राष्ट्रीय प्रौद्योगिकी संस्थान राउरकेला

National Institute of Technology Rourkela

MaThCryst

INTERNATIONAL SCHOOL ON FUNDAMENTAL CRYSTALLOGRAPHY AND WORKSHOP ON STRUCTURAL PHASE TRANSITIONS

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ICTP The Abdus Salam International Centre for Theoretical Physics

IUCr

SERB INDIA

Indian National Science Academy

ROURKELA INTERNATIONAL CRYSTALLOGRAPHY SCHOOL

REPRESENTATIONS OF CRYSTALLOGRAPHIC GROUPS IV

DATABASES AND TOOLS OF THE BILBAO CRYSTALLOGRAPHIC SERVER

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BILBAO CRYSTALLOGRAPHIC SERVER

Space Groups Retrieval Tools

GENPOS	Generators and General Positions of Space Groups
WYCKPOS	Wyckoff Positions of Space Groups
HKLCOND	Reflection conditions of Space Groups
MAXSUB	Maximal Subgroups of Space Groups
SERIES	Series of Maximal Isomorphic Subgroups of Space Groups
WYCKSETS	Equivalent Sets of Wyckoff Positions
NORMALIZER	Normalizers of Space Groups
KVEC	The k-vector types and Brillouin zones of Space Groups
SYMMETRY OPERATIONS	Geometric interpretation of matrix column representations of symmetry operations
IDENTIFY GROUP	Identification of a Space Group from a set of generators in an arbitrary setting

Representation Theory Applications

REPRES	Space Groups Representations
Representations PG	Irreducible representations of the crystallographic Point Groups
Representations SG	Irreducible representations of the Space Groups
Get_irreps	Irreps and order parameters in a space group-subgroup phase transition
Get_mirreps	Irreps and order parameters in a paramagnetic space group-magnetic subgroup phase transition
DIRPRO	Direct Products of Space Group Irreducible Representations
CORREL	Correlations relations between the irreducible representations of a group-subgroup pair
POINT	Point Group Tables
SITESYM	Site-symmetry induced representations of Space Groups
COMPATIBILITY RELATIONS	Compatibility relations between the irreducible representations of a space group

Databases of Representations

Representations of space and point groups

wave-vector data

Brillouin zones
representation domains
parameter ranges

POINT

character tables
multiplication tables
symmetrized products

Retrieval tools

Database on Representations of Point Groups

group-subgroup relations

Point Group Tables of C_{6v}(6mm)

Character Table

C_{6v}(6mm)	#	1	2	3	6	m_d	m_v	functions
Mult.	-	1	1	2	2	3	3	.
A_1	Γ_1	1	1	1	1	1	1	z,x^2+y^2,z^2
A_2	Γ_2	1	1	1	1	-1	-1	J_z
B_1	Γ_3	1	-1	1	-1	1	-1	.
B_2	Γ_4	1	-1	1	-1	-1	1	.
E_2	Γ_6	2	2	-1	-1	0	0	(x^2-y^2,xy)
E_1	Γ_5	2	-2	-1	1	0	0	$(x,y),(xz,yz),(J_x,J_y)$

[List of irreducible representations in matrix form]

The Rotation Group D(L)

L	2L+1	A_1	A_2	B_1	B_2	E_2	E_1
0	1	1	.	.	.	.	.
1	3	1	.	.	.	.	1
2	5	1	.	.	.	1	1
3	7	1	.	1	1	1	1
4	9	1	.	1	1	2	1
5	11	1	.	1	1	2	2
6	13	2	1	1	1	2	2
7	15	2	1	1	1	2	3
8	17	2	1	1	1	3	3
9	19	2	1	2	2	3	3
10	21	2	1	2	2	4	3

Point Subgroups

Subgroup	Order	Index
6mm	12	1
6	6	2
3m	6	2
3	3	4
mm2	4	3
2	2	6
m	2	6
1	1	12

character tables
matrix representations
basis functions

Direct (Kronecker) products of representations

Point-group Database

Multiplication Table

C_{6v}(6mm)	A_1	A_2	B_1	B_2	E_2	E_1
A_1	A_1	A_2	B_1	B_2	E_2	E_1
A_2	.	A_1	B_2	B_1	E_2	E_1
B_1	.	.	A_1	A_2	E_1	E_2
B_2	.	.	.	A_1	E_1	E_2
E_2	.	.	.	.	$A_1+A_2+E_2$	$B_1+B_2+E_1$
E_1	.	.	.	.	.	$A_1+A_2+E_2$

Symmetrized Products of Irreps

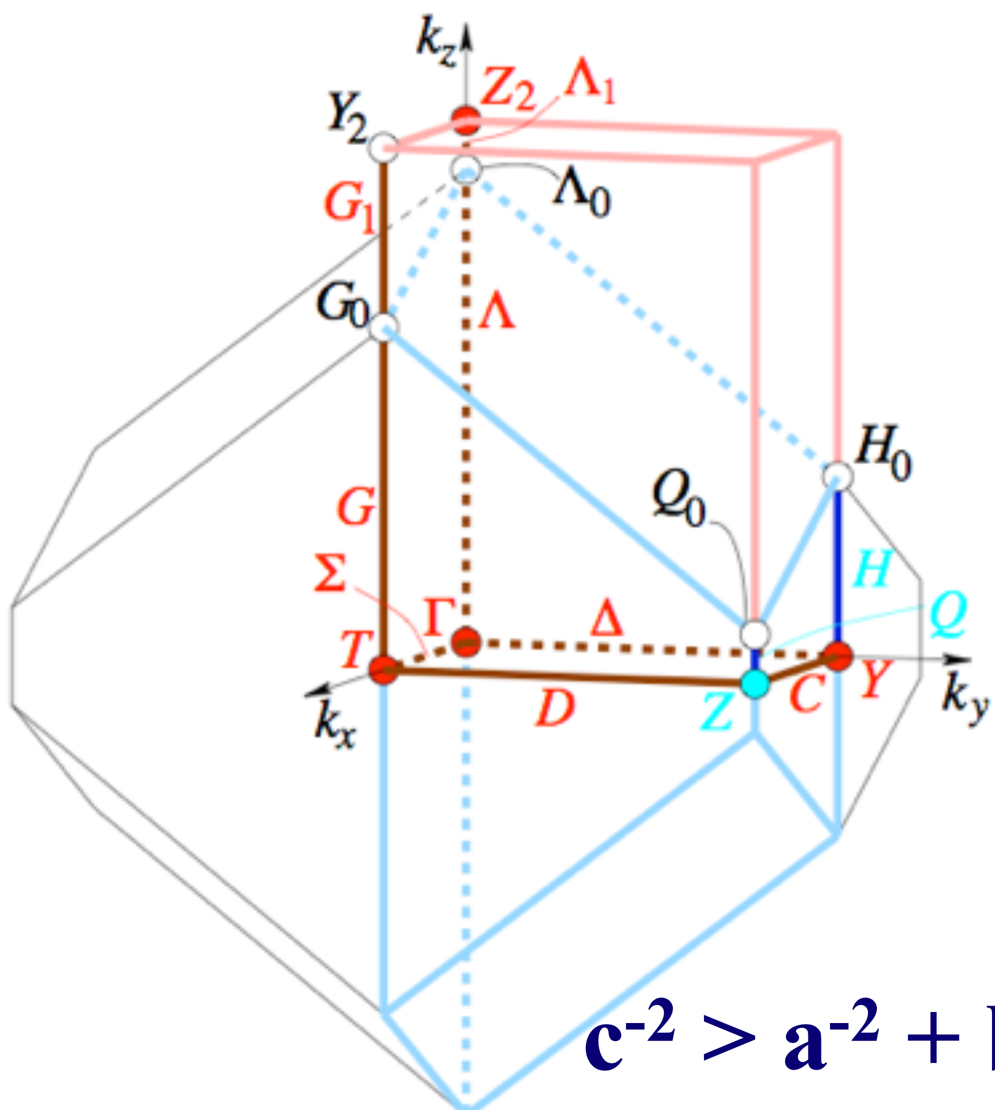
C_{6v}(6mm)	A_1	A_2	B_1	B_2	E_2	E_1
$[A_1 \times A_1]$	1	.	.	.	.	.
$[A_2 \times A_2]$	1	.	.	.	.	.
$[B_1 \times B_1]$	1	.	.	.	.	.
$[B_2 \times B_2]$	1	.	.	.	.	.
$[E_2 \times E_2]$	1	.	.	.	1	.
$[E_1 \times E_1]$	1	.	.	.	1	.

Irreps Decompositions

C_{6v}(6mm)	A_1	A_2	B_1	B_2	E_2	E_1
V	1	.	.	.	.	1
$[V^2]$	2	.	.	.	1	1
$[V^3]$	2	.	1	1	1	2
$[V^4]$	3	.	1	1	3	2
A	.	1	.	.	.	1
$[A^2]$	2	.	.	.	1	1
$[A^3]$	.	2	1	1	1	2
$[A^4]$	3	.	1	1	3	2
$[V^2]\text{x}V$	3	1	1	1	2	4
$[[V^2]^2]$	5	.	1	1	4	3
$\{V^2\}$	.	1	.	.	.	1
$\{A^2\}$	.	1	.	.	.	1
$\{[V^2]^2\}$	1	2	1	1	2	3

Brillouin Zone Database
Crystallographic Approach

Reciprocal space groups		Symmorphic space groups
Brillouin zones	↔	IT unit cells
Representation domain		Asymmetric unit
Wave-vector symmetry		Wyckoff positions



$$c^{-2} > a^{-2} + b^{-2}$$

The k-vector Types of Group 22 [*F*222]

k-vector description			Wyckoff Position			ITA description
CDML*		Conventional-ITA	ITA			Coordinates
Label	Primitive					
GM	0,0,0	0,0,0	a	2	222	0,0,0
T	1,1/2,1/2	0,1,1	b	2	222	0,1/2,1/2
T~T$_2$			b	2	222	1/2,0,0
Z	1/2,1/2,0	0,0,1	c	2	222	0,0,1/2
Y	1/2,0,1/2	0,1,0	d	2	222	0,1/2,0
Y~Y$_2$			d	2	222	1/2,0,1/2
SM	0,u,u ex	2u,0,0	e	4	2..	x,0,0 : 0 < x <= sm$_0$
U	1,1/2+u,1/2+u ex	2u,1,1	e	4	2..	x,1/2,1/2 : 0 < x < u$_0$
U~SM$_1$=[SM$_0$ T$_2$]			e	4	2..	x,0,0 : 1/2-u$_0$=sm$_0$ < x < 1/2
SM+SM$_1$=[GM T$_2$]			e	4	2..	x,0,0 : 0 < x < 1/2
A	1/2,1/2+u,u ex	2u,0,1	f	4	2..	x,0,1/2 : 0 < x <= a$_0$
C	1/2,u,1/2+u ex	2u,1,0	f	4	2..	x,1/2,0 : 0 < x < c$_0$

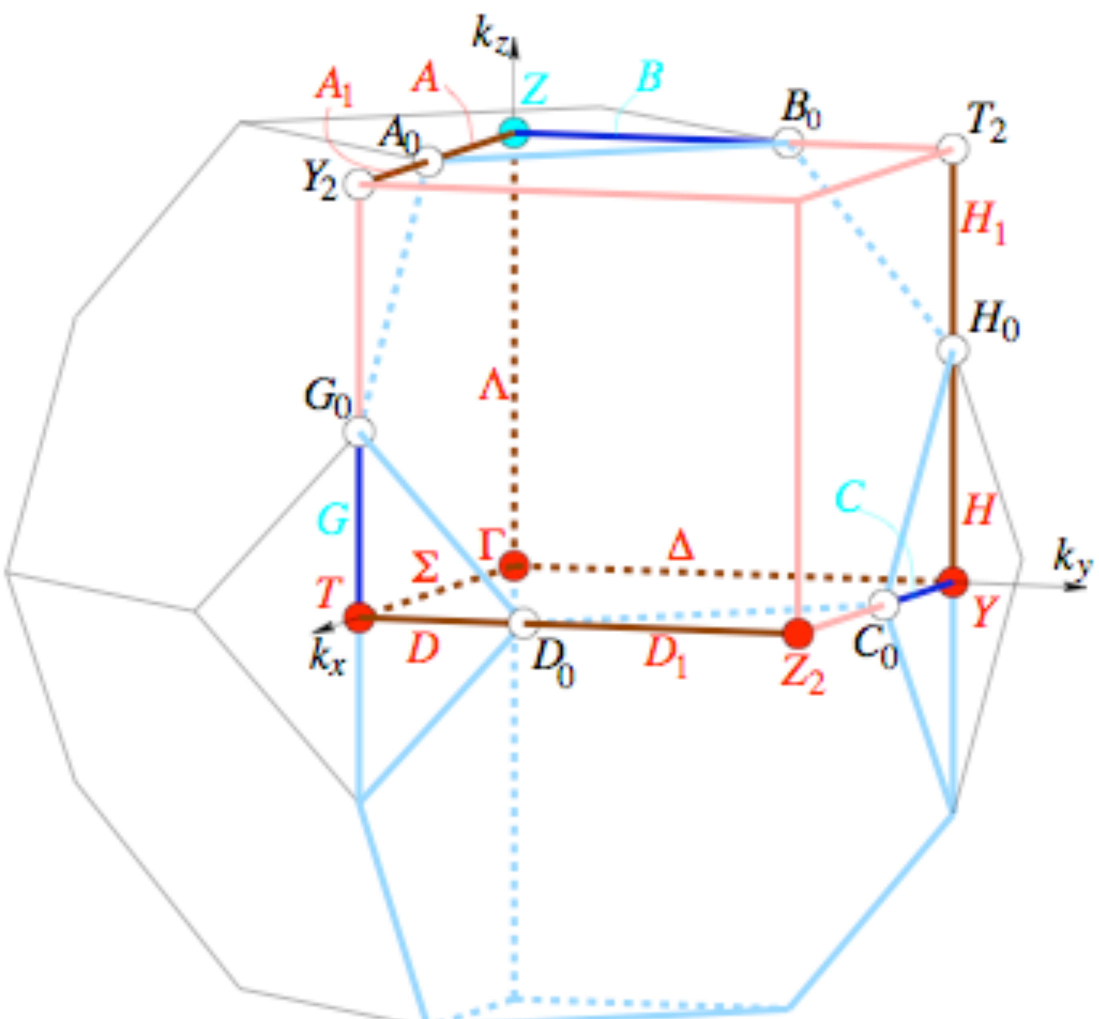
Example:

