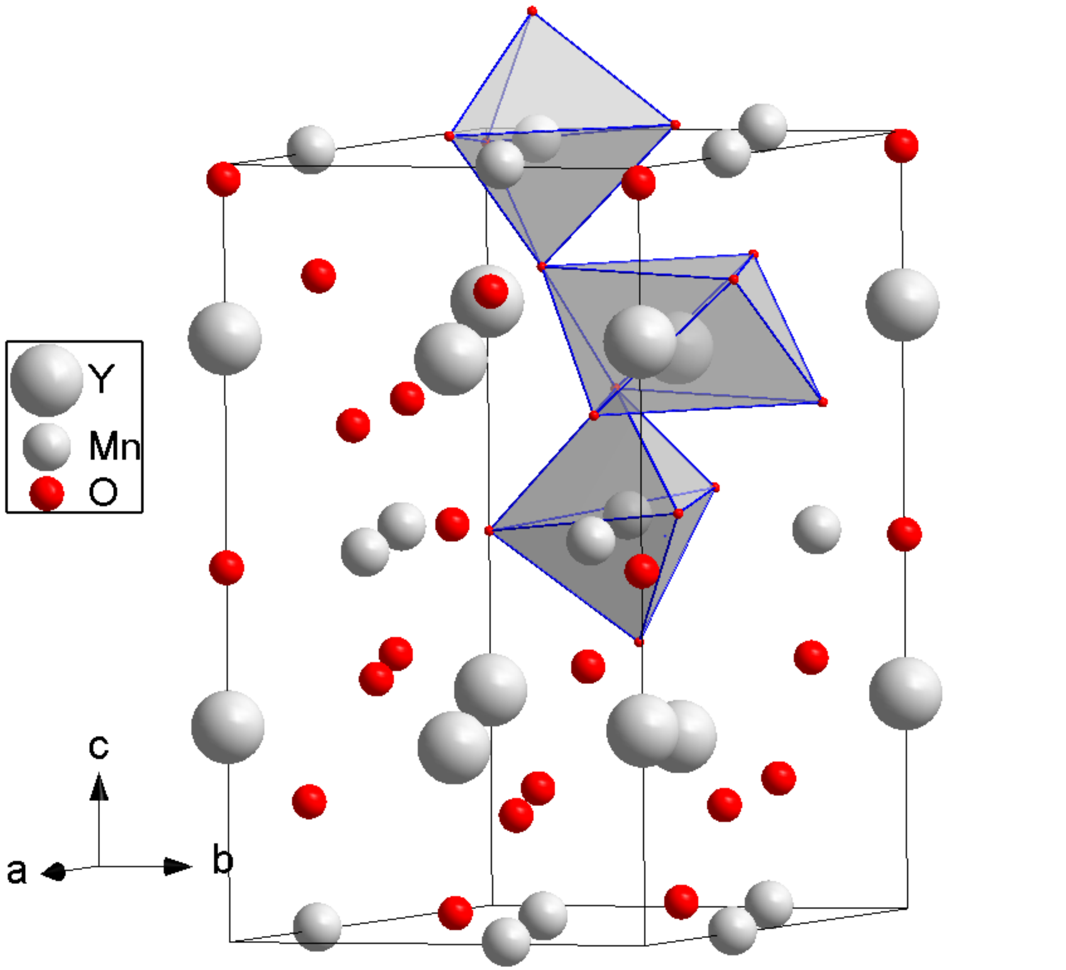
Magnetic Structures of h-$YMnO_3$

Detian Yang

04/26/202$\boldsymbol{E}$

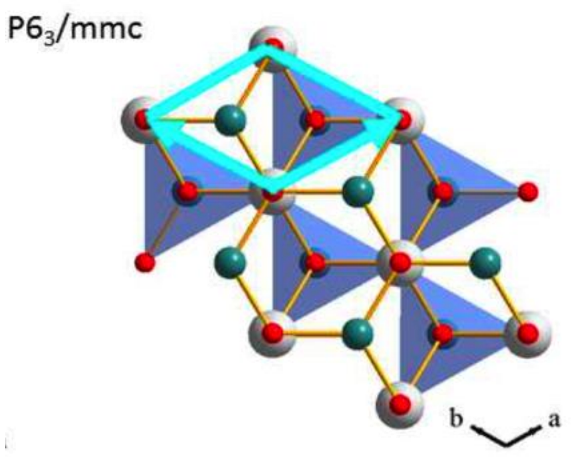
Crystal Structure and Symmetry: $P6_3cm$

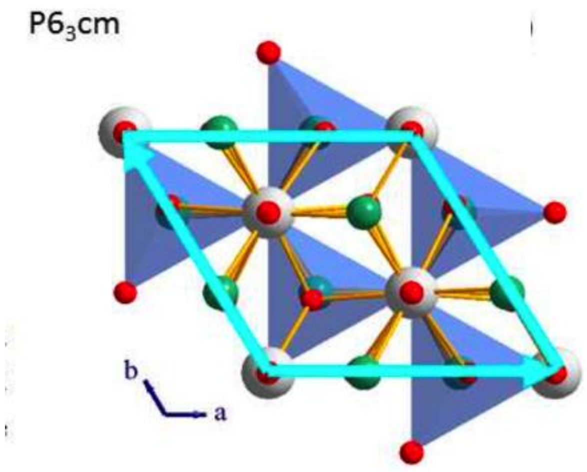
Magnetic Symmetry: $P6_3cm \otimes I$



O:8; Mn 6; R 6

A	B	C
	O (3)	Mn(3)
		O(3)
	R(3)	
O(3)		
Mn(3)	O(3)	
O(3)		
	R(3)	
		O(3)
	O	Mn





'The spins being axial vectors, one writes down a Hamiltonian, invariant under spin reversal and symmetry operations of crystallographic group, in terms of vectors which form the basis of irreducible representations. All invariants of order 2 which enter the Hamiltonian are products of two base vectors belonging to the same representation. "

