REPRESENTATIONS OF CRYSTALLOGRAPHIC GROUPS II.

SPACE GROUPS

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Irreducible Representations of Space Groups

Method: Construct the irreps of the space group G starting from the irreps of one of its normal subgroups $H \lhd G$

1. Construct all irreps of H
2. Distribute the irreps of H into orbits under G and select a representative
3. Determine the little group for each representative
4. Find the small (allowed) irreps of the little group
5. Construct the irreps of G by induction from the the small (allowed) irreps of the little group

Representations of the Translation subgroup

Born-von Karman boundary

$$(\mathbf{I}, \mathbf{t}_i)^{N_i} = (\mathbf{I}, \mathbf{N}_i) = (\mathbf{I}, \mathbf{o})$$

$$(\mathbf{I}, \mathbf{N}\,\mathbf{t}); \quad \mathbf{N}\,\mathbf{t} = (N_1 t_1, N_2 t_2, N_3 t_3)$$

$$\Gamma^{(q_1\, q_2\, q_3)}[(\mathbf{I}, \mathbf{t})] = e^{-2\pi i (q_1 \frac{t_1}{N_1} + q_2 \frac{t_2}{N_2} + q_3 \frac{t_3}{N_3})},$$

with $\mathbf{t} = (t_1, t_2, t_3)$;

$q_j = 0, 1, \ldots, N_j - 1$;

$j = 1, 2, 3$; t_k, q_j integers.

number of irreps:
$N_1 N_2 N_3$

Representations of the Translation subgroup

reciprocal space

$L: a_1, a_2, a_3 \longleftrightarrow L^*: a^*_1, a^*_2, a^*_3$

$a_i . a^*_j = 2\pi\delta_{ij}$

$$\Gamma^{(q_1\, q_2\, q_3)}[(\mathbf{I}, \mathbf{t})] = e^{-2\pi i (q_1 \frac{t_1}{N_1} + q_2 \frac{t_2}{N_2} + q_3 \frac{t_3}{N_3})}$$

$k_i = q_i / N_i$

$$\Gamma^{(q_1\, q_2\, q_3)}[(\mathbf{I}, \mathbf{t})] = \Gamma^{\mathbf{k}}[(\mathbf{I}, \mathbf{t})] = \exp -i(\mathbf{k}\, \mathbf{t})$$

$$(k_1, k_2, k_3) \begin{vmatrix} t_1 \\ t_2 \\ t_3 \end{vmatrix}$$

Representations of the Translation subgroup

unit cell of reciprocal space

$k' = k + K$

$\Gamma^{k'} = \exp(-i(k+K)t) = \exp{-i(k.t)} = \Gamma^{k}$

first Brillouin zone (Wigner-Seitz cell)

$|k| \leq |K-k|, \forall K \in L^*$

crystallographic unit cell

$0 \leq |k| < 1$

Orbits of irreps of the Translation subgroup. Little group.

conjugation of irreps of T

$$\Gamma^{k'}(I,t)= \Gamma^{k}((W,w)^{-1}(I,t)(W,w)),\ (I,t)\in T,\quad (W,w)\in G$$

$$\Gamma^{k'}(I,t)= \Gamma^{k}(I,W^{-1}t)=\exp\text{-}i(k\,.(W^{-1}t)) = \exp\text{-}i((k\,W^{-1}).t)$$

$$k'= k\,W + K$$

little co-group of k: $\overline{G}^{k}$

$$k= k\,W + K,\ K\in L^{*}$$

special and general

$$\overline{G}^{k} =\{1\} \quad \overline{G}^{k} >\{1\}$$

Orbits of irreps of the Translation subgroup. Little group.

star of k: k*

$\overline{G}^k < \overline{G}$

$\overline{G} = \overline{G}^k + W_2 \overline{G}^k + \ldots + W_m \overline{G}^k$

$k^* = \{k' = kW_m + K, W_m\}$

Little group G^k

$G^k = \{(W,w) \in G \mid W \in \overline{G}^k\}$

representation domain

exactly one k-vector from each star

Little-group irreps
(Allowed irreps of the little group)

CASE 1:

1. **k** is a vector of the interior of the BZ
   OR
2. $\mathcal{G}^{\mathbf{k}}$ is a symmorphic space group.

allowed irreps $\mathbf{D}^{\mathbf{k},i}$:

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

Here $\overline{\mathbf{D}}^{\mathbf{k},i}$ is an irrep of $\overline{\mathcal{G}}^{\mathbf{k}}$,

Little-group irreps
(Allowed irreps of the little group)

CASE 2:

1. **k** is a vector on the surface of the BZ AND
2. $\mathcal{G}^{\mathbf{k}}$ is a nonsymmorphic space group.