Brillouin zone Database

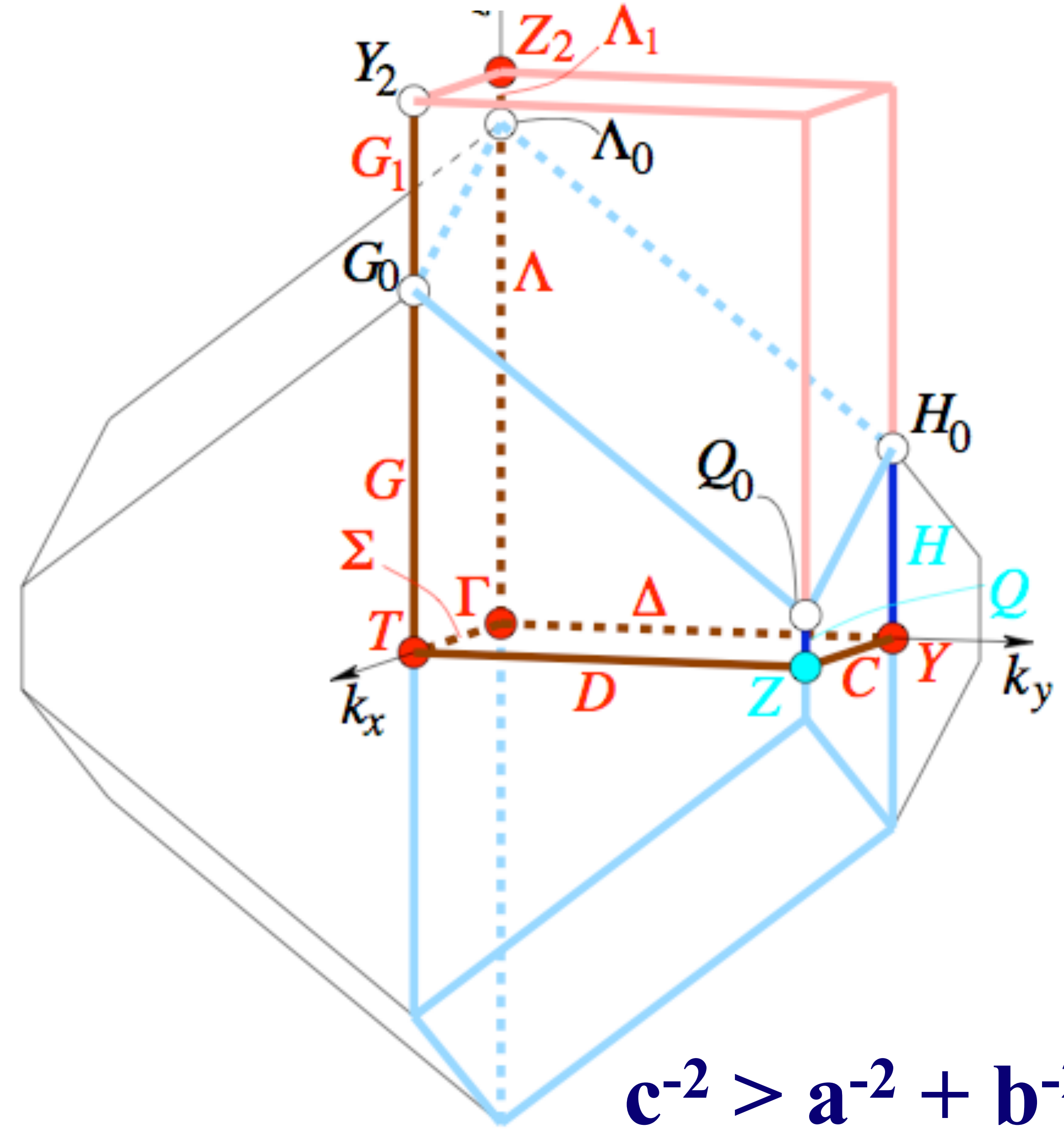
The k-vector Types of Group 22 [*F*222]

Brillouin zone

(Diagram for arithmetic crystal class 222F)

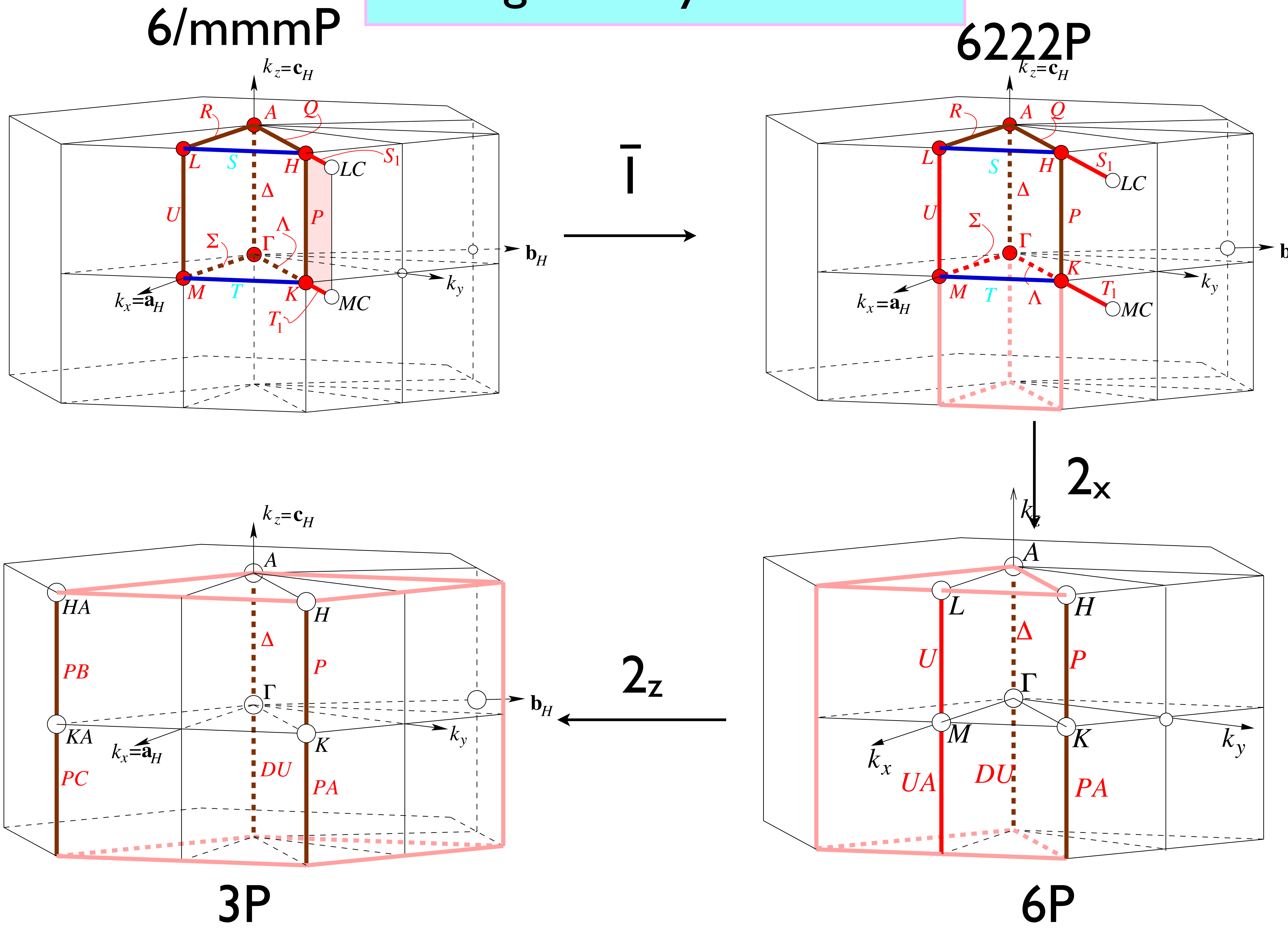


$c^{-2} < a^{-2} + b^{-2}$



$c^{-2} > a^{-2} + b^{-2}$

Hexagonal crystal classes



PROCEDURE FOR THE CONSTRUCTION OF SPACE-GROUP REPRESENTATIONS

Procedure for the construction of the irreps of space groups.

1. space-group information

(a) Decomposition of the space group $\mathcal{G}$ in cosets relative to its translation subgroup $\mathcal{T}$, see IT A (1996)

$$\mathcal{G} = \mathcal{T} \cup (\mathbf{W}_2, \mathbf{w}_2)\,\mathcal{T} \cup \ \ldots \ \cup (\mathbf{W}_p, \mathbf{w}_p)\,\mathcal{T}$$

(b) Choice of a convenient set of generators of $\mathcal{G}$, see IT A (1996)

2. k-vector information

(a) $\mathbf{k}$ vector from the representation domain of the BZ

(b) Little co-group $\overline{\mathcal{G}}^{\mathbf{k}}$ of $\mathbf{k}$:

$$\overline{\mathcal{G}}^{\mathbf{k}} = \{\widetilde{\mathbf{W}}_i \in \overline{\mathcal{G}} : \ \mathbf{k} = \mathbf{k}\,\widetilde{\mathbf{W}}_i + \mathbf{K}, \ \mathrm{k} \in \mathbf{L}^*\}$$

(c) $\mathbf{k}$-vector star $\star(\mathbf{k})$

$\star(\mathbf{k}) = \{\mathbf{k}, \mathbf{k}_2, \ldots, \mathbf{k}_s\}$, with $\mathbf{k} = \mathbf{k}\,\overline{\mathbf{W}}_j$, $j = 1, \ldots s$, where $\overline{W}_j$ are the coset representatives of $\overline{\mathcal{G}}$ relative to $\overline{\mathcal{G}}^{\mathbf{k}}$.