Group Theoretical Strategy

$$T^{-E} = T^{\dagger}$$

$$T^{-E} = -T^{\dagger}$$

$$[\boldsymbol{H}, \boldsymbol{T}] = \boldsymbol{0} \qquad \forall \boldsymbol{T} \in \{\boldsymbol{Symmetry\ Group}: |\langle\Psi|\Phi\rangle|^2 = |\langle T\Psi|T\Phi\rangle|^2\}$$

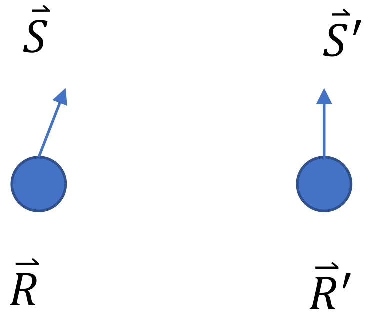
System state space$\{\Phi\}$: Hilbert Vector Space (complete metric space with inner product)

Unitary operator	Orthornomal basis	Representation	irreducible basis	irreducible Representation
$\boldsymbol{T}$	→	$\begin{bmatrix} & \cdots & \\ \vdots & \ddots & \vdots \\ & \cdots & \end{bmatrix}$	→	$\begin{bmatrix} D_{\boldsymbol{E}} & & \\ & D_{2;\boldsymbol{EE}} & D_{2;\boldsymbol{E}2} \\ & D_{2;2\boldsymbol{E}} & D_{2;22} \end{bmatrix}$
		Unitary Matrix		Diagonalized to the extreme

irreducible basis: Physical field, Symmetry-protected States, preferred state, Magnetic order,…

Symmetry → Interaction → Physical States

Microscopic Method (Matrix Method)



Spin Interaction

$$H = \sum_{\vec{R}\vec{R}'} W(\vec{R}, \vec{R}')$$

$$W(\vec{R}, \vec{R}') = -2 \sum_{\alpha,\beta} A_{\alpha\beta}(\vec{R}, \vec{R}') S_\alpha(\vec{R}) S'_\beta(\vec{R}') \qquad \alpha, \beta = x, y, z$$

$$\mathbf{A}(\vec{R}, \vec{R}') = \mathbf{A}_{Sym}(\vec{R}, \vec{R}') + \mathbf{A}_{Anti}(\vec{R}, \vec{R}') = \frac{\boldsymbol{E}}{3} A_{\alpha\alpha}\delta_{\alpha\beta} + \sum_\gamma \varepsilon_{\alpha\beta\gamma} D_\gamma + \boldsymbol{\phi}_{\alpha\beta}$$

Scalar   Polar vector   Traceless tensor

$$\mathbf{A}_{Sym;\alpha\beta} = \frac{\boldsymbol{E}}{2}(A_{\alpha\beta} + A_{\beta\alpha}) \qquad \mathbf{A}_{Anti;\alpha\beta} = \frac{\boldsymbol{E}}{2}(A_{\alpha\beta} - A_{\beta\alpha}) = \sum_\gamma \varepsilon_{\alpha\beta\gamma} D_\gamma \qquad D_\gamma(\vec{R}, \vec{R}') = \frac{\boldsymbol{E}}{2} \varepsilon_{\alpha\beta\gamma} \mathbf{A}_{Anti;\alpha\beta}(\vec{R}, \vec{R}')$$

$$\mathbf{A}_{Sym;\alpha\beta} = \frac{\boldsymbol{E}}{3} A_{\alpha\alpha}\delta_{\alpha\beta} + \boldsymbol{\phi} \qquad A_{\alpha\alpha} \equiv A_{xx} + A_{yy} + A_{zz} \coloneqq 3J \qquad \boldsymbol{\phi}_{\alpha\beta} \equiv \left[\frac{\boldsymbol{E}}{2}(A_{\alpha\beta} + A_{\beta\alpha}) - \frac{\boldsymbol{E}}{3} A_{\alpha\alpha}\delta_{\alpha\beta}\right]$$

Dzialoshinski-Moriya Interaction

$$\sum_{\alpha,\beta} \mathbf{A}_{Anti;\alpha\beta}(\vec{R}, \vec{R}') S_\alpha(\vec{R}) S'_\beta(\vec{R}') = \sum_{\alpha,\beta,\gamma} \varepsilon_{\alpha\beta\gamma} D_\gamma(\vec{R}, \vec{R}') S_\alpha(\vec{R}) S'_\beta(\vec{R}') = \vec{D}(\vec{R}, \vec{R}') \cdot \left(\vec{S}(\vec{R}) \times \vec{S}'(\vec{R}')\right)$$

$$W(\vec{R}, \vec{R}') = -2\left[J(\vec{R}, \vec{R}')\vec{S}(\vec{R}) \cdot \vec{S}'(\vec{R}') + \vec{D}(\vec{R}, \vec{R}') \cdot \left(\vec{S}(\vec{R}) \times \vec{S}'(\vec{R}')\right) + \vec{S}(\vec{R}) \cdot \boldsymbol{\phi}(\vec{R}, \vec{R}') \cdot \vec{S}'(\vec{R}')\right]$$