allowed irreps $\mathbf{D}^{\mathbf{k},i}$:
induced from allowed irreps $\mathbf{D}^{\mathbf{k},i}_{\mathcal{H}_0^{\mathbf{k}}}$ of $\mathcal{H}_0$ where
$\mathcal{H}_0$ is a symmorphic subgroup of $\mathcal{G}^{\mathbf{k}}$

$$\mathcal{G} \triangleright \mathcal{H}_1 \triangleright \mathcal{H}_2 \ \ldots \ \triangleright \mathcal{H}_0 \triangleright \ \ldots \ \triangleright \mathcal{T}$$

PROCEDURE FOR THE CONSTRUCTION OF

THE IRREDUCIBLE REPRESENTATIONS OF SPACE GROUPS

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) **k** vector from the representation domain of the BZ

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

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

(e) Decomposition of $\mathcal{G}$ relative to $\mathcal{G}^{\mathbf{k}}$

An obvious choice of coset representatives of $\mathcal{G}$ relative to $\mathcal{G}^{\mathbf{k}}$ is the set of of elements $\{q_i = (\overline{W}_i, \overline{w}_i),\ i = 1,\ \ldots,\ s\}$ where $\overline{W}_i$ are the coset representatives of $\overline{\mathcal{G}}$ relative to $\overline{\mathcal{G}}^{\mathbf{k}}$

$$\mathcal{G} = \mathcal{G}^{\mathbf{k}} \cup (\overline{W}_2, \overline{w}_2)\, \mathcal{G}^{\mathbf{k}} \cup\ \ldots\ (\overline{W}_s, \overline{w}_s)\, \mathcal{G}^{\mathbf{k}}$$

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).

subgroup irrep matrix

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

induction matrix

a) Construction of the induction matrix

The elements of the little group $\mathcal{G}^{\mathbf{k}}$ and the coset representatives $\{q_1, q_2, \ldots, q_s\}$ of G relative to $\mathcal{G}^{\mathbf{k}}$ are necessary for the construction of the induction matrix

$$M(W,w)_{ij} = \begin{cases} 1 \text{ if } q_i^{-1}(W,w)q_j \in \mathcal{G}^{\mathbf{k}} \\ 0 \text{ if } q_i^{-1}(W,w)q_j \notin \mathcal{G}^{\mathbf{k}} \end{cases}$$

0	1	0	0
0	0	1	0
1	0	0	0
0	0	0	1

dim M=s x s

monomial matrix

$(\boldsymbol{W}_l, \boldsymbol{w}_l)$	q_i	q_i^{-1}	$q_i^{-1}(\boldsymbol{W}_l, \boldsymbol{w}_l)$	$q_i^{-1}(\boldsymbol{W}_l, \boldsymbol{w}_l)q_j$	$M(\boldsymbol{W}_l, \boldsymbol{w}_l$
...	...	...	...	...	

(b) Matrices of the irreps $\mathbf{D}^{\star\mathbf{k},m}$ of $\mathcal{G}$:

$$\mathbf{D}^{\star\mathbf{k},m}(\boldsymbol{W}_l,\ \boldsymbol{w}_l)_{i\mu,j\nu} = M(\boldsymbol{W}_l,\ \boldsymbol{w}_l)_{ij}\,\mathbf{D}^{\mathbf{k},m}(\widetilde{\boldsymbol{W}}_p,\ \tilde{\boldsymbol{w}}_p)_{\mu\nu},$$

where $(\widetilde{\boldsymbol{W}}_p,\ \tilde{\boldsymbol{w}}_p) = q_i^{-1}\,(\boldsymbol{W}_l,\ \boldsymbol{w}_l)\,q_j$.

0	1	0	0
0	0	1	0
1	0	0	0
0	0	0	1

All irreps of the space group $\mathcal{G}$ for a given **k** vector are obtained considering all allowed irreps of the little group $\mathcal{G}^{\mathbf{k}}$ $\mathbf{D}^{\mathbf{k},m}$ obtained in step 3.

EXERCISES

Problem 1.

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

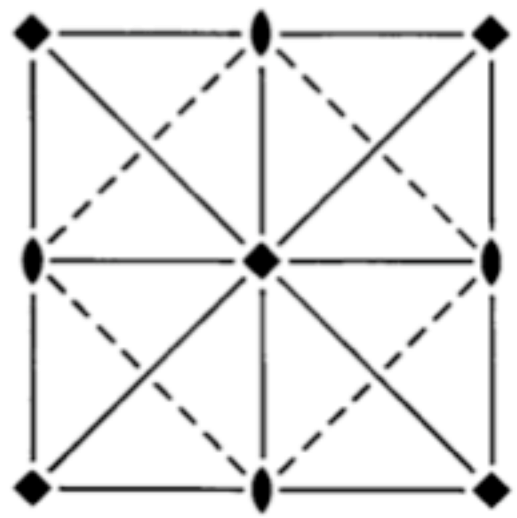
(i) Determine the little groups, the **k**-vector stars, the number and the dimensions of the little-group irreps, the number and the dimensions of the corresponding irreps of the group *P4mm*.