(d) Determination of the little group $\mathcal{G}^{\mathbf{k}}$

$$\mathcal{G}^{\mathbf{k}} = \{(\widetilde{\mathbf{W}}_i, \widetilde{\mathbf{w}}_i) \in \mathcal{G} : \widetilde{\mathbf{W}}_i \in \overline{\mathcal{G}}\}$$

3. Allowed (small) irreps of $\mathcal{G}^{\mathbf{k}}$

(a) If $\mathcal{G}^{\mathbf{k}}$ is a symmorphic space group or $\mathbf{k}$ is inside the BZ, then the non-equivalent allowed irreps $\mathbf{D}^{\mathbf{k},i}$ of $\mathcal{G}^{\mathbf{k}}$ are related to the non-equivalent irreps $\overline{\mathbf{D}}^{\mathbf{k},i}$ of $\overline{\mathcal{G}}^{\mathbf{k}}$ in the following way:

$$\mathbf{D}^{\mathbf{k},i}(\widetilde{\mathbf{W}}_i, \widetilde{\mathbf{w}}_i) = \exp -(i\,\mathbf{k}\,\mathbf{w}_i)\,\overline{\mathbf{D}}^{\mathbf{k},i}(\widetilde{\mathbf{W}}_i)$$

(b) If $\mathcal{G}^{\mathbf{k}}$ is a non-symmorphic space group and $\mathbf{k}$ is on the surface of the BZ, then:

i. Look for a symmorphic subgroup $\mathcal{H}_0^{\mathbf{k}}$ (or an appropriate chain of normal subgroups) of index 2 or 3

ii. Find the allowed irreps $\mathbf{D}_{\mathcal{H}_0}^{\mathbf{k}\,i}$ of $\mathcal{H}_0^{\mathbf{k}}$, *i. e.* those for which is fulfilled $\mathbf{D}_{\mathcal{H}_0}^{\mathbf{k},i}(\mathbf{I},\mathbf{t}) = \exp -(i\,\mathbf{k},\mathbf{t})\,\mathbf{I}$ and distribute them into orbits relative to $\mathcal{G}^{\mathbf{k}}$

iii. Determine the allowed irrpes of $\mathcal{G}^{\mathbf{k}}$ using the results for the induction from the irreps of normal subgroups of index 2 or 3

Induction procedure

4. Induction procedure for the construction of the irreps $\mathbf{D}^{\star\mathbf{k},i}$ of $\mathcal{G}$ from the allowed irreps $\mathbf{D}^{\mathbf{k},i}$ of $\mathcal{G}$
The representation matrices of $\mathbf{D}^{\star\mathbf{k},i}(\mathcal{G})$ for any element of $\mathcal{G}$ can be obtained if the matrices for the generators $\{(\mathbf{W}_l, \mathbf{w}_l),\ l = 1, \ldots, k\}$ of $\mathcal{G}$ are available (step 1a).

$$\boldsymbol{D}^{Ind}(g) = \boldsymbol{M}(g) \otimes \boldsymbol{D}^{(j)}(h)$$

subgroup irrep matrix

induction matrix

EXERCISES

Problem 1.

Consider the **k**-vectors Γ(000) and **X** (0½0) of the group ***P4mm***

(i) Determine the little groups, the **k**-vector stars, the number and the dimensions of the little-group irreps, the number and the dimensions of the corresponding irreps of the group ***P4mm***

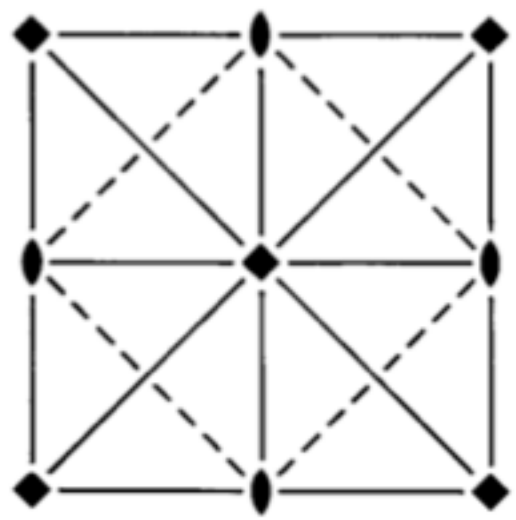
(ii) Calculate a set of coset representatives of the decomposition of the group ***P4mm*** with respect to the little group of the **k**-vectors Γ(000) and **X**, and construct the corresponding full space group irreps of ***P4mm***

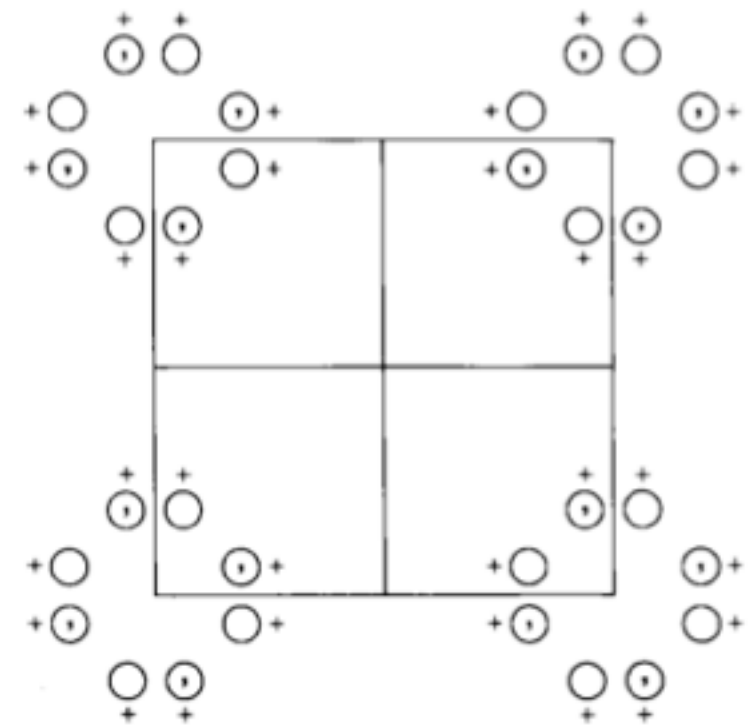
International Tables for Crystallography (2006). Vol. A, Space group 99, pp. 382–383.

$P4mm$ C_{4v}^{1} $4mm$ Tetragonal

No. 99 $P4mm$ Patterson symmetry $P4/mmm$

ITA space-group data (selection)





Origin on $4mm$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le 1$; $x \le y$

Symmetry operations

(1) 1	(2) 2 $0,0,z$	(3) 4^+ $0,0,z$	(4) 4^- $0,0,z$
(5) m $x,0,z$	(6) m $0,y,z$	(7) m $x,\bar{x},z$	(8) m x,x,z

General position

(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$
(5) $x,\bar{y},z$	(6) $\bar{x},y,z$	(7) $\bar{y},\bar{x},z$	(8) y,x,z

5.5 Crystal class $4mm$

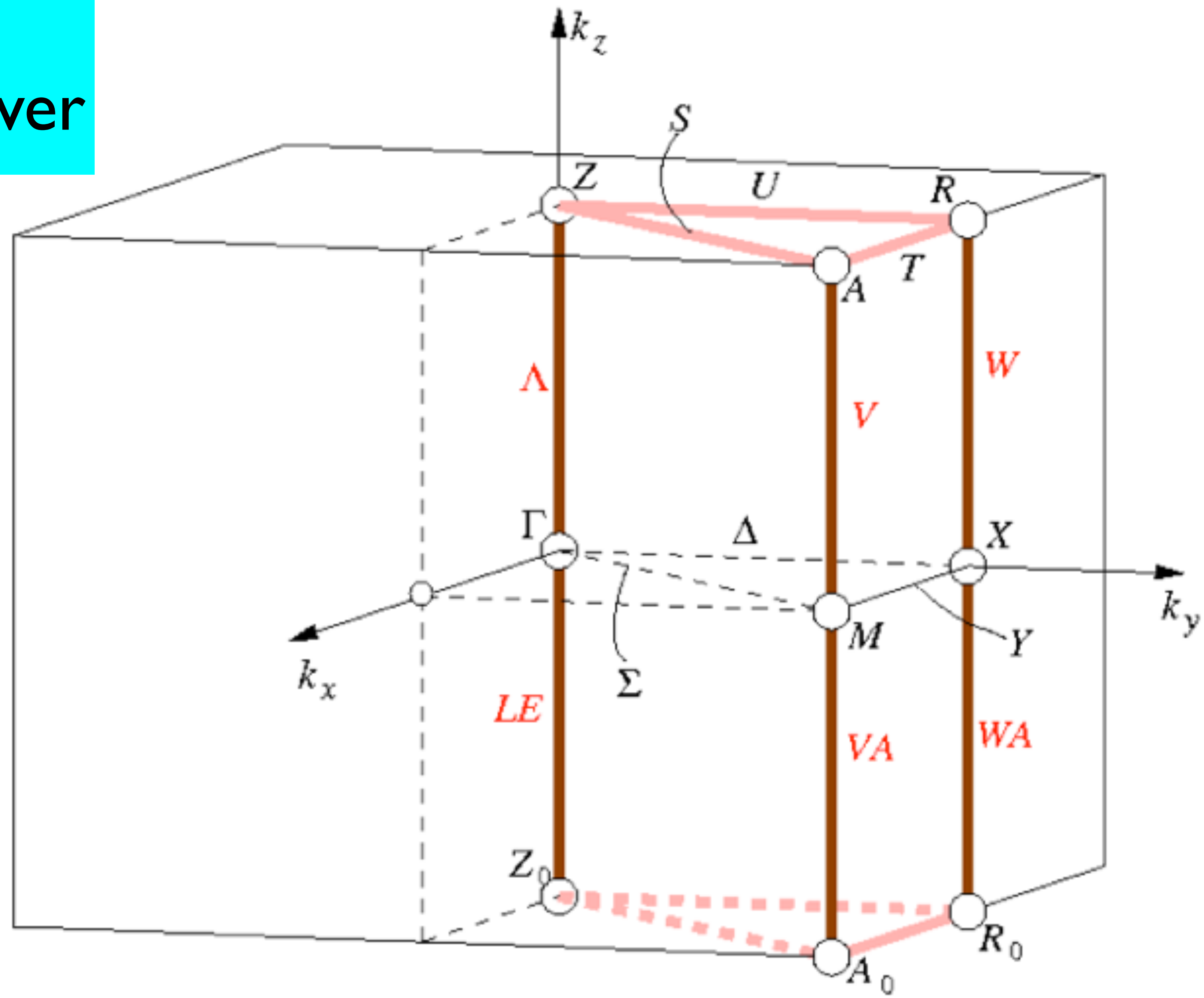
5.5.1 Arithmetic crystal class $4mmP$

Fig. 5.5.1.1 Diagram for arithmetic crystal class $4mmP$

$P4mm - C_{4v}^1$ (99) to $P4_2bc - C_{4v}^8$ (106)

Reciprocal-space group $(P4mm)^*$, No. 99 see Tab. 5.5.1.1

Brillouin Zone Database BilbaoCrystServer



SOLUTION

Problem 1

Irreps of P4mm, Γ(000) and X(01/20)

1. Space-group information

(a) Decomposition of *P4mm* relative to its translation subgroup;

coset representatives from IT A (1996):

$(\mathbf{1},\mathbf{o}), (\mathbf{2}_z,\mathbf{o}), (\mathbf{4},\mathbf{o}), (\mathbf{4}^{-1},\mathbf{o}),$
$(\mathbf{m}_{yz},\mathbf{o}), (\mathbf{m}_{xz},\mathbf{o}), (\mathbf{m}_{x\bar{x}},\mathbf{o}), (\mathbf{m}_{xx},\mathbf{o})$

(b) generators of *P4mm* from IT A (1996)
$\mathbf{t}_1, \mathbf{t}_2, \mathbf{t}_3, (\mathbf{2}_z,\mathbf{o}), (\mathbf{4},\mathbf{o}), (\mathbf{m}_{yz},\mathbf{o})$

2. $\vec{k}$-vector information

(a) X (0, 1/2, 0)

(b) little co-group $\overline{\mathcal{G}}^X = \{\mathbf{1},\ \mathbf{2}_z,\ \mathbf{m}_{yz},\ \mathbf{m}_{xz}\} = 2_z m_{yz} m_{xz}$

$$e.g.,\ X\,2_z = (0,\,1/2,\,0)\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix} = (0,\,-1/2,\,0) = (0,\,1/2,\,0) + (0,\,\bar{1},\,0)$$

And the little co-group of Γ(000)?

(c) $\vec{k}$-vector star: $\star X = \{(0, 1/2, 0), (1/2, 0, 0)\}$ coset representative of $\overline{G} = 4mm$ relative to $\overline{G}^{\mathbf{k}} = 2_z m_{yz} m_{xz}$, HM symbol $mm2$

$$4mm = 2_z m_{yz} m_{xz} \cup \mathbf{m}_{xx}\, 2_z m_{yz} m_{xz}$$

(d) little group $\mathcal{G}^X = P2_z m_{yz} m_{xz}$, HM symbol $Pmm2$

(e) decomposition of $P4mm$ relative to $P2_z m_{yz} m_{xz}$

$$P4mm = P2_z m_{yz} m_{xz} \cup (\mathbf{m}_{xx}, \mathbf{o}) P2_z m_{yz} m_{xz}$$

And for the point Γ(000)?