Isotropic Exchange   **Antisymmetric D-M Interaction**   **Anisotropic term**

Crystalline field
Dipolar interaction
Pseudo-dipolar interaction

Isotropic Exchange: Static Equilibrium

$$H_{H-N} = \sum_{\vec{R}\vec{R}'} W(\vec{R}, \vec{R}')$$

$$W(\vec{R}, \vec{R}') = -2J(\vec{R}, \vec{R}')\vec{S}(\vec{R}) \cdot \vec{S}'(\vec{R}')$$
$$= -2\tilde{J}(\vec{R}, \vec{R}')\vec{\sigma}(\vec{R}) \cdot \vec{\sigma}(\vec{R}')$$

$$\vec{\sigma}(\vec{R}) \equiv \vec{S}(\vec{R})/S(\vec{R})$$

$$\tilde{J}(\vec{R}, \vec{R}') \equiv S(\vec{R})J(\vec{R}, \vec{R}')S(\vec{R}')$$

$$\frac{\delta H_{H-N}}{\delta \vec{\sigma}(\vec{R})} = 0, [\sigma(\vec{R})]^2 = \boldsymbol{E}$$

Or

$$\frac{d\sigma(\vec{R})}{dt} = \sum_{\vec{R}'} 2\tilde{J}(\vec{R}, \vec{R}')\vec{\sigma}(\vec{R}') \times \vec{\sigma}(\vec{R})$$

→ $\sigma(\vec{R}) \parallel \sum_{\vec{R}'} 2\tilde{J}(\vec{R}, \vec{R}')\vec{\sigma}(\vec{R}')$ → $\lambda(\vec{R})\sigma(\vec{R}) = \sum_{\vec{R}'} 2\tilde{J}(\vec{R}, \vec{R}')\vec{\sigma}(\vec{R}')$

$$H_{H-N} = -\sum_{\vec{R}} \lambda(\vec{R})[\sigma(\vec{R})]^2 = -\sum_{\vec{R}} \lambda(\vec{R})$$

$\lambda(\vec{R})$: Exchange energy of $\vec{S}(\vec{R})$ interacting with all neighbors

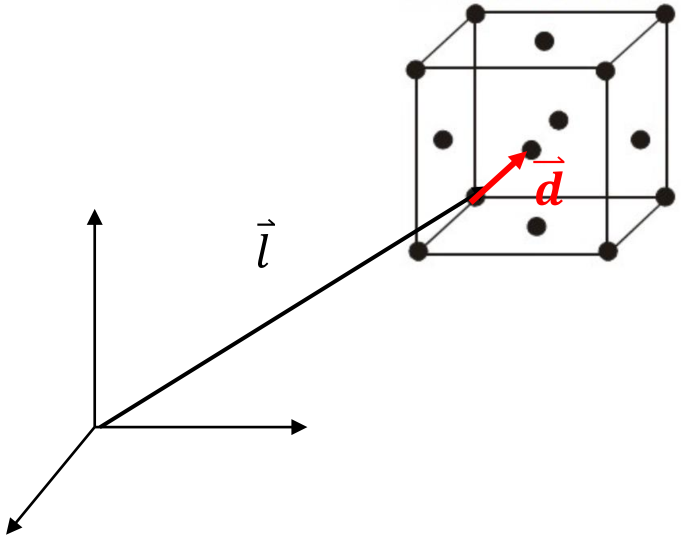
$$\frac{d\vec{I}}{dt} = Torque = \vec{\mu} \times \vec{B} \qquad \vec{\mu} = \gamma\vec{I}$$

$$H = -\vec{\mu} \cdot \vec{B}$$

$[\boldsymbol{H}, \boldsymbol{T}] = \boldsymbol{0}$ → $\lambda(\vec{R})$ is same for crystallographic equivalent atoms

Spin configuration of lowest energy of crystallographic symmetry.

$\lambda(\vec{R}_i)\sigma(\vec{R}_i) = \sum_{\vec{R}'} 2\tilde{J}(\vec{R}_i, \vec{R}')\vec{\sigma}(\vec{R}')$ $\quad i = \boldsymbol{E}, 2, \ldots n$



$$\lambda_i T_i(\vec{k}) = \sum_j \xi_{ij}(\vec{k}) T_j(\vec{k})$$

$$T_i(\vec{k}) \equiv \sum_{\vec{R}_i} \sigma(\vec{R}_i) e^{i\vec{k}\cdot\vec{R}_i} / N \qquad \xi_{ij}(\vec{k}) \equiv \sum_{\vec{R}_i} \tilde{J}(\vec{R}_i, \vec{R}_j) e^{i\vec{k}\cdot(\vec{R}_i - \vec{R}_j)}$$

$$\left(\boldsymbol{\xi}(\vec{\boldsymbol{k}}) - \boldsymbol{\lambda}\right)\boldsymbol{T}(\vec{\boldsymbol{k}}) = \mathbf{0}$$

Magnetic States are given by $\boldsymbol{T}(\vec{\boldsymbol{k}})$

Magnetic Structures of h-YMnO3: Irreducible Basis in Spin Space

crystallographic space group $\boldsymbol{F}$ $P6_3cm$

↓

Nontrivial Magnetic Group: $\boldsymbol{DE}\cup(\boldsymbol{F}-\boldsymbol{D})\boldsymbol{E'}$

