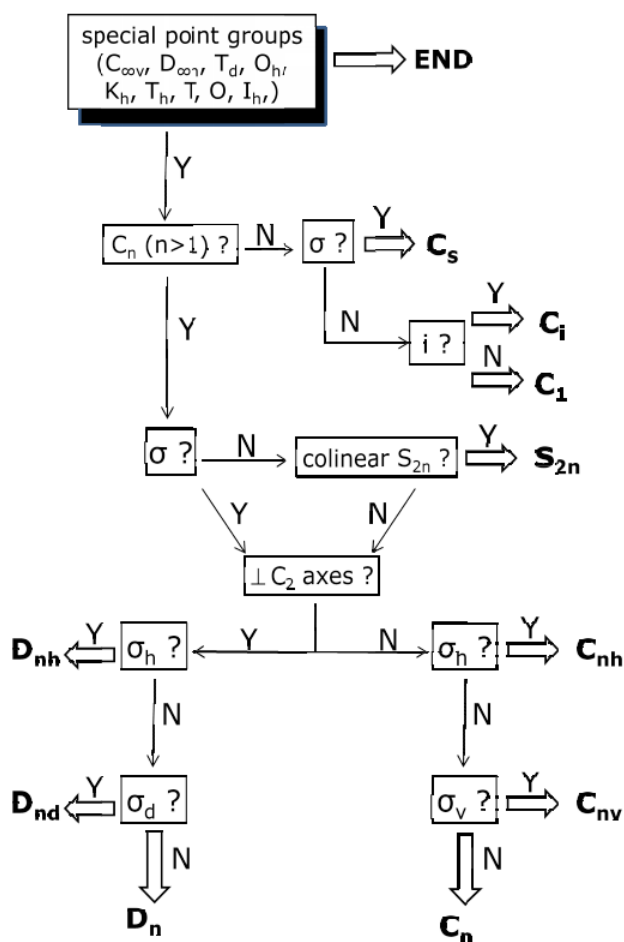
A pure rotational subgroup of  $T_d$ , contains only the  $C_n$ 's of  $T_d$  point group

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

**I<sub>h</sub>** : generators are  $C_3$ ,  $C_5$ ,  $i$  ( $h = 120$ )  $\implies$  the icosahedral point group

**K<sub>h</sub>** : generators are  $C_\phi$ ,  $C_\phi'$ ,  $i$  ( $h = \infty$ )  $\implies$  the spherical point group

Flow chart for assigning molecular point groups:



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