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5.04 Principles of Inorganic Chemistry II
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5.04, Principles of Inorganic Chemistry II
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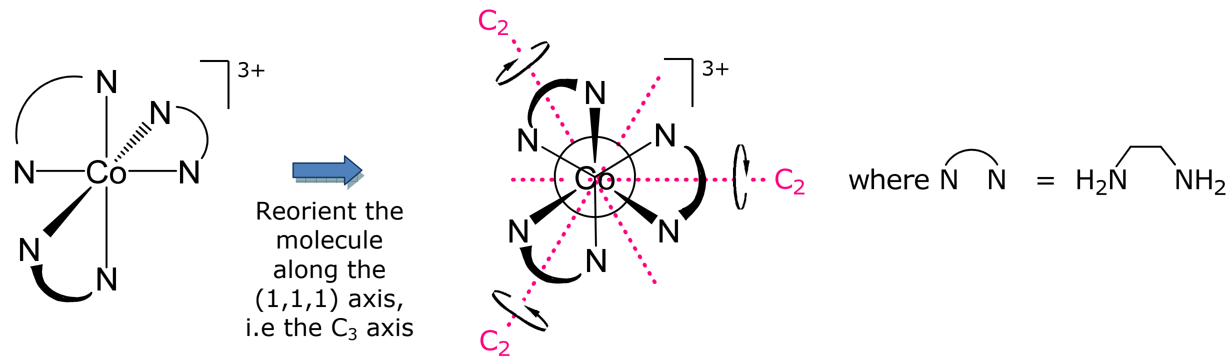
Lecture 5: Molecular Point Groups 2

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 $n\perp C_2$ ($h = 2n$)

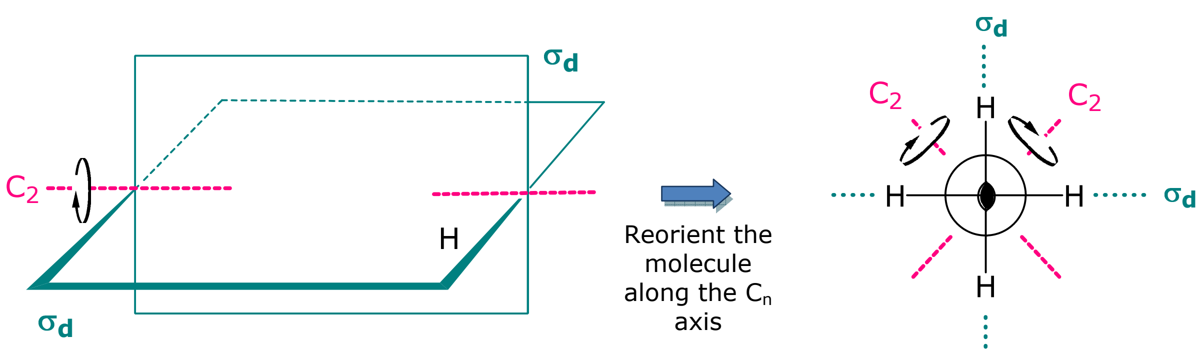
Example: $Co(en)_3^{3+}$ is in the D_3 point group,



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.

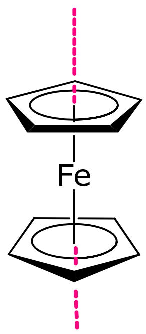
D_{nd} : C_n, $n\perp C_2$, $n\sigma_d$ (dihedral mirror planes bisect the $\perp C_2$s)

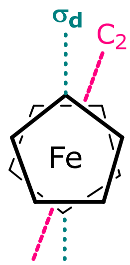
Example: allene is in the D_{2d} point group,



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





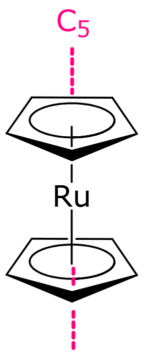
	S_{10}^2	S_{10}^4	S_{10}^6	S_{10}^8
	≡	≡	≡	≡
E	C_5	C_5^2	C_5^3	C_5^4

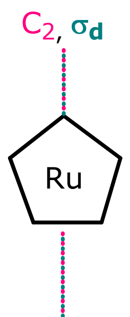
$5\sigma_d$ (generated with C_5 axis)

$5\perp C_2$ (generated with C_5 axis)

S_{10},	S_{10}^3,	S_{10}^5,	S_{10}^7,	S_{10}^9
		≡		
		i		

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



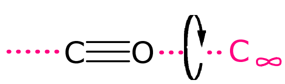


	S_{10}^2	S_{10}^4	S_{10}^6	S_{10}^8
	≡	≡	≡	≡
E,	C_5,	C_5^2,	C_5^3,	C_5^4
$5\sigma_v$				
$5\perp C_2$				
S_5,	S_5^3,	S_5^5,	S_5^7,	S_5^9
		≡		
		σ_h		

when n is even, $\frac{n}{2}\sigma_v$ and $\frac{n}{2}\sigma_v'$

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

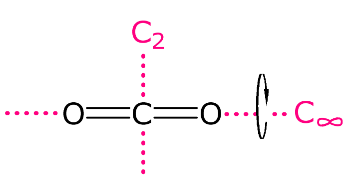
linear molecules without an inversion center



a σ_v is easily identified as the plane of the paper, by virtue of the C_∞, $\infty\sigma_v$s are generated

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

linear molecules with an inversion center

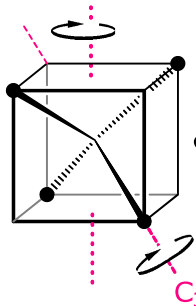


the C_∞, generates $\infty\sigma_v$ and ∞C_2

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)

C_2, S_4 through each face



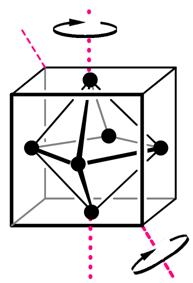
σ_d's through each edge

C_3 through each corner

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)

C_2, C_4, S_4 through each face



σ_h bisect faces of cube
σ_d contains edges of cube
C_2 bisect edges of cube

C_3, S_6 through each corner

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_h : generators are C_3, C_5, i (h = 120) ➡ the icosahedral point group

K_h : generators are C_ϕ, C_ϕ', i (h = ∞) ➡ the spherical point group

Flow chart for assigning molecular point groups: