Lect 6 Ponit group — proper point group

§ The proper point groups — rotatiun $\det O = 1$

n-fold axis — Schoenflies symbol C_n — $R(\hat{n}, \frac{2\pi}{n})$

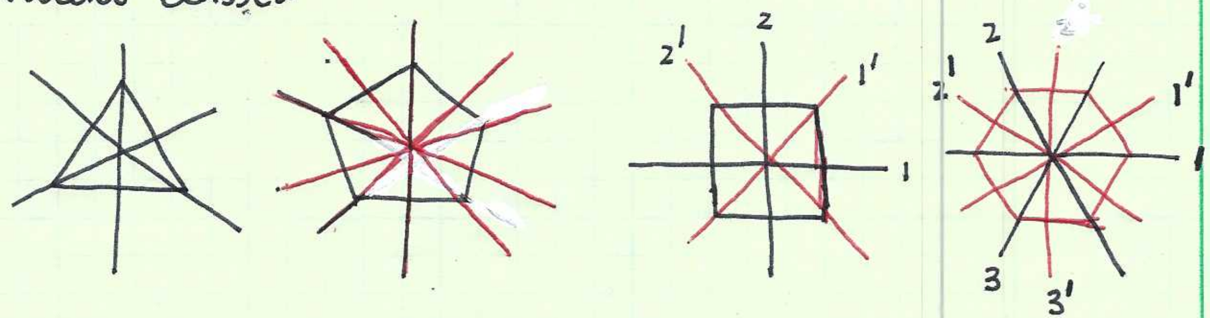
international notatiun n

1° groups with only one axis — C_n or n

2° groups with 2-fold axes but only one n-fold axis $n \geq 2$.

D_n or $n2$ for n odd, and $n22$ for n even.

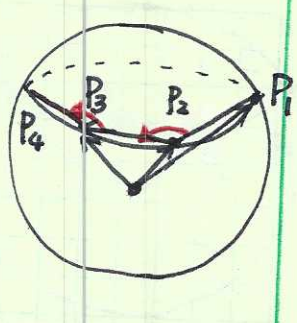
The 2-fold axes need to be perpendicular to the n-fold axis, otherwise they will generate new n-fold axes. The n-fold axis generates n 2-fold axes. $n22$ for D_{2n} means the alternating 2-fold axes fall into two non-equivalent classes.



3° groups with more than one principle axis $n > 2$.

If two axes $n > 2$ and $n' > 2$ are present, the actiun of $C_{n'}$ will at least creat a new n-fold axes. Below we will show that if we have 2 n-fold axis, $(n > 2)$, their mutual actiun will generate a bunch of axes. The directions of these n-fold axes form regular polyhedrons on the unit sphere. This impose strong anstraint on possible anfigurations.

Pick up 2 directiun of n-fold axes on the unit sphere, whose distance to each other is the closest. They are denoted as P_1, P_2. Around the P_2 axis, Perform C_n^1 rotation, then P_1 axis is rotated to P_3.



$P_1 P_2 P_3$ determine a plane, which cuts the sphere and the intersection is a circle. The points P_1, P_2, P_3 on the circle can be repeated: Around the P_3 axis, perform C_n^1 rotation, we arrive another P_4 axis on the circle.

Finally, this process needs to come back to P_1, i.e., $P_1 P_2 \cdots P_s$ form a regular polygon with s-sides.

If we start from P_1 and perform another C_n rotation, we get another axis P_2' from P_2. Then we can repeat another process, and arrive at anothe regular polygon. All the n-fold axes are equivalent, and can be used for the above processes. Hence, all the n-fold axes form a

repeating

regular poly-hedra, — $\boxed{\text{Platonic Solids!}}$

We denote (s, m): s is # of sides of a face, and m is # of faces meeting at a vertex. Then according to $V - E + F = 2$.

$$V = F \cdot S/m, \quad E = F \cdot S/2$$

where V # of vertex, E # of edges, F # of faces.

$$\Rightarrow \frac{F \cdot S}{m} - \frac{F \cdot S}{2} + F = 2$$

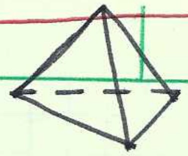
$$\Rightarrow \frac{1}{m} + \frac{1}{S} = \frac{1}{2} + \frac{2}{F \cdot S},$$

because $F \geq 4$, $S \geq 3$

$$\Rightarrow \frac{2}{F \cdot S} \leq 1/6$$

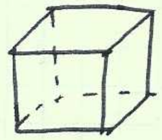
$$\boxed{\frac{1}{2} < \frac{1}{m} + \frac{1}{S} \leq \frac{2}{3}}$$

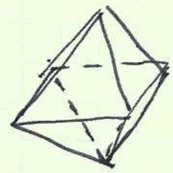
Solutions 1) $m = s = 3$, $F = 4$



2) $m=3$, $s=4$, or $m=4$, $s=3$,

$F = 6$ $\qquad$ $F = 8$

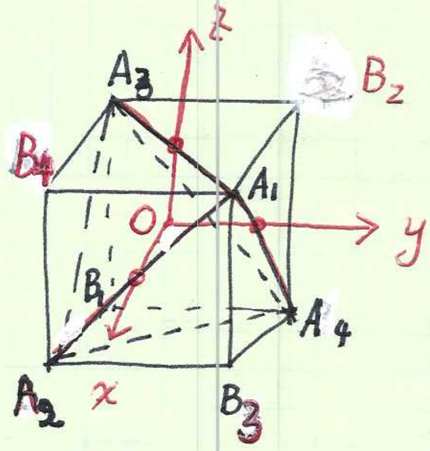




3) $m=3$, $s=5$, $F=12$, or $s=3$ $m=5$, $F=20$

dodecahedron $\qquad$ icosahedron

T (tetrahedron) (23)



- The x, y, z-axis, use $T_{x,y,z}$ to represent $\pi/2$ rotation, then only $T_x^2, T_y^2, T_z^2 \in T$. (They are 2-fold axes)

- The body diagonal direction rotation 3-fold axes

R_1: $(e_x+e_y+e_z)/\sqrt{3}$, R_2: $(e_x-e_y-e_z)/\sqrt{3}$ — rotation $\frac{2}{3}\pi$

R_3: $(-e_x-e_y+e_z)/\sqrt{3}$, R_4: $(-e_x+e_y-e_z)/\sqrt{3}$

and R_1^2, R_2^2, R_3^2, R_4^2. (This group is generated by 2-fold 3-fold axes not at right angle)

	E	T_x^2	T_y^2	T_z^2	R_1	R_1^2	R_2	R_2^2	R_3	R_3^2	R_4	R_4^2
A_1	1	3	4	2	1	1	3	4	4	2	2	3
A_2	2	4	2	1	4	3	2	2	1	4	3	1
A_3	3	1	3	4	2	4	4	1	3	3	1	2
A_4	4	2	1	3	3	2	1	3	2	1	4	4

S_4's even permutation, i.e. A_4 – alternating group.

The productable is not very instructive, nevertheless it has the following structure

	$\{E \quad T^2\}$	$\{R\}$	$\{R^2\}$
E, T^2	T	R	R^2
$\{R\}$	R	R^2	T
$\{R^2\}$	R^2	T	R

T - 2-fold axis operation

R - 3-fold axis with $\frac{2}{3}\pi$ rotation

R^2 - 3-fold axis with $\frac{4}{3}\pi$ rotation

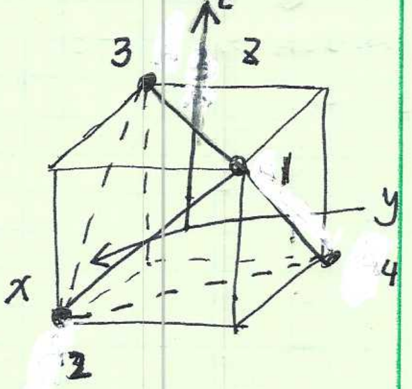
This shows that $\{E, T_x^2, T_y^2, T_z^2\}$ is a normal subgroup, which is D_2, and the quotient group $T/D_2 = C_3$. Then the C_3's representations are also T's

There are 4 classes: $E, \{T^2\}, \{R\}, \{R^2\} \Rightarrow 1^2+1^2+1^2+3^2=12$.
There exist three 1D Reps, which come for C_3, and one 3D Rep.

	E	$3T^2$	$4R$	$4R^2$
A	1	1	1	1
E	1	1	ω	ω^2
E'	1	1	ω^2	ω
T	3	-1	0	0

A and T are real Rep
E and E' are complex

by using $\sum_M \chi_M^*(C_\alpha) C_M(C_\beta) = \frac{|G|}{n_{C_\alpha}} \delta_{\alpha\beta}$



· Example: consider a molecular orbit consists of $|1\rangle$, $|2\rangle$, $|3\rangle$, and $|4\rangle$. It's reps

χ:	E	$3T^2$	$4R$	$4R^2$
	4	0	1	1

$\Rightarrow \quad \chi = A \oplus T$

A: $|\psi_A\rangle = \frac{1}{2}(|1\rangle + |2\rangle + |3\rangle + |4\rangle)$

T: $|\psi_{E,x}\rangle = \frac{1}{2}[|1\rangle + |2\rangle - |3\rangle - |4\rangle]$, $|\psi_{E,y}\rangle = \frac{1}{2}[|1\rangle - |2\rangle - |3\rangle + |4\rangle]$

$|\psi_{E,z}\rangle = \frac{1}{2}[|1\rangle - |2\rangle + |3\rangle - |4\rangle]$

$|\psi_{Ex,y,z}\rangle$ have the symmetry of P_x, P_y, P_z, and $A \longrightarrow S$.

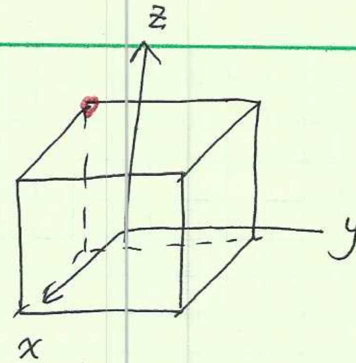
We use $|\psi_{Ex}\rangle$, $|\psi_{Ey}\rangle$ and $|\psi_{Ez}\rangle$ as bases to construct its 3d Rep

$E \begin{pmatrix} 1 & & \\ & 1 & \\ & & 1 \end{pmatrix}$ $T_x^2 \begin{pmatrix} 1 & & \\ & -1 & \\ & & -1 \end{pmatrix}$ $T_y^2 \begin{pmatrix} -1 & & \\ & 1 & \\ & & -1 \end{pmatrix}$ $T_z^2 \begin{pmatrix} -1 & & \\ & -1 & \\ & & 1 \end{pmatrix}$

$(x \to y \to z)$

$R_1 \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$ $R_2 \begin{pmatrix} 0 & 0 & -1 \\ -1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$ $R_3 \begin{pmatrix} 0 & 0 & -1 \\ 1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix}$ $R_4 \begin{pmatrix} 0 & 0 & 1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix}$

R_1^2: $\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$ R_2^2: $\begin{pmatrix} 0 & -1 & 0 \\ 0 & 0 & 1 \\ -1 & 0 & 0 \end{pmatrix}$ R_3^2: $\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & -1 \\ -1 & 0 & 0 \end{pmatrix}$ R_4^2: $\begin{pmatrix} 0 & -1 & 0 \\ 0 & 0 & -1 \\ 1 & 0 & 0 \end{pmatrix}$



☆ O - group

T group is a normal subgroup of the O-group, and its index is 2. The coset contains 12 elements

$\{T_x, T_x^3, T_y\ T_y^3\ T_z\ T_z^3, S_1, S_2, S_3\ S_4\ S_5\ S_6\}$

where $T_{x,y,z}$, $T^3_{x,y,z}$ are the rotation $\frac{\pi}{2}$, $\frac{3\pi}{2}$ around x. y. z axes,

$S_1 \sim S_6$ are 2-fold axes passing the middle points of opposite edges.

① The 2-fold axes ⊥ the body diagonal axis ⇒ the body diagonal axis becomes bilateral. Hence, the 8 3-fold axis rotations belong to one class. Now we have 5 classes

$$E, \underset{\uparrow C_4^2}{\{3T^2\}}, \underset{\uparrow C_3'}{\{8R\}}, \underset{C_4'}{\{6T\}}, \underset{C_2''}{\{6S\}}$$

② # of irreducible representations $1^2+1^2+2^2+3^2+3^2 = 24$

③ T is an invariant (normal) subgroup — quotient group C_2

The quotient group gives rise to 2 1D representations A_1, A_2.

D_2 is another invariant subgroup — quotient group D_3

: D_3 gives a 2D represent E.

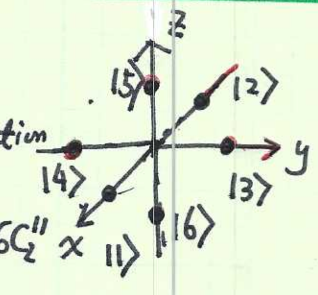
	E	$3C_4^2$	$8C_3'$	$6C_4$	$6C_2''$
A_1	1	1	1	1	1
A_2	1	1	1	-1	-1
E	2	2	-1	0	0
T_1	3	-1	0	1	-1
T_2	3	-1	0	-1	1

′, and ″ represent two new axes.

$$\chi_{A_2} \cdot \chi_{T_1} = \chi_{T_2}$$

Combine with orthonormal condition we can figure out χ_{T_1} and χ_{T_2}.

Conside six atomic orbitals $|1\rangle, |2\rangle, \cdots |6\rangle$ (vertices of an octahedron). Such a representation for the O-group, its χ for $E,\ 3C_4^2,\ 8C_3',\ 6C_4,\ 6C_2''$ are $\{6, 2, 0, 2, 0\}$



$$\Rightarrow (\chi_{A_1}^* \cdot \chi)\cdot \frac{1}{24} = (6 + 3\times 2 + 6\times 2)\frac{1}{24} = 1$$

$$(\chi_E^* \cdot \chi)\frac{1}{24} = (6\times 2 + 3\times 2\times 2)\frac{1}{24} = 1$$

$$(\chi_{T_1}^* \cdot \chi)\frac{1}{24} = (6\times 3 + 3\times 2\times(-1) + 6\times 1\times 2) = 1$$

$\boxed{A_1 \oplus E \oplus T_1}$

Basis $|\psi_{A_1}\rangle = \frac{1}{\sqrt{6}}[|1\rangle + |2\rangle + |3\rangle + |4\rangle + |5\rangle + |6\rangle]$ — $|s\rangle$ symmetry

$$|\psi_{T_1}^x\rangle = \frac{1}{\sqrt{2}}[|1\rangle - |2\rangle], \quad |\psi_{T_1}^y\rangle = \frac{1}{\sqrt{2}}[|3\rangle - |4\rangle], \quad |\psi_{T_1}^z\rangle = \frac{1}{\sqrt{2}}[|5\rangle - |6\rangle]$$

$$\uparrow \qquad\qquad \uparrow \qquad\qquad \uparrow$$

$$|P_x\rangle \qquad\qquad |P_y\rangle \qquad\qquad |P_z\rangle$$

under these bases, for those T group elements, we have the same matrices as before.

$$T_x^1: \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix} \quad T_y^1: \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{bmatrix} \quad T_z^1: \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$T_x^3: \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{bmatrix} \quad T_y^3: \begin{bmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix} \quad T_z^3: \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

$$S_{xy}: \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & & -1 \end{bmatrix} \quad S_{yz}: \begin{bmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \quad S_{zx}: \begin{bmatrix} & & 1 \\ & -1 & \\ 1 & & \end{bmatrix}$$

$$S_{-xy}: \begin{bmatrix} 0 & -1 & \\ -1 & 0 & \\ & & -1 \end{bmatrix} \quad S_{\underline{y}z}: \begin{bmatrix} -1 & & \\ & & -1 \\ & -1 & \end{bmatrix} \quad S_{\underline{z}x}: \begin{bmatrix} & & -1 \\ & -1 & \\ -1 & & \end{bmatrix}$$

For T_2-representation: the representation matrices for the T-group operations are the same as T_1, and those for $6C_4'$ and $6C_2''$ have an opposite sign, i.e. $T_2 = A_1 \otimes T_1$.

☆ Now we can form the basis for the E-representation

$$|\psi_E^+\rangle = \frac{1}{\sqrt{6}}\left[\overset{z^2}{|5\rangle+|6\rangle} + \omega\big(\overset{x^2}{|1\rangle+|2\rangle}\big) + \omega^2\big(\overset{y^2}{|3\rangle+|4\rangle}\big)\right] \qquad \boxed{z^2-r^2 \pm i(x^2-y^2)}$$

e_g orbitals

$$|\psi_E^-\rangle = \frac{1}{\sqrt{6}}\left[|5\rangle+|6\rangle + \omega^2[|1\rangle+|2\rangle] + \omega[|3\rangle+|4\rangle]\right]$$

For $H = \{E\ T_x^2,\ T_y^2,\ T_z^2\}$: $\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ ← invariant subgroup

$R_1 H = \{R_1\ R_2\ R_3\ R_4\}$, $R_1^2 H = \{R_1^2, R_2^2\ R_3^2\ R_4^2\}$

$T_z H = \{T_z\ T_z^3\ S_{xy}, S_{-xy}\}$ $T_x H = \{T_x, T_x^3, S_{yz}\ S_{-yz}\}$ $T_y H = \{T_y, T_y^3, S_{xz}, S_{-xz}\}$