D any index 2 subgroup of F

E: identity; E' time reversing

$P6'_3c'm$, $P6'_3cm'$, $*P6_3c'm'$

↓

Little Group $\boldsymbol{G_{\vec{k}}}$ $P6_3cm$

↓

Irreducible Representations of crystallographic space group $P6_3cm$ ← Fundamentals of Group Theory

magnetic group

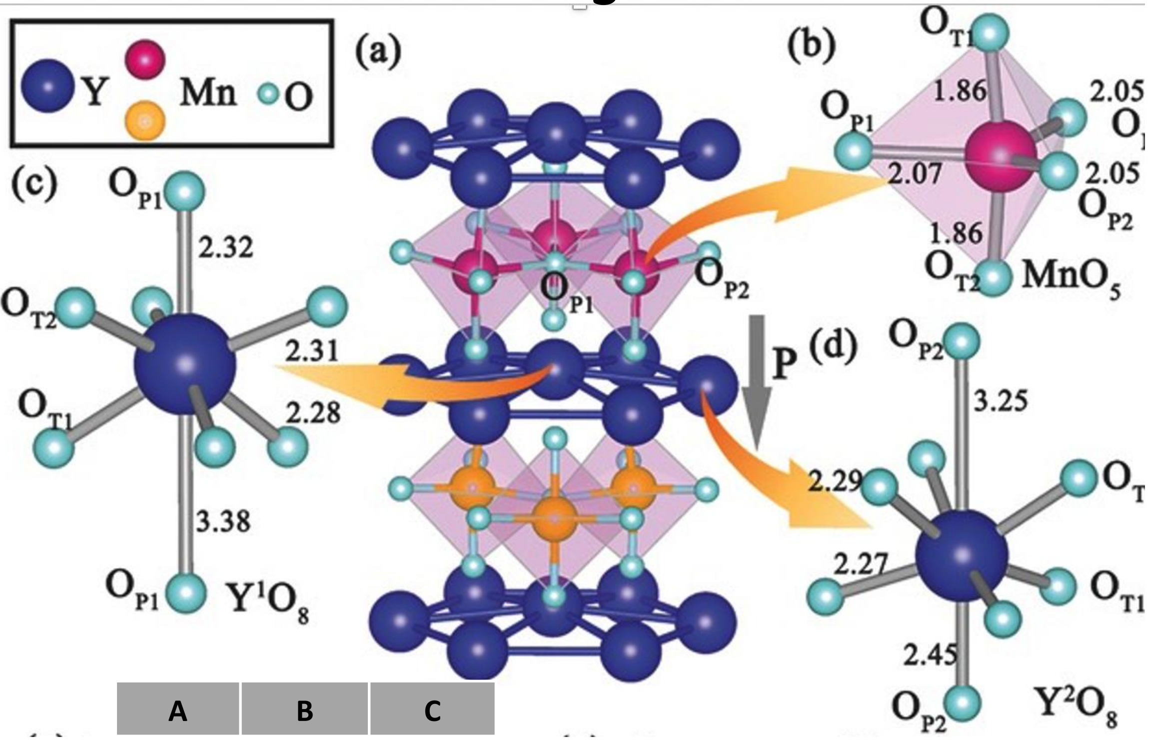
↓

Irreducible Representations and Basis in 18(6x3)-D state space

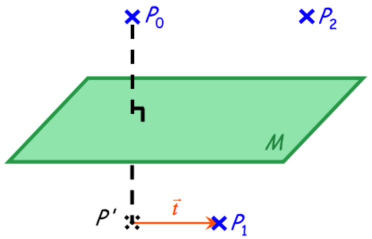
↓

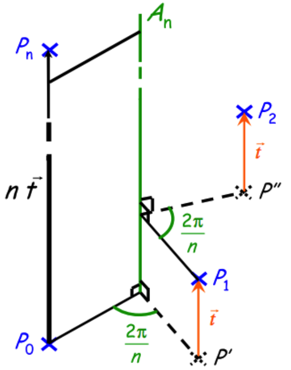
Irreducible Representations and Basis Compatible with Experimental Observations