3. Allowed irreps of $\mathcal{G}^X$

Because $\mathcal{G}^X$ is a symmorphic group,

$$\mathbf{D}^{X,i}(\widetilde{W}_i,\,\tilde{w}_i) = \exp-(i\,\mathbf{X}\,\tilde{\mathbf{w}}_i)\,\overline{\mathbf{D}}^{X,i}(\widetilde{W}_i)$$

$P2_zmm$	$(\mathit{1},\,\boldsymbol{o})$	$(\mathit{2},\,\boldsymbol{o})$	$(\boldsymbol{m}_{yz},\,\boldsymbol{o})$	$(\boldsymbol{m}_{xz},\,\boldsymbol{o})$	$(\mathit{1},\,\boldsymbol{t})$
$\boldsymbol{D}^{X,1}$	1	1	1	1	$\exp-(i\,\mathbf{X}\,\mathbf{t})$
$\boldsymbol{D}^{X,2}$	1	1	-1	-1	$=\exp-(i\pi n_2)$
$\boldsymbol{D}^{X,3}$	1	-1	1	-1	$=(-1)^{n_2}$
$\boldsymbol{D}^{X,4}$	1	-1	-1	1	

$\boldsymbol{t}$ is the column of integer coefficients $(n_1,\,n_2,\,n_3)$

And for the point Γ(000)?

4. Induction procedure

Generators of $P4mm$: $\langle(\boldsymbol{W}_l, \boldsymbol{w}_l)\rangle = \langle(\boldsymbol{1}, \boldsymbol{t}_i), (\boldsymbol{4}, \boldsymbol{o}), (\boldsymbol{m}_{yz}, \boldsymbol{o})\rangle$

Representatives of $P2_z m_{yz} m_{xz}$ relative to $\mathcal{T}$:

$\{(\widetilde{W}_j, \widetilde{w}_j)\} = \{(\boldsymbol{1}, \boldsymbol{o}), (\boldsymbol{2}_z, \boldsymbol{o}), (\boldsymbol{m}_{yz}, \boldsymbol{o}), (\boldsymbol{m}_{xz}, \boldsymbol{o})\}$

Coset representatives of $P4mm$ relative to $P2_z m_{yz} m_{xz}$:

$\{q_1, q_2\} = \{(\boldsymbol{1}, \boldsymbol{o}), (\boldsymbol{m}_{xx}, \boldsymbol{o})\}$.

Induction matrix

$(\boldsymbol{W}_l, \boldsymbol{w}_l)$	q_i	q_i^{-1}	$q_i^{-1}(\boldsymbol{W}_l, \boldsymbol{w}_l)$	q_j	$q_i^{-1}(\boldsymbol{W}_l, \boldsymbol{w}_l)q_j = (\widetilde{W}_j, \widetilde{w}_j)$	$M_{ij} \neq 0$
$(\boldsymbol{1}, \boldsymbol{t})$	$(\boldsymbol{1}, \boldsymbol{o})$	$(\boldsymbol{1}, \boldsymbol{o})$	$(\boldsymbol{1}, \boldsymbol{t})$	$(\boldsymbol{1}, \boldsymbol{o})$	$(\boldsymbol{1}, \boldsymbol{t})$	11
	$(\boldsymbol{m}_{xx}, \boldsymbol{o})$	$(\boldsymbol{m}_{xx}, \boldsymbol{o})$	$(\boldsymbol{m}_{xx}, \boldsymbol{m}_{xx}\boldsymbol{t})$	$(\boldsymbol{m}_{xx}, \boldsymbol{o})$	$(\boldsymbol{1}, \boldsymbol{m}_{xx}\boldsymbol{t})$	22
$(\boldsymbol{m}_{yz}, \boldsymbol{o})$	$(\boldsymbol{1}, \boldsymbol{o})$	$(\boldsymbol{1}, \boldsymbol{o})$	$(\boldsymbol{m}_{yz}, \boldsymbol{o})$	$(\boldsymbol{1}, \boldsymbol{o})$	$(\boldsymbol{m}_{yz}, \boldsymbol{o})$	11
	$(\boldsymbol{m}_{xx}, \boldsymbol{o})$	$(\boldsymbol{m}_{xx}, \boldsymbol{o})$	$(\boldsymbol{4}^{-1}, \boldsymbol{o})$	$(\boldsymbol{m}_{xx}, \boldsymbol{o})$	$(\boldsymbol{m}_{xz}, \boldsymbol{o})$	22
$(\boldsymbol{4}, \boldsymbol{o})$	$(\boldsymbol{1}, \boldsymbol{o})$	$(\boldsymbol{1}, \boldsymbol{o})$	$(\boldsymbol{4}, \boldsymbol{o})$	$(\boldsymbol{m}_{xx}, \boldsymbol{o})$	$(\boldsymbol{m}_{yz}, \boldsymbol{o})$	12
	$(\boldsymbol{m}_{xx}, \boldsymbol{o})$	$(\boldsymbol{m}_{xx}, \boldsymbol{o})$	$(\boldsymbol{m}_{xz}, \boldsymbol{o})$	$(\boldsymbol{1}, \boldsymbol{o})$	$(\boldsymbol{m}_{xz}, \boldsymbol{o})$	21

(b) Matrices of the irreps $\mathbf{D}^{*X,\,i}$ of $\mathcal{G}$

$$\mathbf{D}^{*X,\,i}(\boldsymbol{1},\boldsymbol{t}) = \left(\begin{array}{c|c} \mathbf{D}^{X,\,i}(\boldsymbol{1},\boldsymbol{t}) & \boldsymbol{O} \\ \hline \boldsymbol{O} & \mathbf{D}^{X,\,i}(\boldsymbol{1},\boldsymbol{m}_{xx}\boldsymbol{t}) \end{array}\right);$$

$$\mathbf{D}^{*X,\,i}(\boldsymbol{m}_{yz},\,\boldsymbol{o}) = \left(\begin{array}{c|c} \mathbf{D}^{X,\,i}(\boldsymbol{m}_{yz},\,\boldsymbol{o}) & \boldsymbol{O} \\ \hline \boldsymbol{O} & \mathbf{D}^{X,\,i}(\boldsymbol{m}_{xz},\,\boldsymbol{o}) \end{array}\right)$$

$$\mathbf{D}^{*X,\,i}(\boldsymbol{4},\boldsymbol{o}) = \left(\begin{array}{c|c} \boldsymbol{O} & \mathbf{D}^{X,\,i}(\boldsymbol{m}_{yz},\,\boldsymbol{o}) \\ \hline \mathbf{D}^{X,\,i}(\boldsymbol{m}_{xz},\,\boldsymbol{o}) & \boldsymbol{O} \end{array}\right)$$

Table of irreps $\mathbf{D}^{*X,i}$ for the generators of $P4mm$ $\boldsymbol{t}$ =

	$(\boldsymbol{m}_{yz}, \boldsymbol{o})$	$(\boldsymbol{4}, \boldsymbol{o})$	$(\boldsymbol{1}, \boldsymbol{t})$
$\mathbf{D}^{*X,1}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} (-1)^{n_2} & 0 \\ 0 & (-1)^{n_1} \end{pmatrix}$
$\mathbf{D}^{*X,2}$	$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$	$\begin{pmatrix} (-1)^{n_2} & 0 \\ 0 & (-1)^{n_1} \end{pmatrix}$
$\mathbf{D}^{*X,3}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$	$\begin{pmatrix} (-1)^{n_2} & 0 \\ 0 & (-1)^{n_1} \end{pmatrix}$
$\mathbf{D}^{*X,4}$	$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} (-1)^{n_2} & 0 \\ 0 & (-1)^{n_1} \end{pmatrix}$

EXERCISES

Problem 1.

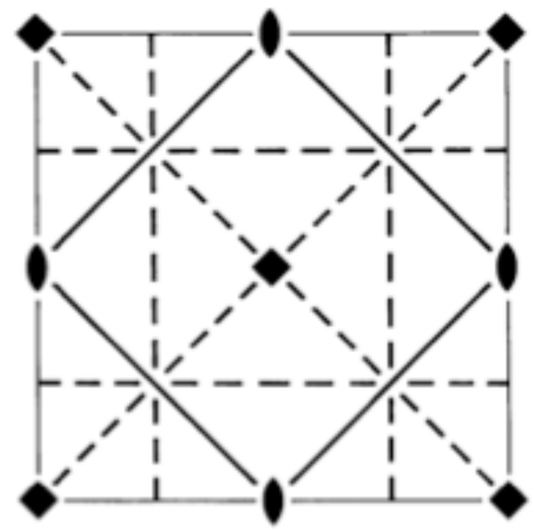
Consider the **k**-vectors Γ(000) and **X** (0½0) of the group ***P4bm***

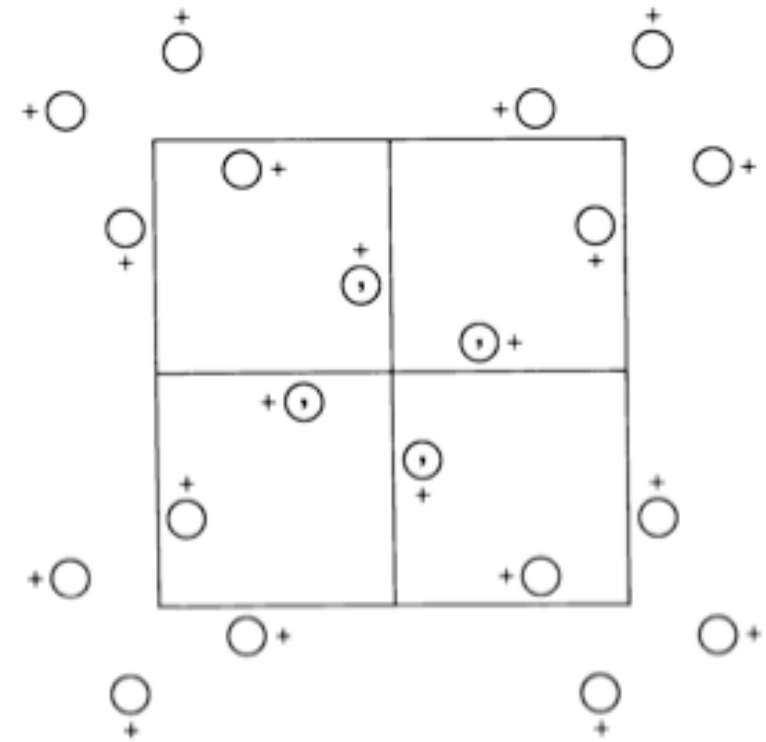
(i) Determine the little groups, the **k**-vector stars, the number and the dimensions of the little-group irreps, the number and the dimensions of the corresponding irreps of the group ***P4bm***

(ii) Calculate a set of coset representatives of the decomposition of the group ***P4bm*** with respect to the little group of the **k**-vectors Γ(000) and **X**, and construct the corresponding full space group irreps of ***P4bm***

$P4bm$ C_{4v}^{2} $4mm$

No. 100 $P4bm$ Patterson syı





Origin on $41g$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le 1$; $y \le \frac{1}{2} - x$

Symmetry operations

(1) 1	(2) 2 $0,0,z$	(3) 4^{+} $0,0,z$	(4) 4^{-} $0,0,z$
(5) a $x,\frac{1}{4},z$	(6) b $\frac{1}{4},y,z$	(7) m $x+\frac{1}{2},\bar{x},z$	(8) $g(\frac{1}{2},\frac{1}{2},0)$ x,x,z

General position

(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$
(5) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(6) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	(7) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	(8) $y+\frac{1}{2},x+\frac{1}{2},z$

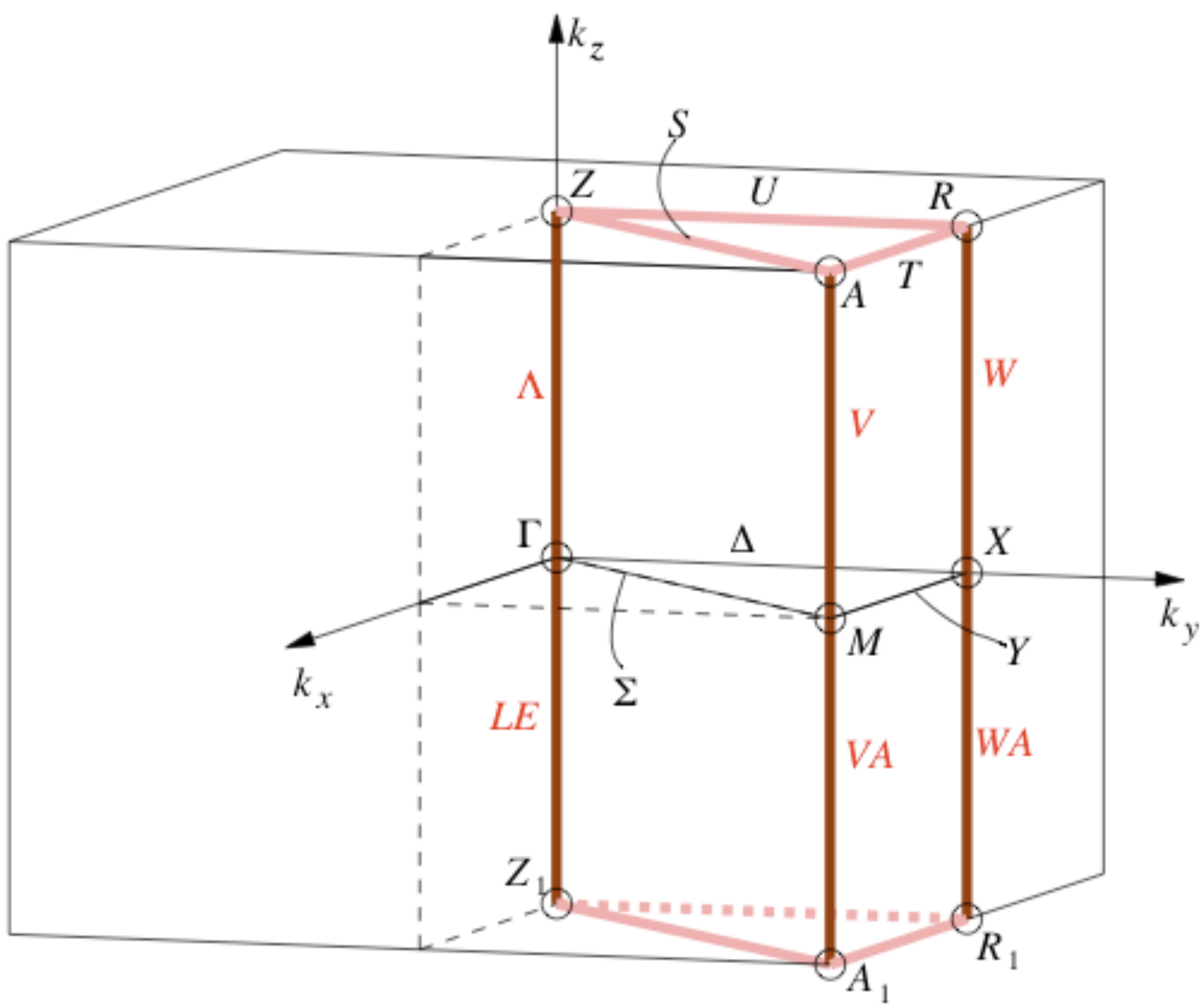
5.5 Crystal class $4mm$

5.5.1 Arithmetic crystal class $4mmP$

Fig. 5.5.1.1 Diagram for arithmetic crystal class $4mmP$

$P4mm - C_{4v}^1$ (99) to $P4_2bc - C_{4v}^8$ (106)

Reciprocal-space group $(P4mm)^*$, No. 99 see Tab. 5.5.1.1



EXERCISES

Problem 2

Consider a general ***k***-vector of a space group G. Determine its little co-group, the ***k***-vector star. How many arms has its star? How many full-group irreps will be induced and of what dimension? Write down the matrix of the full-group irrep of a general ***k***-vector of a translation.

SOLUTION

Problem 2

general k-vector k

irrep of T: Γ^k

little co-group $\overline{G}^k = \{1\}$

little group $G^k = T$

star of k, $k^* = \{kW_i, W_i \in \overline{G}\}$

allowed irrep: Γ^k

induction procedure

(W,w)	q_j	$(W,w)q_j$	q_i	$q_i^{-1}(W,w)q_j$	M_{ij}
(1,t)	(W_j,w_j)				

SOLUTION

Problem 2

$k^* = \{k, k', k'', \ldots, k^n\}$

$D^{k^*}(l,t) =$

exp-ikt					
	exp-ik't			0	
		exp-ik''t			
			…		
	0			…	
					$\exp{-ik^n t}$

Computing Programs
Representations of point and space groups

Representation Theory Applications	
REPRES	Space Groups Representations
DIRPRO	Direct Products of Space Group Irreducible Representations
CORREL	Correlations Between Representations
POINT	Point Group Tables
SITESYM	Site-symmetry induced representations of Space Groups

Solid State Theory Applications	
SAM	Spectral Active Modes (IR and RAMAN Selection Rules)
NEUTRON	Neutron Scattering Selection Rules
SYMMODES	Primary and Secondary Modes for a Group - Subgroup pair
AMPLIMODES	Symmetry Mode Analysis

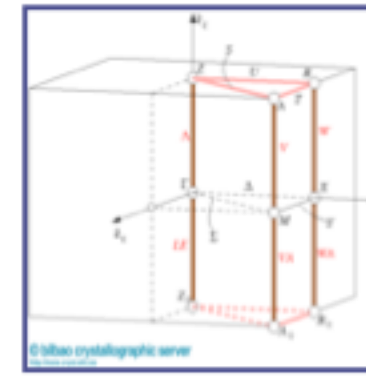
Problem: Representations of space groups REPRES

Space Group Number: Please, enter the sequential number of group as given in *International Tables for Crystallography*, Vol. A or choose it	99

next

REPRES

link to Brillouin zone database



- You can introduce the **k**-vector choosing one from the table:

Option 1

k-vector data

Choose one	CDML		Wyckoff position	
	k-vector label	Coordinates	Multiplicity	Letter
○	LD	0,0,u	1	a
○	V	1/2,1/2,u	1	b
○	W	0,1/2,u	2	c
○	C	u,u,v	4	d
○	B	0,u,v	4	e
○	F	u,1/2,v	4	f
○	GP	u,v,w	8	g

⊙ Or you can introduce the **k**-vector coordinates, relative to the basis you have chosen, as any three decimal numbers or fractions:

Option 2

k vector data	
Reciprocal basis	primitive (CDML)
Coordinates	k_x ☐ k_y ☐ k_z ☐

REPRES

k-vector data: option 1

Choose one	CDML		Wyckoff position	
	k-vector label	Coordinates	Multiplicity	Letter
○	LD	0,0,u	1	a
○	V	1/2,1/2,u	1	b
○	W	0,1/2,u	2	c
○	C	u,u,v	4	d
○	B	0,u,v	4	e
○	F	u,1/2,v	4	f
○	GP	u,v,w	8	g

Choose one	Label	Coordinates (CDML)
○	GM	0,0,0
○	Z	0,0,1/2
○	LD	0,0,u
⊙	LE	0,0,-u

u:

continue

REPRES

INPUT Options

- **Optional:** If you wish to see the full-group irreps for the generator check this ☐
- **Optional:** If you wish to change conventional (ITA) basis check this ☐

non-conventional setting

Rotation	1	0	0
	0	1	0
	0	0	1
Origin shift	0	0	0

- **Optional:** If you wish to see the irreps for arbitrary space group element check this ☐

arbitrary element

Rotational part			**Traslation**
1	0	0	0
0	1	0	0
0	0	1	0

continue

Space-group data

REPRES: output

$$G=\langle (W_1,w_1),\dots,(W_k,w_k) \rangle$$

```
Space group  G99 , number 99
Lattice type : tP

Number of generators : 4

         1                         2                         3                         4
  1   0   0        0     -1   0   0        0      0  -1   0        0      1   0   0        0
  0   1   0        0      0  -1   0        0      1   0   0        0      0  -1   0        0
  0   0   1        0      0   0   1        0      0   0   1        0      0   0   1        0
```

$$G=T+(W_2,w_2)T+\dots+(W_n,w_n)T$$

```
Number of elements : 8

         1                         2                         3                         4
  1   0   0        0     -1   0   0        0      0  -1   0        0      0   1   0        0
  0   1   0        0      0  -1   0        0      1   0   0        0     -1   0   0        0
  0   0   1        0      0   0   1        0      0   0   1        0      0   0   1        0

         5                         6                         7                         8
  1   0   0        0     -1   0   0        0      0  -1   0        0      0   1   0        0
  0  -1   0        0      0   1   0        0     -1   0   0        0      1   0   0        0
  0   0   1        0      0   0   1        0      0   0   1        0      0   0   1        0
```

REPRES: output

k-vector and its star *k

```
K-vector X :
   in primitive basis :   0.000  0.500  0.000
   in standard dual basis        :   0.000  0.500  0.000

The star of the k-vector has the following 2 arms :
   0.000  0.500  0.000
   0.500  0.000  0.000
```

Little group $G^X=\{(W_i,w_i)|W_ik=k+K, (W_i,w_i)\in G\}$

```
The little group of the k-vector has the following 4
elements as translation coset representatives :

          1                          2                          3                          4
  1  0  0      0       -1  0  0      0        1  0  0      0       -1  0  0      0
  0  1  0      0        0 -1  0      0        0 -1  0      0        0  1  0      0
  0  0  1      0        0  0  1      0        0  0  1      0        0  0  1      0
```

Little group G^X

```
 The little group of the k-vector has  4  allowed irreps.
 The matrices, corresponding to all of the little group elements are :

  Irrep (X)(1) ,  dimension 1
        1                2                3                4
 (1.000,  0.0)   (1.000,  0.0)   (1.000,  0.0)   (1.000,  0

  Irrep (X)(2) ,  dimension 1
        1                2                3                4
 (1.000,  0.0)   (1.000,  0.0)   (1.000,180.0)   (1.000,180.0)
```

Allowed (small) irreps $D^{X,1}$

Coset decomposition

REPRES: output

```
The space group has the following 2 elements as
coset representatives relative to the little group :

         1                        2
  1  0   0      0        0 -1   0      0
  0  1   0      0        1  0   0      0
  0  0   1      0        0  0   1      0
```

$$G=G^X+q_2G^X+...+q_kG^X$$

Full-group irreps: Characters

$$\Sigma\ D^{*X,i}(W,w)_{ii}$$

```
General position characters:
Gen Pos:      1                2                3
X1       (2.000,  0.0) (2.000,  0.0) (0.000,  0.0)
X2       (2.000,  0.0) (2.000,  0.0) (0.000,  0.0)
X4       (2.000,  0.0) (2.000,180.0) (0.000,  0.0)
X3       (2.000,  0.0) (2.000,180.0) (0.000,  0.0)
```

Physically-irreducible irreps

```
Physically-irreducible representations:
   *X1   *X2   *X4   *X3
```

$$D^{*X,i} \oplus (D^{*X,i})^*$$

Coset decomposition

REPRES: output

```
The space group has the following 2 elements as
coset representatives relative to the little group :

          1                         2
  1   0   0       0       0  -1   0       0
  0   1   0       0       1   0   0       0
  0   0   1       0       0   0   1       0
```

$$G=G^{X}+q_2G^{X}+...+q_kG^{X}$$

Full-group irreps: Induction procedure

```
Generator number 3
Induction matrix :
0 1
1 0

Block (1,2) :
(1.000,  0.0)
Block (2,1) :
(1.000,  0.0)

Generator number 4
Induction matrix :
1 0
0 1

Block (1,1) :
(1.000,  0.0)
Block (2,2) :
(1.000,  0.0)
```

Full-group irrep — induction matrix — small irrep matrix

$$D^{*X,i}(W,w)_{mi,nj} = M(W,w)_{m,n}D^{X,i}(W^k,w^k)_{i,j}$$

$$(W^k,w^k)=(q_m)^{-1}(W,w)q_n$$

EXERCISES

Problem 1

(a) Obtain the irreps for the space group *P4mm* for the **k**-vectors Γ(000) and X(01/20) using the program REPRES.

(b) Use the program REPRES for the derivation of the irreps of a general **k**-vector of the group *P4mm*.

EXERCISES

Problem 2

Obtain the irreps for the space group *P4bm* for the **k**-vectors Γ(000) and X(01/20) using the program REPRES.