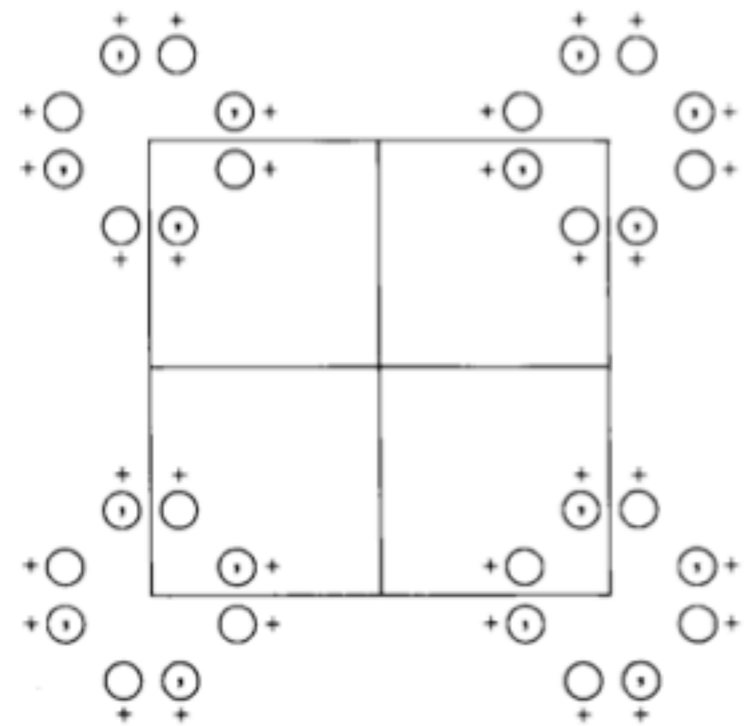
(ii) Calculate a set of coset representatives of the decomposition of the group *P4mm* with respect to the little group of the **k**-vectors and **X**, and construct the corresponding full space group irreps of *P4mm*.