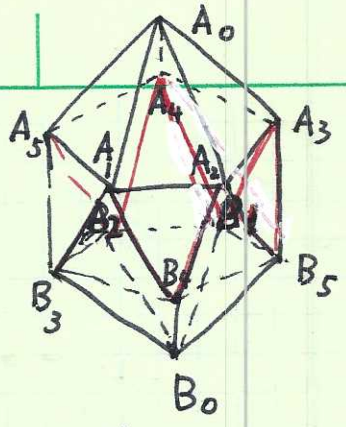
Hence: $R_1 (x\to y\to z)$: $\begin{pmatrix} \omega^2 & 0 \\ 0 & \omega \end{pmatrix}$ $R_1^2 H =$ $\begin{pmatrix} \omega & 0 \\ 0 & \omega^2 \end{pmatrix}$

$T_z H$: $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ $T_x H$ $\begin{pmatrix} 0 & \omega \\ \omega^2 & 0 \end{pmatrix}$ $T_y H$: $\begin{pmatrix} 0 & \omega^2 \\ \omega & 0 \end{pmatrix}$

$\omega = e^{-i\frac{2\pi}{3}}$

It's easy to verfy that all Reps are real.

☆ Y group



20 faces, 12 vertexs, 30 edges

6 · five-fold axes $A_0B_0, A_1B_1, \cdots A_5B_5$

10 3-fold axes : connecting opposite face centers

15 2-fold axes: conneting opposite edge centers

sym operations $1 + 6\times 4 + 10\times 2 + 15 = 60$!

all are self-inverse classes.

$$\boxed{\begin{array}{l} 5 \text{ classes } \quad E,\ 12C_5,\ 12C_5^2,\ 20C_3',\ 15C_2' \\ \quad 1^2 + 3^2 + 3^2 + 4^2 + 5^2 = 60 \end{array}}$$

All Reps are real or pseudo-real.

Unfortunately, Y group does not have non-trivial normal subgroup. It has D_5 and T subgroups. D_5: we can take 5-fold axis A_0B_0, and the 5 two-fold axis perpendicular to A_0B_0.

The T subgroup is not easy to see: Let's find 3 orthogonal 2-fold axes: From O to the middle points of A_0A_1, A_3A_4, A_2B_5. The 4 3-fold axes can be formed for O to the centers of triangles $\Delta A_1B_4A_2$, $\Delta A_0A_2A_3$, $\Delta A_0A_4A_5$, $\Delta A_1A_5B_3$. please check.

→ We can use T group to assist the analysis of the character table of the I group. We denote the 3d reps as T_1 and T_2. They need to be still the 3d rep of the T group. Check characters of A, E and E' of the T-group. For the 2-fold axis rotation, they are all 1. Hence if T_1 and T_2 need to decomposed to the sum of A, E and E', their character for the 2-fold axis should be 3. Then for the I group, the 15 2-fold axes contribute $15 \times 3^2 > 60$. i.e. $\boxed{T_1, T_2 \to T.}$

We also denote G as the 4-dimensional rep, and H as the 5-dimensional Rep. Their decomposition must include T. Since all Reps are real or pseudoreal, their characters are also real. Combining these facters, we have

$$\boxed{G \to T \oplus A, \quad H \to T \oplus E \oplus E'.}$$

Based on these, we can write down part of the character table

I	E	$12C_5$	$12C_5^2$	$20C_3'$	$15C_2''$
A	1	1	1	1	1
T_1	3	$1+2\cos\frac{2}{5}\pi$	$1+2\cos\frac{4\pi}{5}$	0	-1
T_2	3	$1+2\cos\frac{4}{5}\pi$	$1+2\cos\frac{2\pi}{5}$	0	-1
G	4	-1	-1	1	0
H	5	0	0	-1	1

In order to determine the characters of the C_5 and C_5^2 classes. We consider the decomposition with respect to D_5. D_5's characters are

D_5	E	$2C_5^1$	$2C_5^2$	$5C_2'$
A_1	1	1	1	1
A_2	1	1	1	-1
E_1	2	$2\cos\frac{2}{5}\pi$	$2\cos\frac{4}{5}\pi$	0
E_2	2	$2\cos\frac{4}{5}\pi$	$2\cos\frac{2\pi}{5}$	0

$$p = 2\cos\frac{2}{5}\pi = \frac{\sqrt{5}-1}{2}$$

$$p^{-1} = -2\cos\frac{4}{5}\pi = \frac{\sqrt{5}+1}{2}$$

Since C_2''s characters are determined we have $\boxed{T_1 = A_2 \oplus E_1, \quad T_2 = A_2 \oplus E_2}$

Then we can complete characters of T_1, T_2, and they satisfy the orthogonal relation.