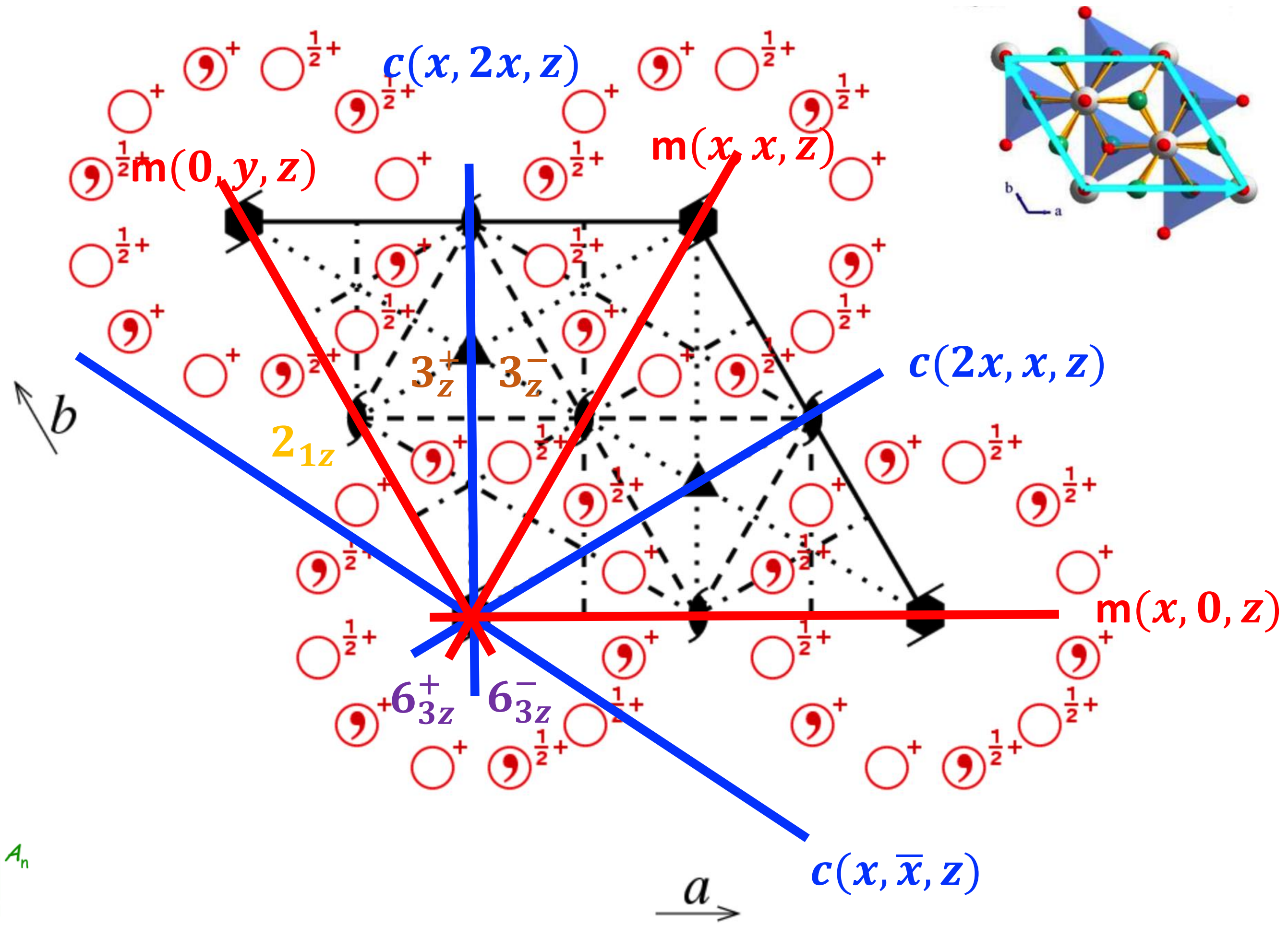
Space Group $P6_3cm$



A	B	C
	O (3)	Mn(3)
		O(3)
	R(3)	
O(3)		
Mn(3)	O(3)	
O(3)		
	R(3)	
		O(3)
	O	Mn







Printed symbol	Symmetry axis	Graphical symbol	Glide translation
1	Identity	none	none
$\bar{1}$	Inversion	○	none
2	Twofold rotation axis	(⊥ paper) (// paper)	none
2_1	Twofold screw axis	(⊥ paper) (// paper)	1/2
3	Threefold rotation axis	⊥ paper ▲	none
3_1	Threefold screw axes		1/3
3_2			2/3
$\bar{3}$	Threefold inversion axis		none

Printed symbol	Symmetry axis	Graphical symbol	Glide translation
4	Fourfold rotation axis	◆	none
4_1	Fourfold screw axes		1/4
4_2			1/2
4_3			3/4
$\bar{4}$	Fourfold inversion axis		none
6	Sixfold rotation axis	⬢	none
6_1	Sixfold screw axes		1/6
6_2			1/3
6_3			1/2
6_4			2/3
6_5			5/6
$\bar{6}$	Sixfold inversion axis		none

printed symbol	symmetry plane	graphical symbol: normal to projection plane	graphical symbol: parallel to projection plane	nature of glide translation
m	reflection plane (mirror plane)			none
a, b, c	'axial' glide plane	$\vec{t}$ // proj. plane; $\vec{t}$ ⊥ proj. plane		$\vec{a}/2, \vec{b}/2$, or $\vec{c}/2$ respectively
e	'double' glide plane			($\vec{a}/2$ and $\vec{b}/2$), ($\vec{b}/2$ and $\vec{c}/2$), or ($\vec{a}/2$ and $\vec{c}/2$); OR $((\vec{a}\pm\vec{b})/2$ and $\vec{c}/2)$, ...etc for tetragonal and cubic lattices
n	'diagonal' glide plane			$(\vec{a}+\vec{b})/2$ or $(\vec{b}+\vec{c})/2$ or $(\vec{a}+\vec{c})/2$; OR $(\vec{a}\pm\vec{b}\pm\vec{c})/2$ for tetragonal and cubic lattices
d	'diamond' glide plane		$\frac{1}{8}$ $\frac{3}{8}$	$(\vec{a}\pm\vec{b})/4$ or $(\vec{b}\pm\vec{c})/4$ or $(\vec{c}\pm\vec{a})/4$; OR $(\pm\vec{a}\pm\vec{b}\pm\vec{c})/4$ for tetragonal and cubic lattices

https://en.wikipedia.org/wiki/Hermann%E2%80%93Mauguin_notation https://doi.org/10.1002/adfm.201505