SUBDUCED SPACE-GROUP REPRESENTATIONS

Problem: SUBDUCED space-group representations

group G

$\{e, g_2, g_3, \ldots, g_i, \ldots, g_n\}$

$\{e, h_2, h_3, \ldots, h_m\}$

subgroup $H<G$

D(G): irrep of G

$\{D(e), D(g_2), D(g_3), \ldots, D(g_i), \ldots, D(g_n)\}$

$\{D(e), D(h_2), D(h_3), \ldots, D(h_m)\}$

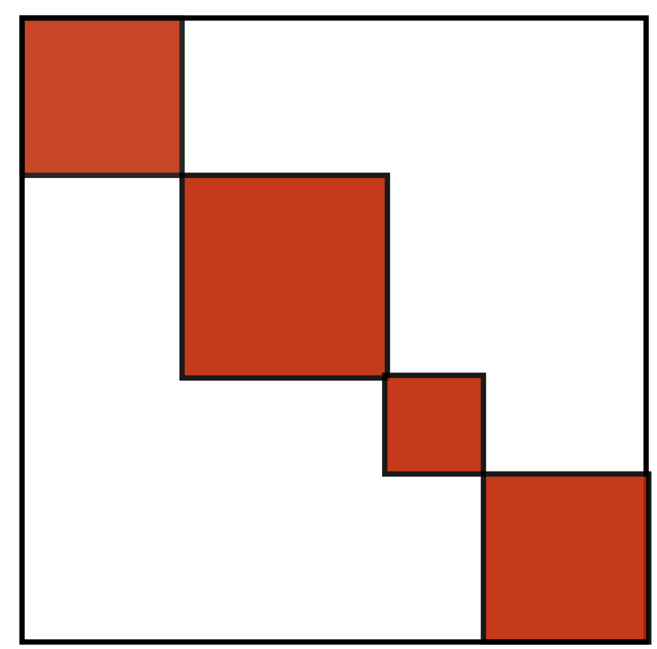
$\{D(G)\downarrow H\}$: subduced rep of $H<G$

$\{D(G)\downarrow H\}$

Subduction

$S^{-1}\{D(G)\downarrow H\}S$

$\bigoplus m_i D_i(H)$



irreps of H

Problem: **Compatibility relations of small (allowed) representations of little groups of a space group G**

Space group G $\left\{ \begin{array}{l} k, G^{k}, D^{k,i} \\ k', G^{k'}, D^{k',j} \end{array} \right.$ such that $k'=k+\delta$

Subduction of little group irreps

in the limit $\delta \longrightarrow 0$

$$D^{k,i}(G^{k}) \downarrow G^{k'} \sim \bigoplus m_j D^{k'j}(G^{k'})$$

Correlations between characters

$$\eta^{k,i}(g^{k'}) = \sum_{j} m_j \, \eta_j^{k'}(g^{k'}) \qquad g^{k'} \in G^{k'}$$

EXAMPLE P4/mmm

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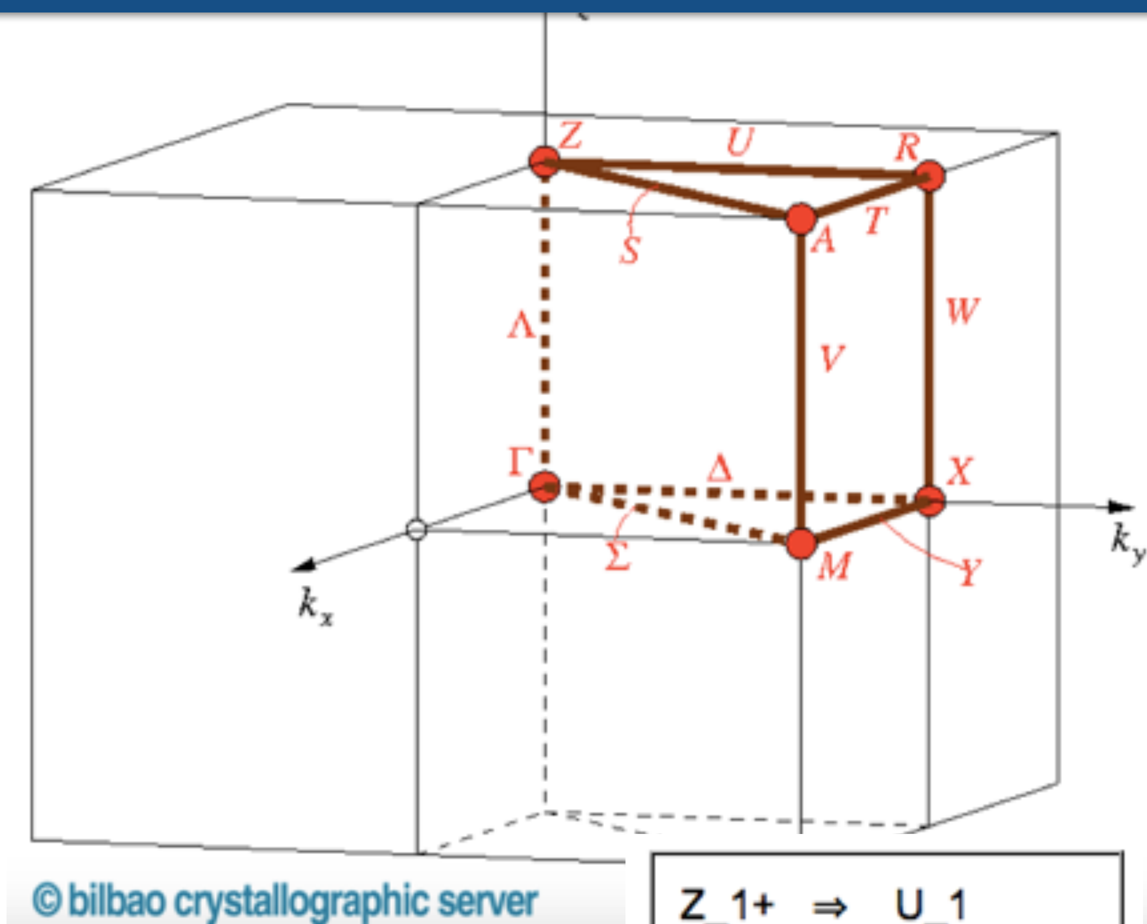
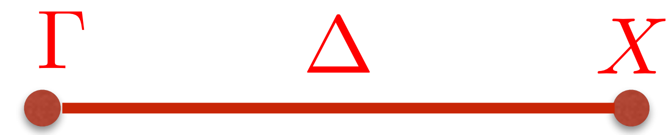
k-vector description		Wyckoff Position		
CDML[1]				
Label	Coefficients			
GM	0,0,0	1	a	4/mmm
Z	0,0,1/2	1	b	4/mmm
M	1/2,1/2,0	1	c	4/mmm
A	1/2,1/2,1/2	1	d	4/mmm
R	0,1/2,1/2	2	e	mmm.
X	0,1/2,0	2	f	mmm.
LD	0,0,u	2	g	4mm
V	1/2,1/2,u	2	h	4mm
W	0,1/2,u	4	i	2mm.
SM	u,u,0	4	j	m.2m
S	u,u,1/2	4	k	m.2m
DT	0,u,0	4	l	m2m.
U	0,u,1/2	4	m	m2m.
Y	u,1/2,0	4	n	m2m.
T	u,1/2,1/2	4	o	m2m.
D	u,v,0	8	p	m..
E	u,v,1/2	8	q	m..
C	u,u,v	8	r	..m
B	0,u,v	8	s	.m.
F	u,1/2,v	8	t	.m.
GP	u,v,w	16	u	1

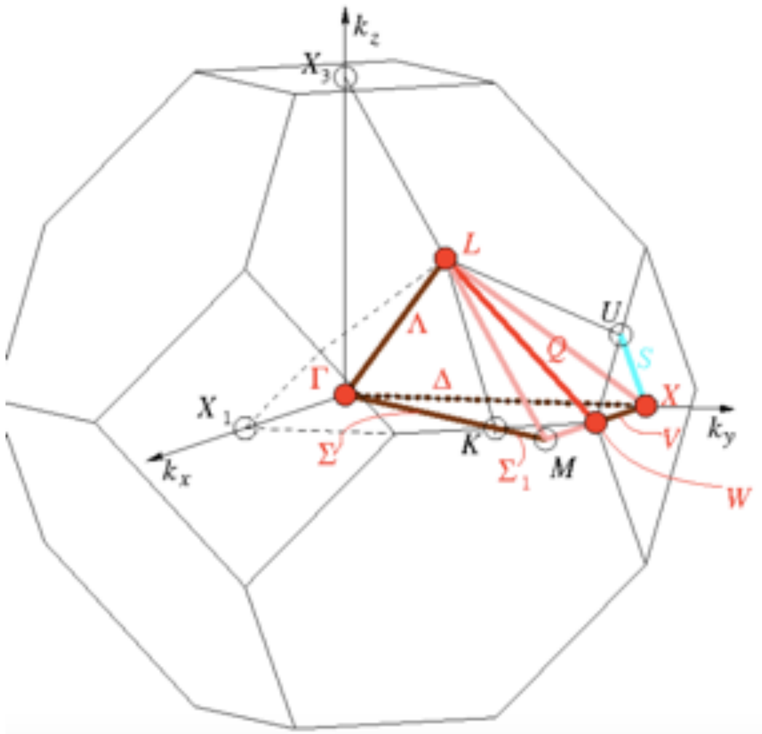


Z_1+ ⇒ LD_1	
Z_1- ⇒ LD_4	
Z_2+ ⇒ LD_2	
Z_2- ⇒ LD_3	
Z_3+ ⇒ LD_4	
Z_3- ⇒ LD_1	
Z_4+ ⇒ LD_3	
Z_4- ⇒ LD_2	

Z_1+ ⇒ U_1
Z_1- ⇒ U_2
Z_2+ ⇒ U_1
Z_2- ⇒ U_2
Z_3+ ⇒ U_4
Z_3- ⇒ U_3
Z_4+ ⇒ U_4
Z_4- ⇒ U_3
Z_5+ ⇒ U_2 + U_3
Z_5- ⇒ U_1 + U_4

EXAMPLE Electronic energy bands of Ge, Fd-3m (227)