· According to orthoagonal relations to T_1 and T_2, we can figuraure out the characters of G, H for C_5 and C_5^2 as shown in the table.

Then we have the decomposition

$$\boxed{G = E_1 \oplus E_2 \quad \text{and} \quad H = E_1 \oplus E_2 \oplus A_1}$$

Example: consider a molecule with a configuration of icosahedroal with 12 atoms. They form a 12 dimensional representation

	E	$12C_5$	$12C_5^2$	$20C_3'$	$15C_2'$
χ	12	2	2	0	0

it's easy to verify that $\boxed{\chi = A \oplus T_1 \oplus T_2 \oplus H}$

Let us treat Y as SO(3) group's subgroup and consider the decomposition of spherical harmonics $Y_{lm}(\theta,\varphi)$. Later, we will know that $Y_{lm}(\theta,\varphi)$ form a $2l+1$ dimensional irreducible rep for SO(3), and the representation matrix is $D^l_{m'm}(\alpha,\beta,\gamma) = \langle lm' | e^{-i\alpha L_z} e^{-i\beta L_y} e^{-i\gamma L_z} | lm \rangle$. The character is simple: for a rotation with θ angle. $\chi^l(\theta) = \sum_{m=-l}^{l} e^{-iml\theta} = \dfrac{\sin(l+\frac{1}{2})\theta}{\sin\frac{\theta}{2}}$.

For

l	$E(\theta=0)$	$12C_5$	$12C_5^2$	$20C_3'$	$15C_2''$
0	1	1	1	1	1
1	3	$\sin\frac{3}{5}\pi/\sin\frac{\pi}{5}$	$\dfrac{\sin\frac{6}{5}\pi}{\sin\frac{2\pi}{5}}$	0	-1
2	5	0	0	-1	1
3	7	$\sin\frac{7}{5}\pi/\sin\frac{\pi}{5}$	$\dfrac{\sin\frac{6}{5}\pi}{\sin 2\pi/5}$	1	-1

It's clear that
$$\boxed{\begin{array}{l} s\text{- state} \leftrightarrow A \\ p\text{- state} \leftrightarrow T_1 \\ d\text{- state} \leftrightarrow H \\ f\text{- state} \leftrightarrow T_2 \oplus G \end{array}}$$

not $\sin\frac{3}{5}\pi / \sin\frac{\pi}{5} = 2\cos\frac{2}{5}\pi + 1 = \frac{\sqrt{5}+1}{2}$

$\sin\frac{6}{5}\pi / \sin\frac{2\pi}{5} = 2\cos\frac{4}{5}\pi + 1 = -\frac{\sqrt{5}-1}{2}$

by noticing $\sin\frac{7}{5}\pi / \sin\frac{\pi}{5} = -\sin\frac{3}{5}\pi / \sin\frac{\pi}{5} = -\frac{\sqrt{5}+1}{2}$

$\sin\frac{4}{5}\pi / \sin\frac{2}{5}\pi = 2\cos\frac{2}{5}\pi = \frac{\sqrt{5}-1}{2}$

\# of A: $\frac{1}{60}\left(7\times1 + 12\left(-\frac{\sqrt{5}+1}{2}\right)\times1 + 12\left(\frac{\sqrt{5}-1}{2}\right)\times1 + 20\times1\times1 + 15\times1\times-1\right)$

$= \frac{1}{60}[0] = 0$

\# of T_1 $\frac{1}{60}\left[3\times7\times1 + \left(-\frac{\sqrt{5}+1}{2}\right)\left(\frac{\sqrt{5}+1}{2}\right)\times12 + \left(\frac{\sqrt{5}-1}{2}\right)\times\left(\frac{\sqrt{5}-1}{2}\right)\times12 + 0 + 15(-1)(-1)\right]$

$= \frac{1}{60}[21 + (-3)\times6\times2 + 15] = 0$

\# of T_2 $\frac{1}{60}\left[3\times7\times1 + \left(-\frac{\sqrt{5}+1}{2}\right)\left(-\frac{\sqrt{5}-1}{2}\right)\times12 + \frac{\sqrt{5}-1}{2}\times\frac{\sqrt{5}+1}{2}\times12 + 0 + 15(-1)\times(-1)\right]$

$= 1/60\,[21 + 12 + 12 + 15] = 1$

\# of G: $\frac{1}{60}\left[4\times7\times1 + \left(-\frac{\sqrt{5}+1}{2}\right)(-1)\times12 + \frac{\sqrt{5}-1}{2}\times(-1)\times12 + 1\times1\times20 + 0\right)$

$= \frac{1}{60}[28 + 12 + 20] = 1$

$\Rightarrow$ The largest degeneracy (no counting spin) is $l=2$, i.e five-fold degeneracy, which can remain under point group. Y is the next highest symmetry, just next to spherical.