Space Group $P6_3cm$: Multiplication Table

D_6 Group

	E	2_{1z}	3_z^+	3_z^-	6_{3z}^+	6_{3z}^-	$c(2x,x,z)$	$c(x,2x,z)$	$c(x,\bar{x},z)$	$m(x,x,z)$	$m(0,y,z)$	$m(x,0,z)$
E	E	2_{1z}	3_z^+	3_z^-	6_{3z}^+	6_{3z}^-	$c(2x,x,z)$	$c(x,2x,z)$	$c(x,\bar{x},z)$	$m(x,x,z)$	$m(0,y,z)$	$m(x,0,z)$
2_{1z}	2_{1z}	E	6_{3z}^-	6_{3z}^+	3_z^-	3_z^+	$m(0,y,z)$	$m(x,0,z)$	$m(x,x,z)$	$c(x,\bar{x},z)$	$c(2x,x,z)$	$c(x,2x,z)$
3_z^-	3_z^-	6_{3z}^+	E	3_z^+	6_{3z}^-	2_{1z}	$c(x,\bar{x},z)$	$c(2x,x,z)$	$c(x,2x,z)$	$m(x,0,z)$	$m(x,x,z)$	$m(0,y,z)$
3_z^+	3_z^+	6_{3z}^-	3_z^-	E	2_{1z}	6_{3z}^+	$c(x,2x,z)$	$c(x,\bar{x},z)$	$c(2x,x,z)$	$m(0,y,z)$	$m(x,0,z)$	$m(x,x,z)$
6_{3z}^-	6_{3z}^+	3_z^+	6_{3z}^+	2_{1z}	E	3_z^-	$m(x,0,z)$	$m(x,x,z)$	$m(0,y,z)$	$c(2x,x,z)$	$c(2x,x,z)$	$c(x,\bar{x},z)$
6_{3z}^+	6_{3z}^-	3_z^-	2_{1z}	6_{3z}^-	3_z^+	E	$m(x,x,z)$	$m(0,y,z)$	$m(x,0,z)$	$c(x,2x,z)$	$c(x,\bar{x},z)$	$c(2x,x,z)$
$c(2x,x,z)$	$c(2x,x,z)$	$m(0,y,z)$	$c(x,\bar{x},z)$	$c(x,2x,z)$	$m(x,0,z)$	$m(x,x,z)$	E	3_z^-	3_z^+	6_{3z}^-	2_{1z}	6_{3z}^+
$c(x,2x,z)$	$c(x,2x,z)$	$m(x,0,z)$	$c(2x,x,z)$	$c(x,\bar{x},z)$	$m(x,x,z)$	$m(0,y,z)$	3_z^+	E	3_z^-	6_{3z}^+	6_{3z}^-	2_{1z}
$c(x,\bar{x},z)$	$c(x,\bar{x},z)$	$m(x,x,z)$	$c(x,2x,z)$	$c(2x,x,z)$	$m(0,y,z)$	$m(x,0,z)$	3_z^-	3_z^+	E	2_{1z}	6_{3z}^+	6_{3z}^-
$m(x,x,z)$	$m(x,x,z)$	$c(x,\bar{x},z)$	$m(x,0,z)$	$m(0,y,z)$	$c(2x,x,z)$	$c(x,2x,z)$	6_{3z}^+	6_{3z}^-	2_{1z}	E	3_z^-	3_z^+
$m(0,y,z)$	$m(0,y,z)$	$c(2x,x,z)$	$m(x,x,z)$	$m(x,0,z)$	$c(x,2x,z)$	$c(x,\bar{x},z)$	2_{1z}	6_{3z}^+	6_{3z}^-	3_z^+	E	3_z^-
$m(x,0,z)$	$m(x,0,z)$	$c(x,2x,z)$	$m(0,y,z)$	$m(x,x,z)$	$c(x,\bar{x},z)$	$c(2x,x,z)$	6_{3z}^-	2_{1z}	6_{3z}^+	3_z^-	3_z^+	E

http://www.math.niu.edu/~beachy/aaol/grouptables2.html

Space Group $P6_3cm$: Character Table

	E	2_{1z}	$3_z^+, 3_z^-$	$6_{3z}^+, 6_{3z}^-$	$c(2x,x,z)$, $c(x,2x,z)$, $c(x,\bar{x},z)$	$m(x,x,z)$ $m(0,y,z)$ $m(x,0,z)$
Γ_1	**1**	1	1	1	**1**	**1**
Γ_2	1	1	1	1	**-1**	**−1**
Γ_3	1	−1	**1**	−1	**1**	**-1**
Γ_4	1	−1	1	−1	**−1**	**1**
Γ_5	2	−2	−2	2	**0**	**0**
Γ_6	2	2	−2	−2	**0**	**0**