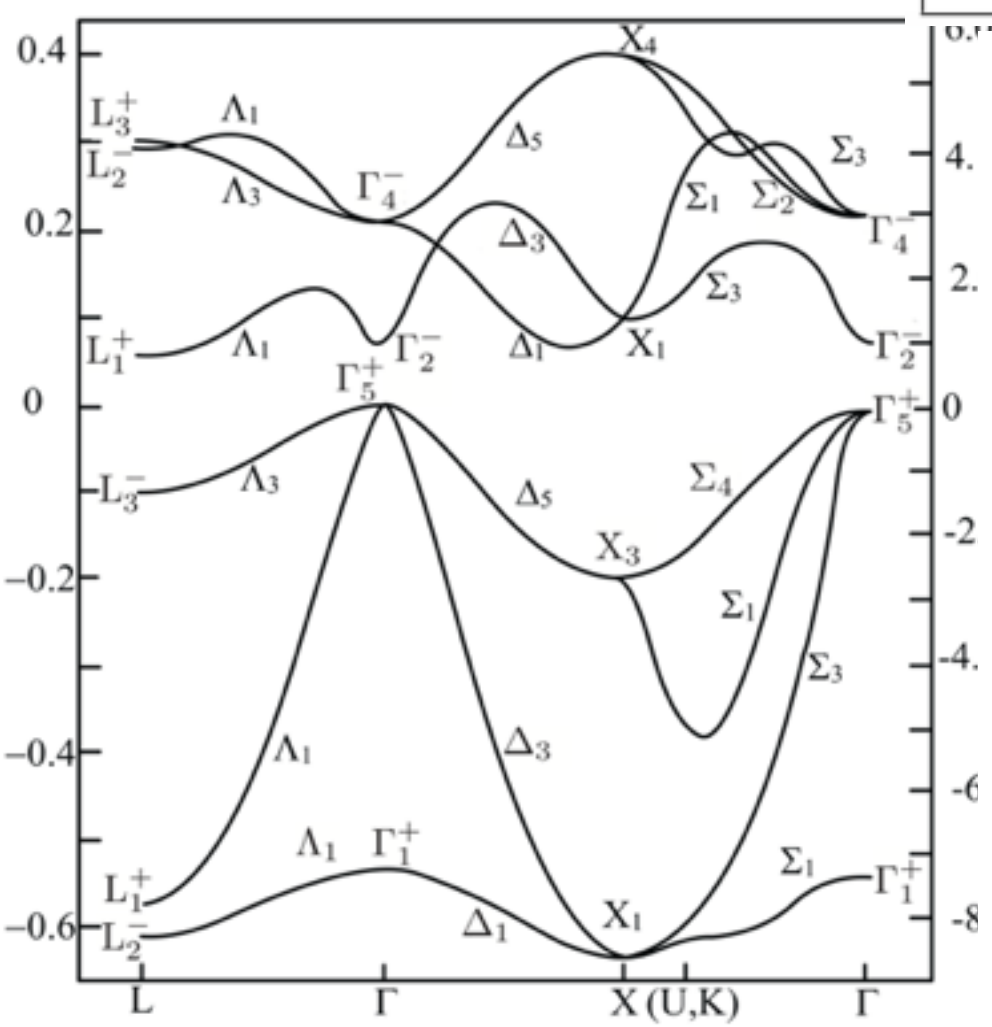


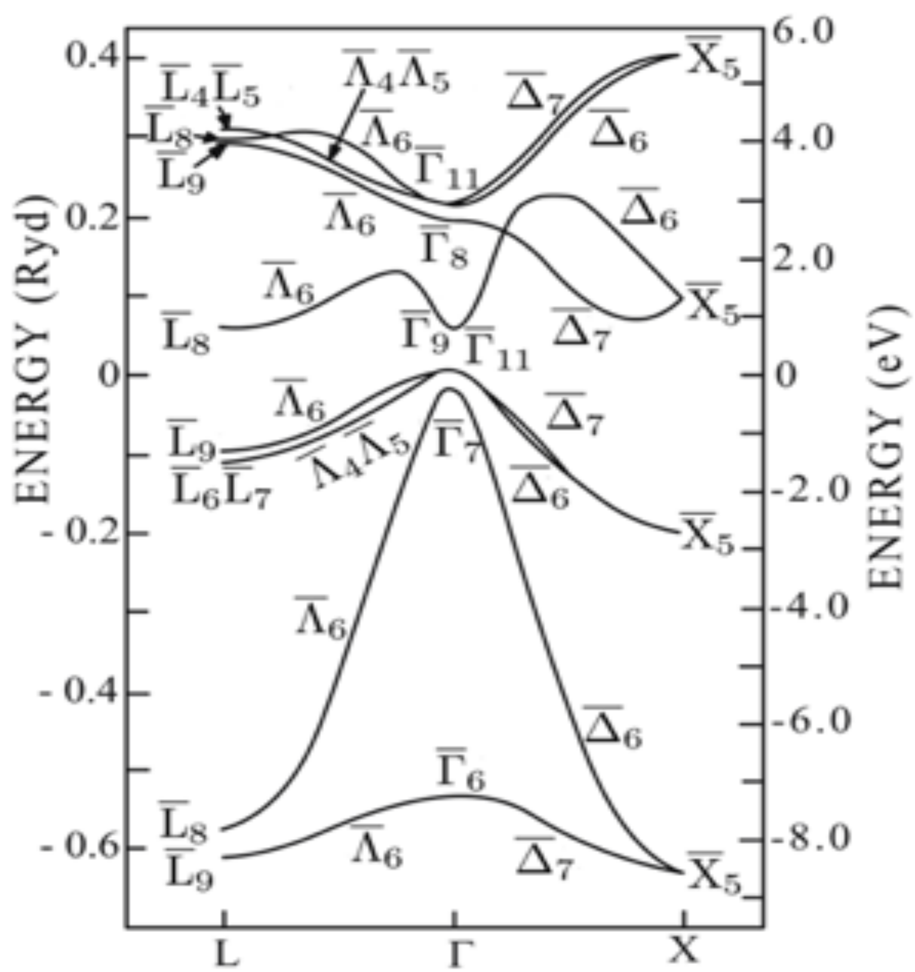
k-vector description		ITA description	
		Wyckoff position	
k-vector label	Conventional basis	Multiplicity	Letter
GM	0,0,0	2	a
X	0,1,0	6	b
L	1/2,1/2,1/2	8	c
W	1/2,1,0	12	d
DT	0,u,0	12	e
LD	u,u,u	16	f
V	u,1,0	24	g
SM (S)	u,u,0	24	h
Q	1/2,1-u,u	48	i
A (B)	v,u,0	48	j
C (J)	v,v,-u	48	k
GP	u,v,w	96	l

Compatibility Relations

$GM_1^+(1) \to DT_1(1)$
$GM_1^-(1) \to DT_4(1)$
$GM_2^+(1) \to DT_2(1)$
$GM_2^-(1) \to DT_3(1)$
$GM_3^+(2) \to DT_1(1) \oplus DT_2(1)$
$GM_3^-(2) \to DT_3(1) \oplus DT_4(1)$
$GM_4^+(3) \to DT_4(1) \oplus DT_5(2)$
$GM_4^-(3) \to DT_1(1) \oplus DT_5(2)$
$GM_5^+(3) \to DT_3(1) \oplus DT_5(2)$
$GM_5^-(3) \to DT_2(1) \oplus DT_5(2)$
$\overline{GM}_6(2) \to \overline{DT}_7(2)$
$\overline{GM}_7(2) \to \overline{DT}_6(2)$
$\overline{GM}_8(2) \to \overline{DT}_7(2)$
$\overline{GM}_9(2) \to \overline{DT}_6(2)$
$\overline{GM}_{10}(4) \to \overline{DT}_6(2) \oplus \overline{DT}_7(2)$
$\overline{GM}_{11}(4) \to \overline{DT}_6(2) \oplus \overline{DT}_7(2)$

$X_1(2) \to DT_1(1) \oplus DT_3(1)$
$X_2(2) \to DT_2(1) \oplus DT_4(1)$
$X_3(2) \to DT_5(2)$
$X_4(2) \to DT_5(2)$
$\overline{X}_5(4) \to \overline{DT}_6(2) \oplus \overline{DT}_7(2)$





Problem: Correlations between representations of space groups

CORREL

group G

$\{e, g_2, g_3, \ldots, g_i, \ldots, g_n\}$

$\{e, h_2, h_3, \ldots, h_m\}$

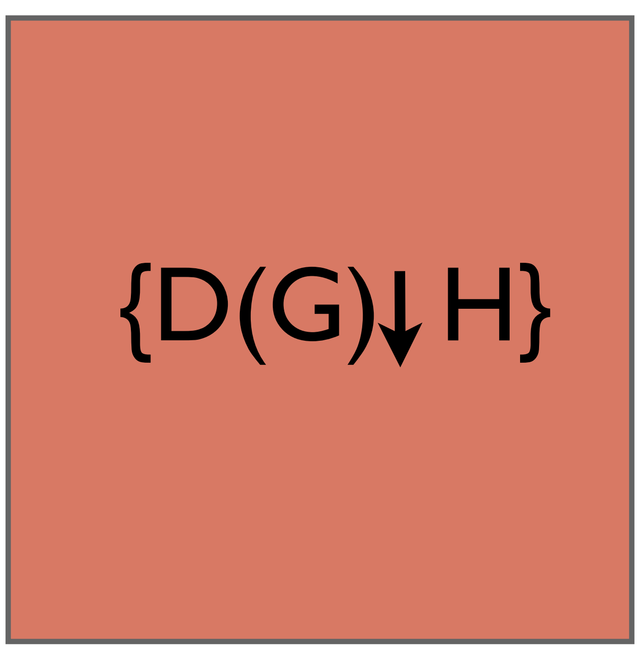
subgroup H<G

D(G): irrep of G

$\{D(e), D(g_2), D(g_3), \ldots, D(g_i), \ldots, D(g_n)\}$

$\{D(e), D(h_2), D(h_3), \ldots, D(h_m)\}$

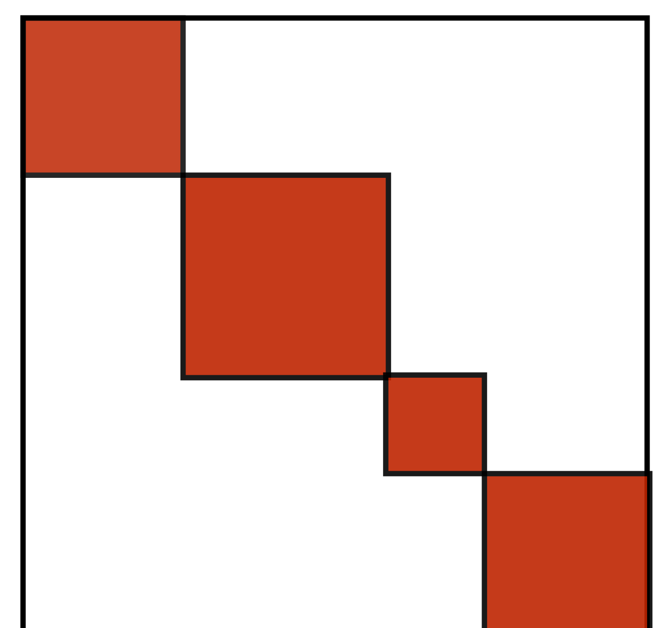
$\{D(G)\downarrow H\}$: subduced rep of H<G



Subduction

$S^{-1}\{D(G)\downarrow H\}S$

$\bigoplus m_i D_i(H)$



irreps of H

Correlations between representations of space groups

Subduction of space group irreps

$$D^{*k_G,i}(G)\downarrow H \sim \bigoplus m_j D^{*k_H,j}(H)$$

Step 1. Correlations between wave vectors

$$^{*}k_G \downarrow H = \sum_{^{*}k_H} (^{*}k_G|^{*}k_H)\,^{*}k_H$$

Step 2. Correlations between characters

$$\eta^{*k_G,i}(G) = \sum_{^{*}k_{H_j}} (^{*}k_{G,i}|^{*}k_{H,j})\ \eta^{*k_{H_j},P}(H)$$

DATA *ITA*1: Maximal Subgroups

Transformation matrix: (P,p)

group G $\{e, g_2, g_3, \ldots, g_i, \ldots, g_{n-1}, g_n\}$

subgroup H<G non-conventional $\{e, \ldots\ldots, g_3, \ldots, g_i, \ldots\ldots\ldots, g_n\}$

(P,p)

subgroup H<G $\{e, h_2, h_3, \ldots, h_m\}$

Problem: Correlations between representations of space groups

CORREL

Supergroup number: Please, enter the sequential number of group as given in *International Tables for Crystallography*, Vol. A or choose it:	221	group G
Subgroup number: Please, enter the sequential number of group as given in *International Tables for Crystallography*, Vol. A or choose it:	99	subgroup H

INPUT data

Enter the transformation matrix below:

Rotational part			Origin Shift
1	0	0	0
0	1	0	0
0	0	1	0

transformation matrix

k vector data	Reciprocal basis	primitive (CDML)
	Coordinates	k_x 0 k_y .5 k_z 0
	Label	X

k-vector data

CORREL: OUTPUT data

$^*k_G$ - vector data

```
K-vector X :
  in primitive basis :   0.000  0.500  0.000
  in dual basis      :   0.000  0.500  0.000

The star *X has the following 3 arms :
  0.000  0.500  0.000
  0.500  0.000  0.000
  0.000  0.000  0.500
```

*k-vector splitting

$$^*k_G = {}^*k_{H,1} + {}^*k_{H,2} + \ldots + {}^*k_{H,k}$$

```
-------------------------------------------------------
Information about splitting
-------------------------------------------------------

The star *X of the supergroup splits the following way
 *X --> 1_*S1 + 1_*S2

Star *S1 = *(  0.000  0.500  0.000)


Star *S2 = *(  0.000  0.000  0.500)
```

Correlations between representations

$$\{D(G)\downarrow H\} \longrightarrow \bigoplus m_i D_i(H)$$

```
--------------------------------------------------
Subduction problem
--------------------------------------------------


Reduction : (*X)(1)  = 1(*S1)(1) + 1(*S2)(1)

Reduction : (*X)(2)  = 1(*S1)(2) + 1(*S2)(2)

Reduction : (*X)(3)  = 1(*S1)(3) + 1(*S2)(2)

Reduction : (*X)(4)  = 1(*S1)(4) + 1(*S2)(1)

Reduction : (*X)(5)  = 1(*S1)(1) + 1(*S2)(3)
```

DIRECT-PRODUCT SPACE-GROUP REPRESENTATIONS

Problem: **Direct product of representations of space groups** — **DIRPRO**

$D_1(G)$: irrep of G

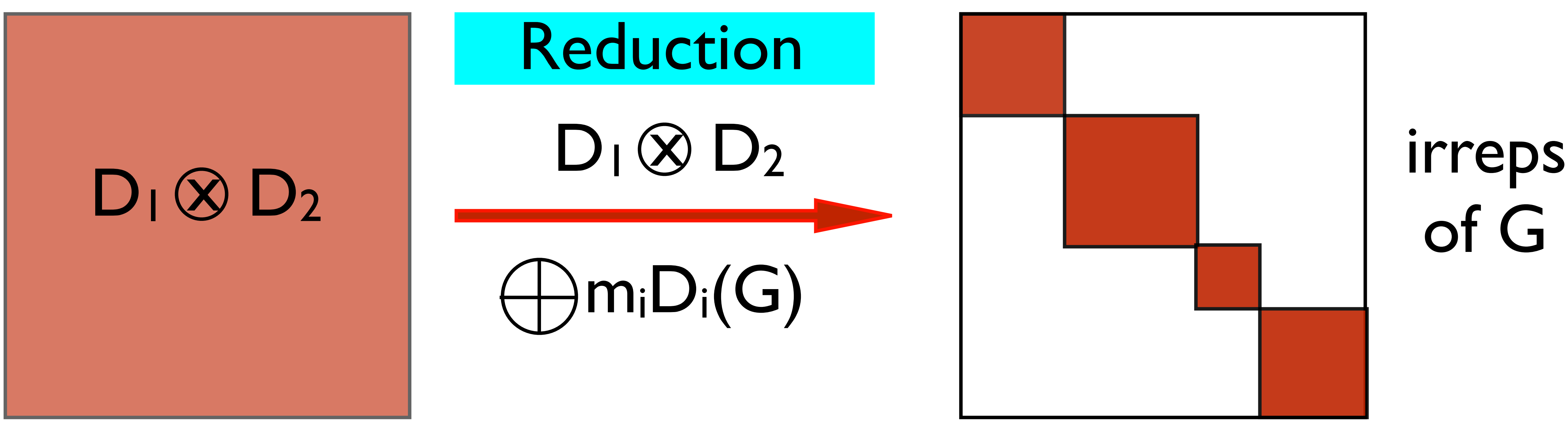
$\{D_1(e), D_1(g_2),\ldots, D_1(g_n)\}$

$D_2(G)$: irrep of G

$\{D_2(e), D_2(g_2),\ldots, D_2(g_n)\}$

Direct-product representation

$$D_1 \otimes D_2 = \{D_1(e) \otimes D_2(e), \ldots, D_1(g_i) \otimes D_2(g_i), \ldots\}$$