☆ improper point groups

- Improper point groups are subgroups of O(3). They contains operations with the 3x3 orthogonal matrice $\det O = -1$, which are not a pure rotation.

- Improper point group must have an invariant proper subgroup H, whose index is 2, i.e. $\boxed{G/H = Z_2}$

- Improper point group can be obtained by adding a single improper element M, as a generater: $\boxed{G = H + MH.}$

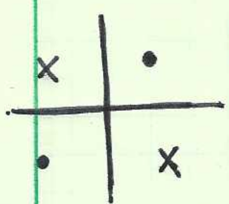
- M can be an <u>inversion I</u>, or <u>a reflection σ</u>, then $M^2 = I$.

  or more generally $\boxed{M = S_{2n} - \text{rotary reflection, such that } M^2 = C_n}$

Classifacation: $\boxed{S_{2n} = C_{2n} \cdot \sigma_h}$

- Rotary reflection groups: For S_{4n}. – 4n cyclic group.

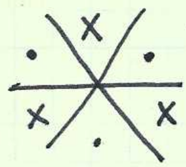
$\bar{4}$



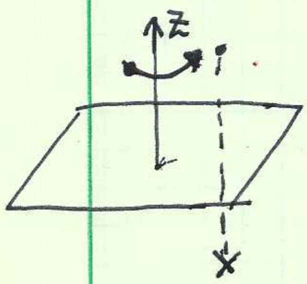
S_4,

For $S_{4n+2} = C_{2n+1} \otimes C_I$, $C_I = \{E, I\}$ ↑ inversion

$\bar{3}$



$(C_{4n+2}\, \sigma_h)^{2n+1} = C_2\, \sigma_h = I$



international symbol $(\overline{2n})$ for n even

$\bar{n}$ for n odd

cyclic abelian group

(horizontal plane reflection)

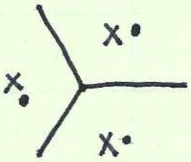
★ C_{nh} groups n/m $C_n \oplus \sigma_h C_n$ — abeliean group

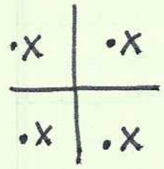
• $C_{2n,h}$ contains inversion. $(C_{2n})^n \sigma_h = C_2 \cdot \sigma_h = I$

then $C_{2n,h} = C_{2n} \otimes \{E, I\}$.

($C_{2n,h}$ and $S_{4n+2,h} = C_n \otimes \{E, I\}$)

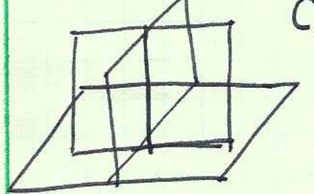
• $C_{2n+1,h}$ does not contain inversion



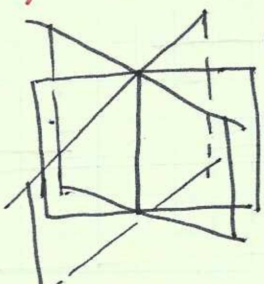


★ C_{nv} groups nm for n odd, nmm for n even

(vectical plane reflection)



C_{2v}



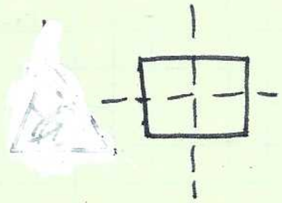
C_{3v}

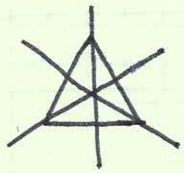
by corresponding

$\sigma_v \longrightarrow C_2'$ (in-plane 2-fold axis)

↑

(vertical plane reflection)





$C_{nv} \simeq D_n$

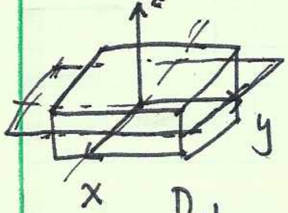
★ D_{nh} groups $\frac{n}{m}\frac{2}{m}\frac{2}{m}$

$D_{nh} = D_n \otimes \{E, \sigma_h\}$ — ∵ σ_h commutes with both C_n and C_2 rotations