$12=1 + 1 + 1 + 1 + 2^2 + 2^2$

http://symmetry.jacobs-university.de/cgi-bin/group.cgi?group=306&option=4

Space Group $P6_3cm$: Irreducible Representations

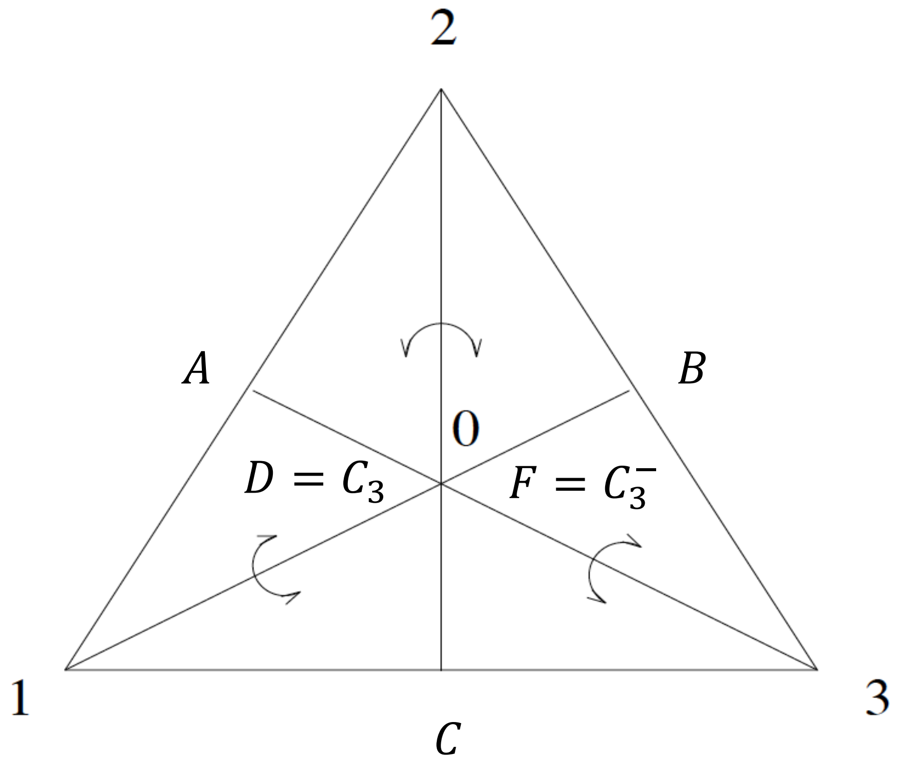
KV	h_1	$h_2/(\boldsymbol{\tau}^a)$	h_3	$h_4/(\boldsymbol{\tau})$	h_5	$h_6/(\boldsymbol{\tau})$	$h_{19}/(\boldsymbol{\tau})$	h_{20}	$h_{21}/(\boldsymbol{\tau})$	h_{22}	$h_{23}/(\boldsymbol{\tau})$	h_{24}
IT	1	6^+_{3z}	3^+_z	2_{1z}	3^-_z	6^-_{3z}	$c(2x,x,z)$	$m(x,x,z)$	$c(x,2x,z)$	$m(0,y,z)$	$c(x,\bar{x},z)$	$m(x,0,z)$
Pos.	x	$x-y$	$\bar{y}$	$\bar{x}$	$\bar{x}+y$	y	x	y	$\bar{x}+y$	$\bar{x}$	$\bar{y}$	$x-y$
	y	x	$x-y$	$\bar{y}$	$\bar{x}$	$\bar{x}+y$	$x-y$	x	y	$\bar{x}+y$	$\bar{x}$	$\bar{y}$
	z	$z+\frac{1}{2}$	z	$z+\frac{1}{2}$	z	$z+\frac{1}{2}$	$z+\frac{1}{2}$	z	$z+\frac{1}{2}$	z	$z+\frac{1}{2}$	z
Γ_1	1	1	1	1	1	1	1	1	1	1	1	1
Γ_2	1	1	1	1	1	1	-1	-1	-1	-1	-1	-1
Γ_3	1	-1	1	-1	1	-1	1	-1	1	-1	1	-1
Γ_4	1	-1	1	-1	1	-1	-1	1	-1	1	-1	1
Γ_5	I	B_1	$-B_2$	$-I$	$-B_1$	B_2	A	C_1	$-C_2$	$-A$	$-C_1$	C_2
Γ_6	I	$-B_1$	$-B_2$	I	$-B_1$	$-B_2$	A	$-C_1$	$-C_2$	A	$-C_1$	$-C_2$

Where: $I=\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$ $A=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$ $B_1=\begin{pmatrix}\omega & 0\\ 0 & \omega^\star\end{pmatrix}$ $B_2=\begin{pmatrix}\omega^\star & 0\\ 0 & \omega\end{pmatrix}$ $C_1=\begin{pmatrix}0 & \omega\\ \omega^\star & 0\end{pmatrix}$ $C_2=\begin{pmatrix}0 & \omega^\star\\ \omega & 0\end{pmatrix}$

$$\boldsymbol{\tau} = (0\ 0\ 1/2),\ \boldsymbol{\omega} = \boldsymbol{e}^{i\frac{\pi}{3}}$$

https://journals.aps.org/prb/abstract/10.1103/PhysRevB.62.9498

Fundamentals of Group Theory: Definitions



$$G = \{g|f(g) = R\}$$

$R :=$

(1) Closedness (relative to multiplication):

$\forall g_1,\ g_2 \in G, \qquad g_3 = g_1 g_2 \in G$

(2) Associativity:

$\forall g_1,\ g_2, g_3 \in G, \quad (g_1 g_2) g_3 = g_1 (g_2 g_3)$

(3) Identity e:

$\exists e \in G, \forall g \in G,\ ge = eg = g$

(4) Inverse:

$\forall g \in G, \exists g^{-1} \in G, g g^{-1} = g^{-1} g = e$

$$F_G := \{F(G)|R\}$$

D_3	E	A	B	C	D	F
E	E	A	B	C	D	F
A	A	E	D	F	B	C
B	B	F	E	D	C	A
C	C	D	F	E	A	B
D	D	C	A	B	F	E
F	F	B	C	A	E	D

F_G	**Order:**N_G	**Subgroup *H***	**Conjugation and Class**
Definition	Number of Elements	$\boldsymbol{H} \subseteq \boldsymbol{G}$ $f(H) = R$	$\forall g \in G, g_1 = g g_2 g^{-1};$ $C_{g_1} := \{g_2 \vert g g_1 g^{-1}, \forall g \in G\}$
D_3	6	$\{E\}, \{E, D, F\},$ $\{E, A\}, \{E, B\},$ $\{E, C\}$	$\{E\}, \{A, B, C\},$ $\{D, F\},$