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

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

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





Origin on $4mm$

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

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 $\;x,x,z$

8 l g

(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

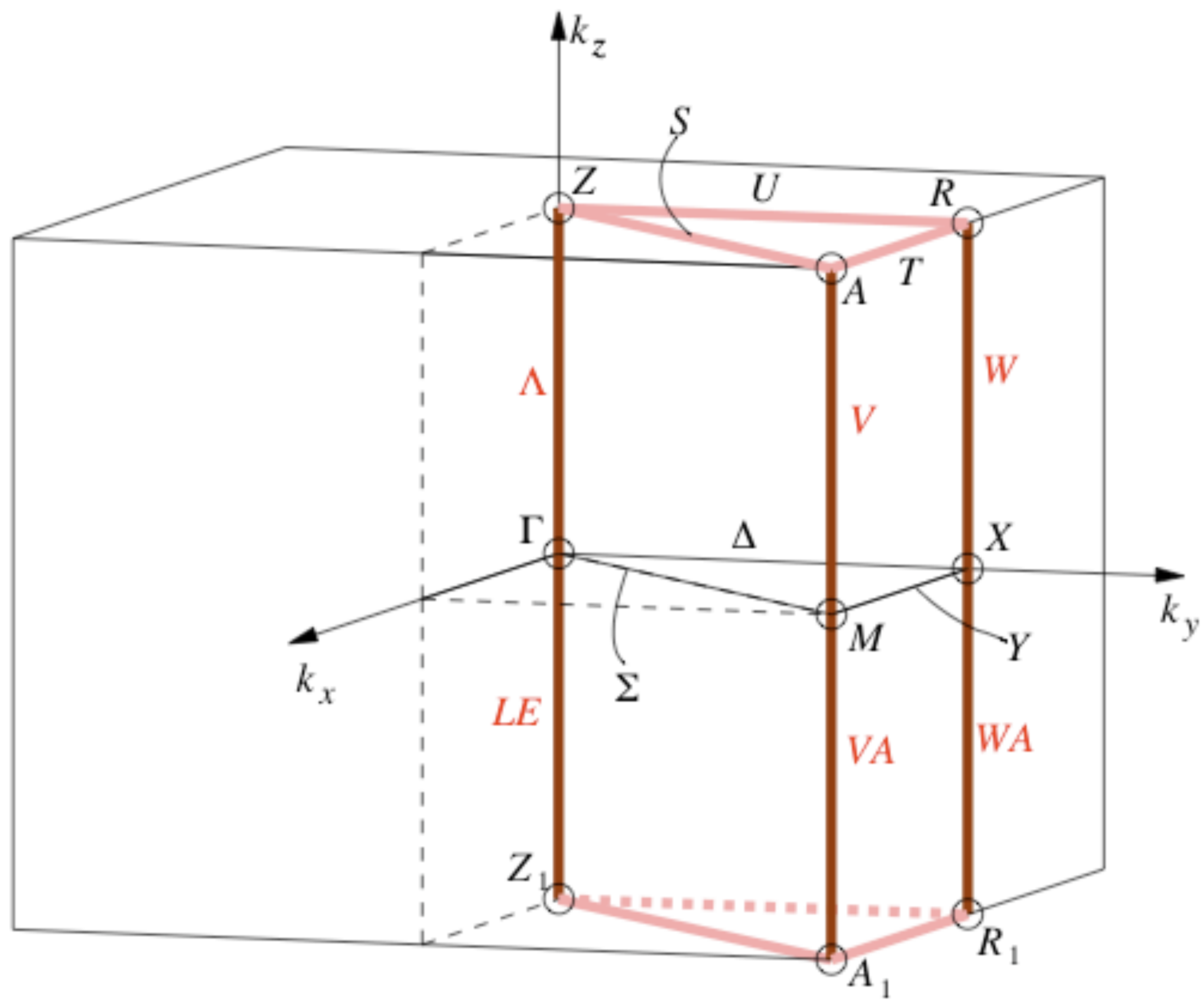
5.5 Crystal class $4mm$

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



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,

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

$P2_zmm$	$(\boldsymbol{1},\, \boldsymbol{o})$	$(\boldsymbol{2},\, \boldsymbol{o})$	$(\boldsymbol{m}_{yz},\, \boldsymbol{o})$	$(\boldsymbol{m}_{xz},\, \boldsymbol{o})$	$(\boldsymbol{1},\, \boldsymbol{t})$
$\boldsymbol{D}^{X,1}$	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 $P4mm$ $\quad t =$

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

EXERCISES

Problem 2

Consider a general k-vector k 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.

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.

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

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

exp-ikt					
	exp-ik't			0	
		exp-ik''t			
	0		...		
				...	
					exp-ik^{n}t

REPRESENTATIONS OF CRYSTALLOGRAPHIC GROUPS

Databases of point and space groups

Representation theory applications

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[The crystallographic site at the Condensed Matter Physics Dept. of the University of the Basque Country]

[Space Groups] [Layer Groups] [Rod Groups] [Frieze Groups] [Wyckoff Sets]

First announcement and pre-registration of a School in 2009 on CrystallographyOnline: InternationalSchoolon theUseandApplications oftheBilbao Crystallographic Server this server

Sections

- Retrieval Tools
- Group-Subgroup
- Representations
- Solid State
- Structure Utilities
- Subperiodic
- ICSDB

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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

Group - Subgroup Relations of Space Groups

SUBGROUPGRAPH	Lattice of Maximal Subgroups
HERMANN	Distribution of subgroups in conjugated classes
COSETS	Coset decomposition for a group-subgroup pair
WYCKSPLIT	The splitting of the Wyckoff Positions
MINSUP	Minimal Supergroups of Space Groups
SUPERGROUPS	Supergroups of Space Groups
CELLSUB	List of subgroups for a given k-index.
CELLSUPER	List of supergroups for a given k-index.
COMMONSUBS	Common Subgroups of Space Groups
COMMONSUPER	Common Supergroups of Two Space Groups