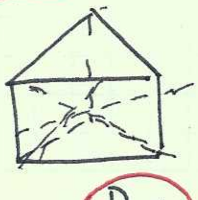
$\sigma_h C_2 \sigma_h = C_2$ (please check)

if n is even: $C_n^{n/2} \sigma_h = C_2 \cdot \sigma_h = I$, which contains inversion

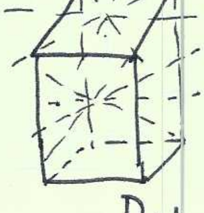
i.e. $D_{2n,h} = \underline{D_{2n} \otimes \{E, I\}}$. $\boxed{D_{2n+1,h} \simeq D_{4n+2}}$



D_{2h},



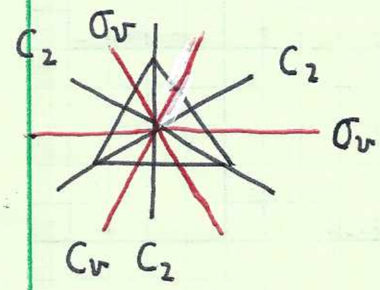
D_{3h}



D_{4h}

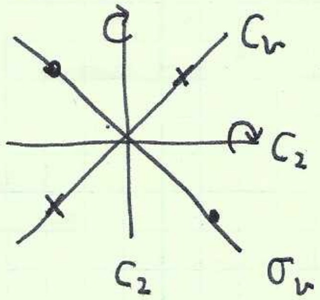
✱ D_{nd} groups

The elements of D_n, combined with a vertical reflection plane middle way between a pair of axis.



For $D_{2n+1,d}$, since C_2 and σ_v can be perpendicular to each other, inversion is included, i.e. $\underline{D_{2n+1,d} = D_{2n+1} \otimes \{E, I\}}$.

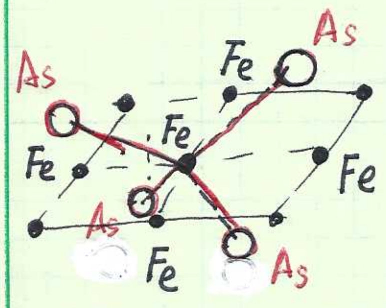
For $D_{2n,d}$



$$C_2 C_v = \begin{pmatrix} 1 & & \\ & -1 & \\ & & -1 \end{pmatrix}\begin{pmatrix} & 1 & \\ 1 & & \\ & & 1 \end{pmatrix} = \begin{pmatrix} & 1 & \\ -1 & & \\ & & -1 \end{pmatrix} = S_4$$

↗ rotation 90° and reflection with reflection to horizontal plane.

→ iron-based super conductor



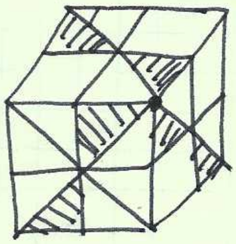
D_{2d}

$$\boxed{D_{2nd} \simeq D_{4n}}$$

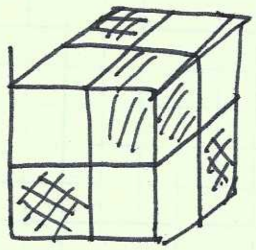
✱ T_d group $\bar{4}3m$, -

The full symmetry of a regular tetrahedron. Add a reflection plane passing one edge and bisecting the opposite edge. T_d has 24 elements $\sim S_4$.

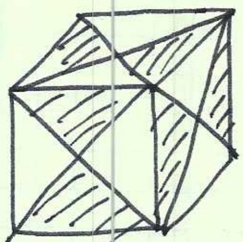
(x) T_h : $\frac{2}{m}\bar{3}$: add an inversion center to T



T



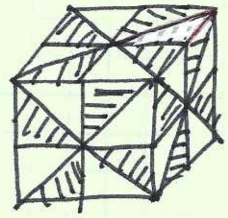
$T_d \simeq O$



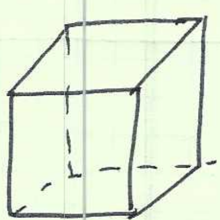
T_h

(x) group O_h : $\frac{4}{m}\bar{3}\frac{2}{m}$

$O_h = O \otimes \{E, I\}$



O



O_h

(x) group $Y_h = Y \otimes \{E, I\}$

improper point groups not containing I : S_{4n}, C_{nv}, $D_{2n+1,h}$, $D_{2n,d}$, T_d