Direct product of representations of space groups

Direct product of space group irreps

$$D^{*k_1,i}(G) \otimes D^{*k_2,j} \sim \bigoplus m_j D^{*k,p}(G)$$

Step 1. Selection rules of wave-vectors stars

$$^*k_1 \otimes {}^*k_2 = \sum_{^*k} ({}^*k_1 {}^*k_2 | {}^*k) {}^*k$$

Step 2. Decomposition of direct product

$$\eta^{*k_1,i1}(G)\ \eta^{*k_2,i2}(G) = \sum_{^*k} ({}^*k_1,i_1 {}^*k_2,i_2 | {}^*k,p)\ \eta^{*k,p}(G)$$

EXERCISES

Problem 4

Consider the space group P4/mmm (No. 123) and its k-vectors X(0 1/2 0) and DT(0 0.27 0). Determine the wave-vector selection rules for the product

$$*DT(0\ 0.27\ 0) \otimes *X(0\ 1/2\ 0).$$

KVEC database

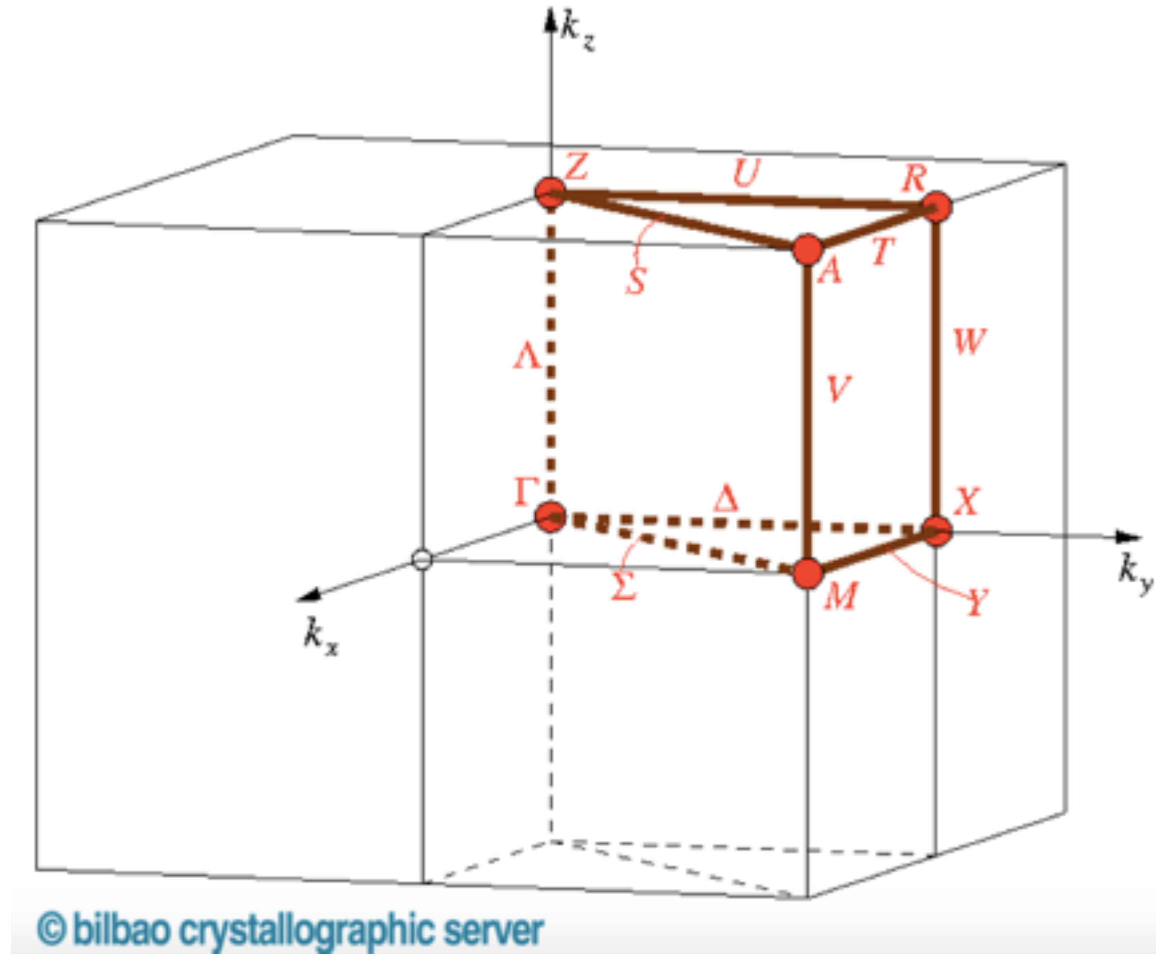
BILBAO CRYSTALLOGRAPHIC SERVER

The k-vector types of space group *P4/mmm* (123)

(Table for arithmetic crystal class 4/mmmP)

P4/mmm-D_{4h}^{1} (123) to $P4_2$/ncm- D_{4h}^{16}(138)

Reciprocal-space group $(P4/mmm)^*$, No.123



k-vector description		ITA description	
		Wyckoff position	
k-vector label	Conventional basis	Multiplicity	Letter
GM	0,0,0	1	a
Z	0,0,1/2	1	b
M	1/2,1/2,0	1	c
A	1/2,1/2,1/2	1	d
R	0,1/2,1/2	2	e
X	0,1/2,0	2	f
LD	0,0,u	2	g
V	1/2,1/2,u	2	h
W	0,1/2,u	4	i
SM	u,u,0	4	j
S	u,u,1/2	4	k
DT	0,u,0	4	l
U	0,u,1/2	4	m
Y	u,1/2,0	4	n
T	u,1/2,1/2	4	o
D	u,v,0	8	p
E	u,v,1/2	8	q
C	u,u,v	8	r
B	0,u,v	8	s
F	u,1/2,v	8	t
GP	u,v,w	16	u

Problem 4

SOLUTION

$$^{*}DT(0\ 0.27\ 0) \otimes {}^{*}X(0\ 1/2\ 0)$$

- **k**-vector label: DT
- The star of the **k**-vector has 4 arms:
  - 0.000 0.270 0.000
  - 0.000 -0.270 0.000
  - 0.270 0.000 0.000
  - -0.270 0.000 0.000
- The point (0,0.27,0) forms part of the line DT
- Little co-group: m2m.
- ITA classification: 4l

- **k**-vector label: X
- The star of the **k**-vector has 2 arms:
  - 0.000 0.500 0.000
  - 0.500 0.000 0.000
- X is a point.
- Little co-group: mmm.
- ITA classification: 2f

$$\sum_{^{*}k} (^{*}k_1\, ^{*}k_2 | ^{*}k)\, ^{*}k$$

- **k**-vector label: DT
- The star of the **k**-vector has 4 arms:
  - 0.000 0.770 0.000
  - 0.000 -0.770 0.000
  - 0.770 0.000 0.000
  - -0.770 0.000 0.000
- The point (0,0.77,0) forms part of the line DT
- Little co-group: m2m.
- ITA classification: 4l

- **k**-vector label: Y
- The star of the **k**-vector has 4 arms:
  - 0.500 0.270 0.000
  - -0.500 -0.270 0.000
  - 0.270 -0.500 0.000
  - -0.270 0.500 0.000
- The point (0.5,0.27,0) forms part of the line Y
- Little co-group: m2m.
- ITA classification: 4n

Problem: Direct product of representations of space groups

DIRPRO

Space Group Number: Please, enter the sequential number of group as given in *International Tables for Crystallography*, Vol. A or choose it:	123

group G

Reciprocal basis	primitive (CDML)

INPUT data

k-vector 1 [coordinates]	k_x 0 k_y 0.27 k_z 0	Label	DT
k-vector 2 [coordinates]	k_x 0 k_y 0.5 k_z 0	Label	X

k-vector data

Get results or Reset form

DIRPRO: OUTPUT data

Space-group data

$$G=\langle (W_1,w_1),\ldots,(W_k,w_k)\rangle$$

```
Space group  G123 , number 123
Lattice type : tP

Number of space group generators : 5

          1                        2                        3                        4
  1  0  0      0       -1  0  0      0        0 -1  0      0       -1  0  0      0
  0  1  0      0        0 -1  0      0        1  0  0      0        0  1  0      0
  0  0  1      0        0  0  1      0        0  0  1      0        0  0 -1      0

          5
 -1  0  0      0
  0 -1  0      0
  0  0 -1      0
```

$$G=T+(W_2,w_2)T+\ldots+(W_n,w_n)T$$

```
Number of space group elements : 16

          1                        2                        3                        4
  1  0  0      0       -1  0  0      0        0 -1  0      0        0  1  0      0
  0  1  0      0        0 -1  0      0        1  0  0      0       -1  0  0      0
  0  0  1      0        0  0  1      0        0  0  1      0        0  0  1      0

          5                        6                        7                        8
 -1  0  0      0        1  0  0      0        0  1  0      0        0 -1  0      0
  0  1  0      0        0 -1  0      0        1  0  0      0       -1  0  0      0
  0  0 -1      0        0  0 -1      0        0  0 -1      0        0  0 -1      0

          9                       10                       11                       12
 -1  0  0      0        1  0  0      0        0  1  0      0        0 -1  0      0
  0 -1  0      0        0  1  0      0       -1  0  0      0        1  0  0      0
  0  0 -1      0        0  0 -1      0        0  0 -1      0        0  0 -1      0

         13                       14                       15                       16
  1  0  0      0       -1  0  0      0        0 -1  0      0        0  1  0      0
  0 -1  0      0        0  1  0      0       -1  0  0      0        1  0  0      0
```

k-vector and its star *k

DIRPRO: output

```
The star *DT has the following 4 arms :
  0.000  0.270  0.000
  0.000 -0.270  0.000
  0.270  0.000  0.000
 -0.270  0.000  0.000

The star *X has the following 2 arms :
  0.000  0.500  0.000
  0.500  0.000  0.000
```

Little group $G^X=\{(W_i,w_i)|W_ik=k+K, (W_i,w_i)\ G\}$

```
--------------------------------------------------------------------------------
Information about the representations
--------------------------------------------------------------------------------

The little group of the k-vector DT(  0.000  0.270  0.000) has the following 4
elements as translation coset representatives :

      1                  2                  3                  4
 1  0  0      0    -1  0  0      0     1  0  0      0    -1  0  0      0
 0  1  0      0     0  1  0      0     0  1  0      0     0  1  0      0
 0  0  1      0     0  0 -1      0     0  0 -1      0     0  0  1      0
```

Little group G^{DT}

```
 The little group of the k-vector has  4  allowed irreps.
 The matrices, corresponding to all of the little group elements are :

  Irrep (DT)(1) ,  dimension 1
      1                2                3                4
(1.000,   0.0)   (1.000,   0.0)   (1.000,   0.0)   (1.000,   0.0)

  Irrep (DT)(2) ,  dimension 1
      1                2                3                4
(1.000,   0.0)   (1.000,   0.0)   (1.000,180.0)   (1.000,180.0)
```

Allowed (small) irreps $D^{DT,1}$

Reduction of the direct product

```
---------------------------------------
Information about the splitting
---------------------------------------

Wave vector selection rules :

*DT x *X  =  1_*S1 + 1_*S2

Star *S1 = *(  0.000  0.770  0.000)

Star *S2 = *(  0.500  0.270  0.000)
```

*k-vector splitting

$$*k_1 \otimes *k_2 = *k_1 + *k_2 + \ldots + *k_k$$

```
------------------------------------------------------------
Reduction problem
------------------------------------------------------------

Reduction : (*DT)(1) x (*X)(1)  =  1(*S1)(1) + 1(*S2)(1)

Reduction : (*DT)(1) x (*X)(2)  =  1(*S1)(2) + 1(*S2)(2)

Reduction : (*DT)(1) x (*X)(3)  =  1(*S1)(3) + 1(*S2)(3)

Reduction : (*DT)(1) x (*X)(4)  =  1(*S1)(4) + 1(*S2)(4)

Reduction : (*DT)(1) x (*X)(5)  =  1(*S1)(2) + 1(*S2)(4)

Reduction : (*DT)(1) x (*X)(6)  =  1(*S1)(1) + 1(*S2)(3)
```

$$D_1(G) \otimes D_2(G)$$

↓

$$\bigoplus m_i D_i(G)$$