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

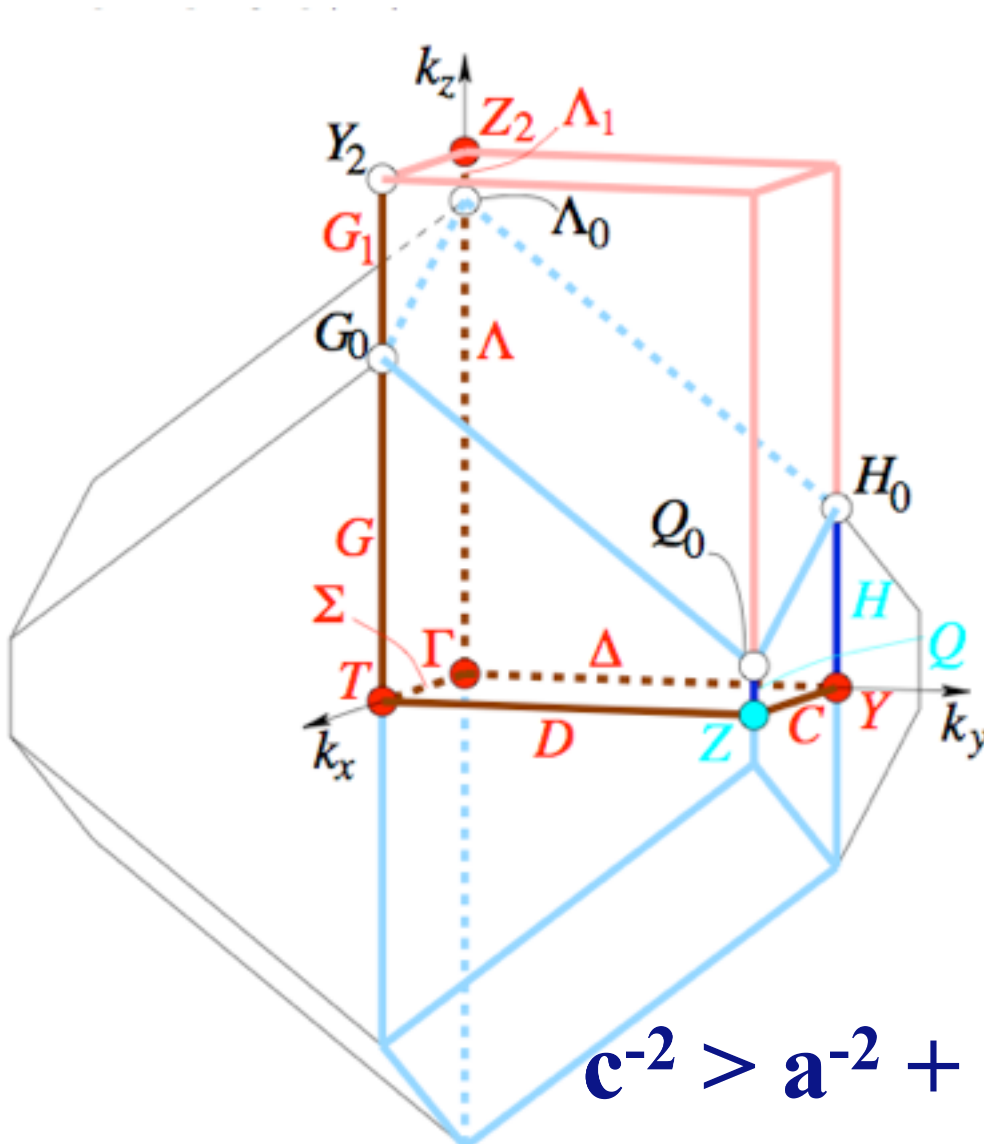
Retrieval tools

Reciprocal-space symmetry
Crystallographic Approach

Reciprocal space groups
Brillouin zones
Representation domain
Wave-vector symmetry

↔

Symmorphic space groups
IT unit cells
Asymmetric unit
Wyckoff positions



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

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

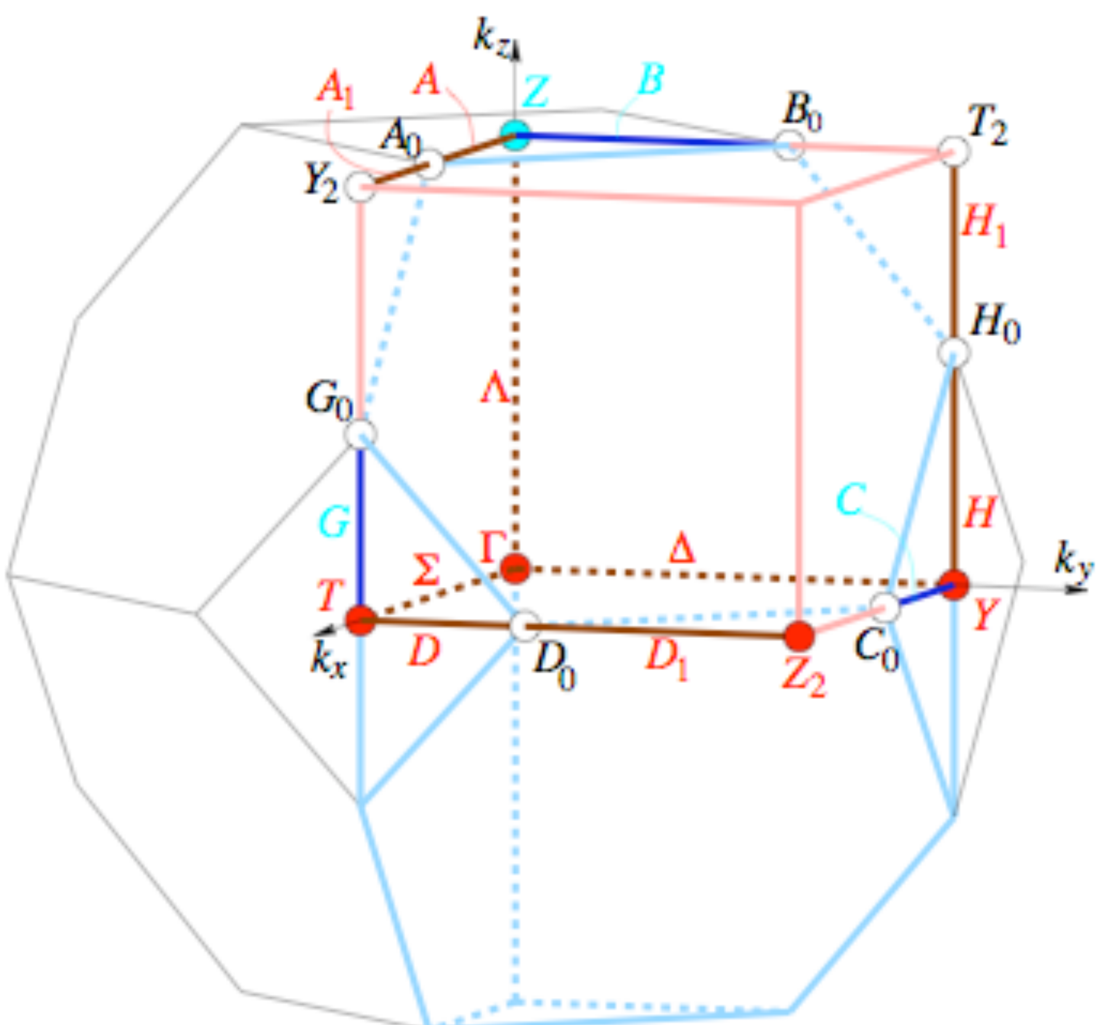
k-vector label CDML		Wyckoff position IT A			Parameters, see IT A
Γ	$0,0,0$	2	a	222	$0,0,0$
T	$0,\frac{1}{2},\frac{1}{2}$	2	b	222	$\frac{1}{2},0,0$
Z	$\frac{1}{2},\frac{1}{2},1$	2	c	222	$\frac{1}{2},\frac{1}{2},0$
$Z \sim Z_2$					$0,0,\frac{1}{2}$
Y	$\frac{1}{2},0,\frac{1}{2}$	2	d	222	$0,\frac{1}{2},0$
$Y \sim Y_2$					$\frac{1}{2},0,0$
Σ	$0,\alpha,\alpha$	4	e	2..	$x,0,0 : 0 < x < \frac{1}{2}$
C	$\frac{1}{2},\alpha,\frac{1}{2}+\alpha$	4	f	2..	$x,\frac{1}{2},0 : 0 < x < \frac{1}{2}$
Δ	$\alpha,0,\alpha$	4	g	.2.	$0,y,0 : 0 < y < \frac{1}{2}$
D	$\alpha,\frac{1}{2},\frac{1}{2}+\alpha$	4	h	.2.	$\frac{1}{2},y,0 : 0 < y < \frac{1}{2}$