Fundamentals of Group Theory: Definitions

$F_G := \{F(G)|R\}$

$\boldsymbol{D_3}$ $\boldsymbol{M(D_3)}$

$E \quad \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$

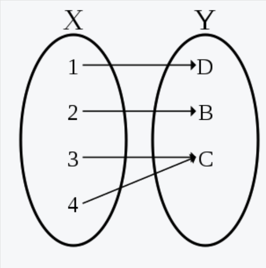
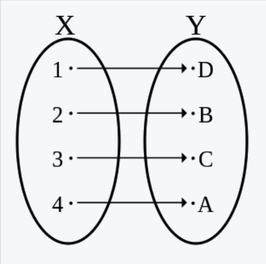
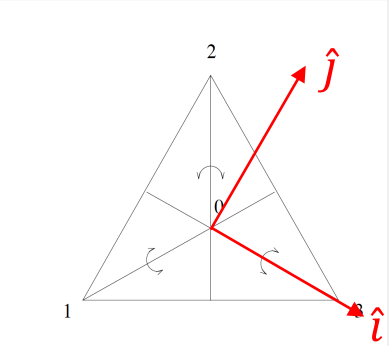
$A \quad \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$

$B \quad \begin{bmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{bmatrix}$

$C \quad \begin{bmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} \end{bmatrix}$

$D \quad \begin{bmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{bmatrix}$

$F \quad \begin{bmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{bmatrix}$

F_G	**Homomorphic && Isomorphic** $m(G) = G'$ **If** $g_3 = g_1\, g_2$ $m(g_3) = m(g_1)\mathrm{m}(g_2)$	**(Unitary)Representation and Representation Space, Basis: reducible& irreducible**	**Character of Group**
Definition	Homomorphic(surjection): $m^{-1}(G') \neq G$ Isomorphic(bijection): $m^{-1}(G') = G$  **surjective-only**  **bijective**	Vector Space $V = \{\alpha_i b_i \| \alpha_i \in R\ or\ C\}$ $\forall g \in G, g b_i = b_j M_{ji}(g), G \to M(G)$ If $b_i \cdot b_j = \delta_{ij}, M^{-1}(G) = M^{\dagger}(G)$ $UM(G)U^{-1} = \Lambda(G)$ $= \begin{bmatrix} D_1(G) & 0 & 0 \\ 0 & D_2(G) & 0 \\ 0 & 0 & D_3(G) \end{bmatrix}$	$\chi(G) = Tr(M(G))$ $\chi(C)$
D_3	$D_3 \to M(D_3)$	 	$\chi(M(E)) = 2;$ $\chi(M(A)) = \chi(M(B))$ $= \chi(M(C)) = 0;$ $\chi(M(D)) = \chi(M(F)) =$ $-1;$

$$
\begin{array}{cccc}
 & E & A & B \\
\Gamma_1 : & (1) & (1) & (1) \\
\Gamma_{1'} : & (1) & (-1) & (-1) \\
\Gamma_2 : & \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} & \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} & \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix} \\
 & C & D & F \\
\Gamma_1 : & (1) & (1) & (1) \\
\Gamma_{1'} : & (-1) & (1) & (1) \\
\Gamma_2 : & \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix} & \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} & \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}
\end{array}
$$

$$
\begin{array}{cccc}
 & E & A & B \\
\Gamma_R : & \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} & \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} & \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ 0 & 0 & \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}
\end{array}
$$

$$
\Gamma_R = \left(\begin{array}{c|c|c} \Gamma_1 & 0 & \mathcal{O} \\ \hline 0 & \Gamma_{1'} & \mathcal{O} \\ \hline \mathcal{O} & \mathcal{O} & \Gamma_2 \end{array}\right)
$$

$$
U\Gamma_R U^{-1} = \Gamma_1 + \Gamma_{1'} + \Gamma_2
$$

Unique

For finite group, all irreducible representations $D(G)$ are unitary representation, i.e., irreducible basis is orthonormal

Fundamentals of Group Theory: Theorems

1. Rearrangement Theorems: $G = \{g_1, \ g_2, g_3, \dots, g_n\}$ $\quad gG = \{gg_1, \ gg_2, gg_3, \dots, gg_n\}$ $\quad \forall g \in G$

$$G = gG$$

2. Orthogonality Theorems for irreducible representations

Γ_1, Γ_2 are two inequivalent irreducible representations

l_1, l_2 are their dimensions

$$\sum_g D^{(l_2)}_{\mu\nu}(g) D^{(l_1)}_{\nu'\mu'}(g^{-1}) = \frac{N_G}{l_1} \delta_{\Gamma_1\Gamma_2} \delta_{\mu\mu'} \delta_{\nu\nu'}$$

3. Orthogonality Theorems for irreducible representations

$$\sum_g \chi^{(l_2)}(g) \chi^{(l_1)}(g^{-1}) = N_G \delta_{\Gamma_1\Gamma_2} \qquad \sum_{C_k} N_k \chi^{(l_2)}(C_k) \chi^{*(l_1)}(C_k) = N_G \delta_{\Gamma_1\Gamma_2}$$

$\{\chi^{(l_j)}(C_k)\}$

$n_C = n_\Gamma$

$$\sum_{\Gamma_j} N_k \chi^{(l_j)}(C_k) \chi^{*(l_j)}(C_{k'}) = N_G \delta_{kk'}$$