Example:

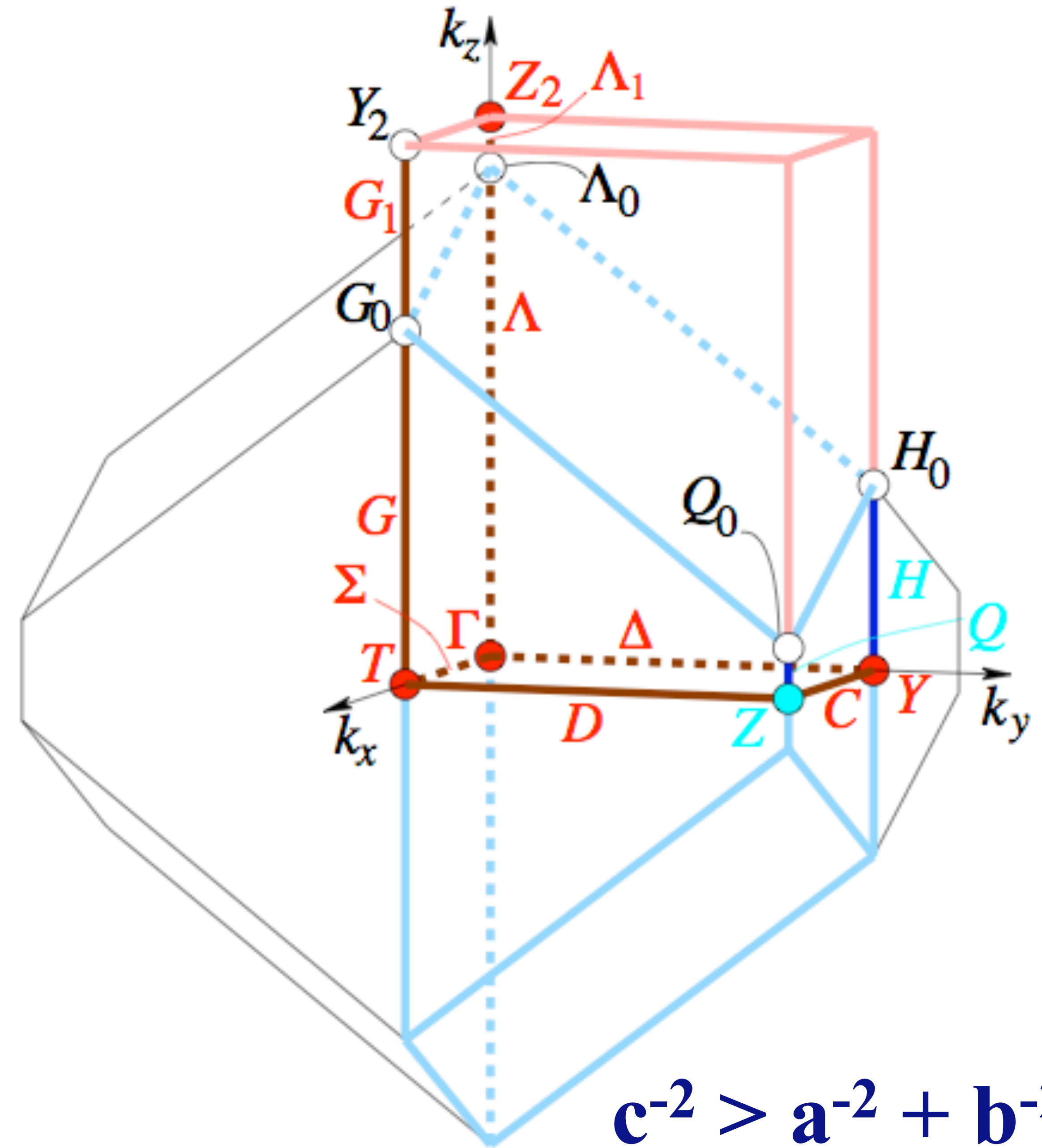
The k-vector Types of Group 22 [*F*222]

Brillouin zone

(Diagram for arithn



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

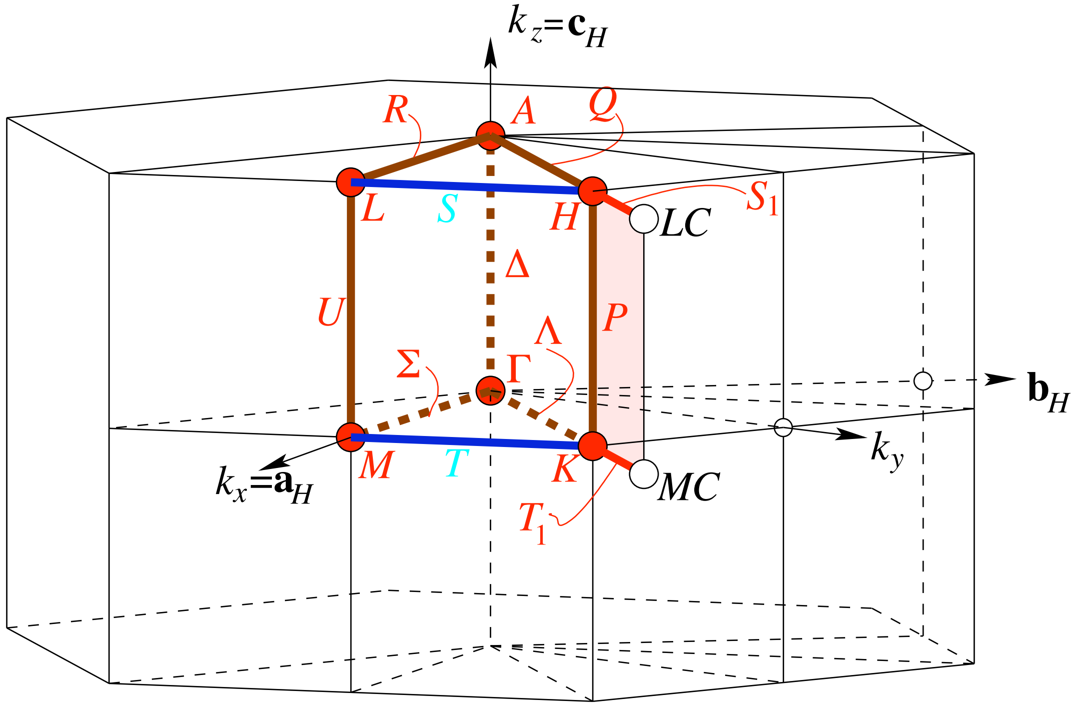


$c^{-2} > a^{-2} + b^{-2}$

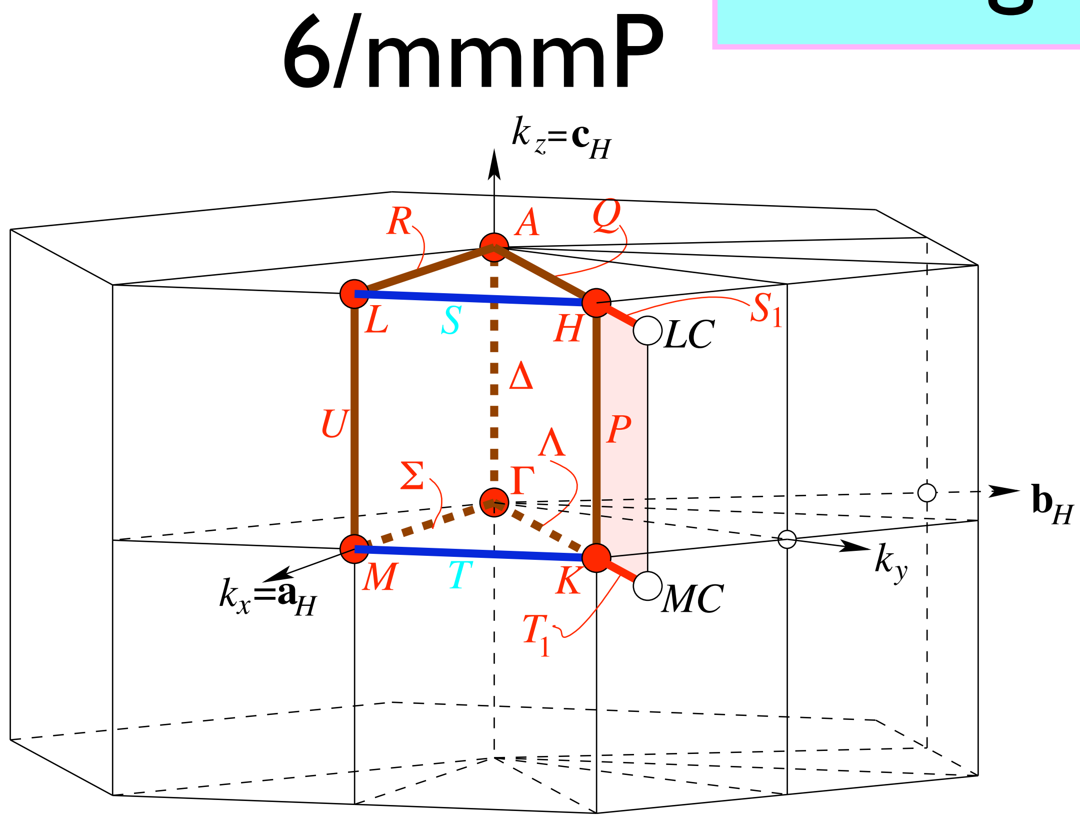
Hexagonal crystal classes

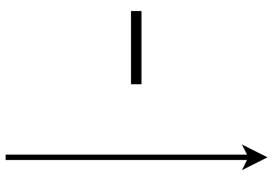
Hexagonal crystal classes

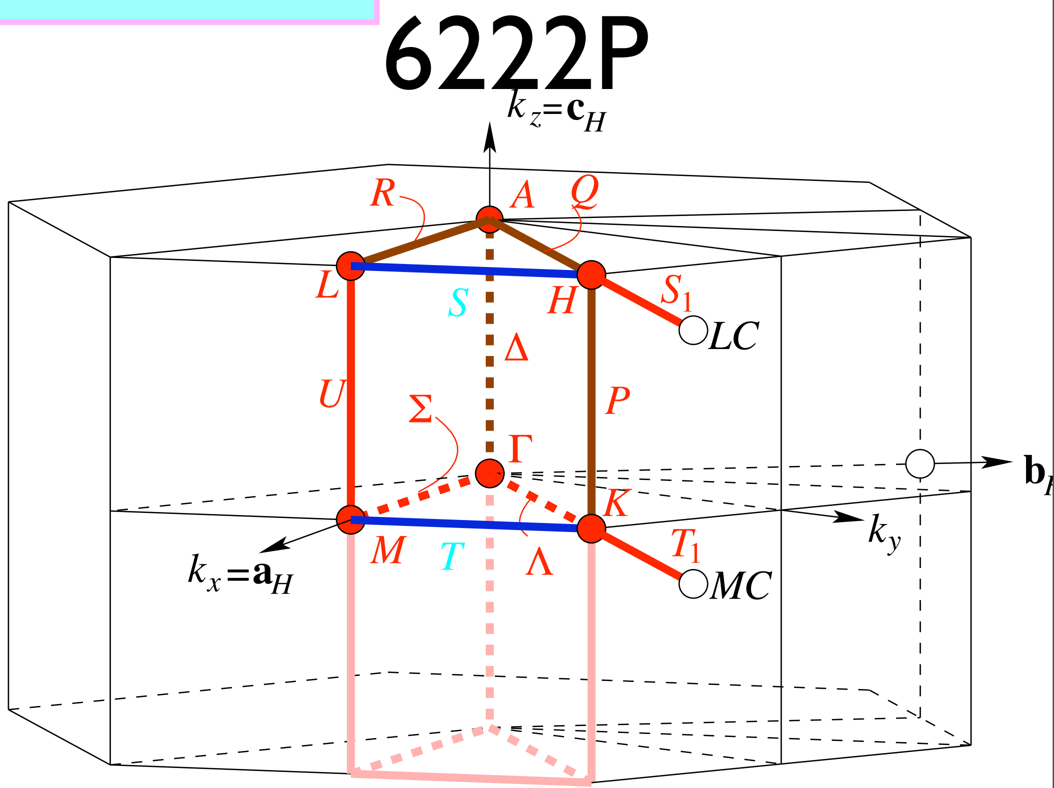
6/mmmP



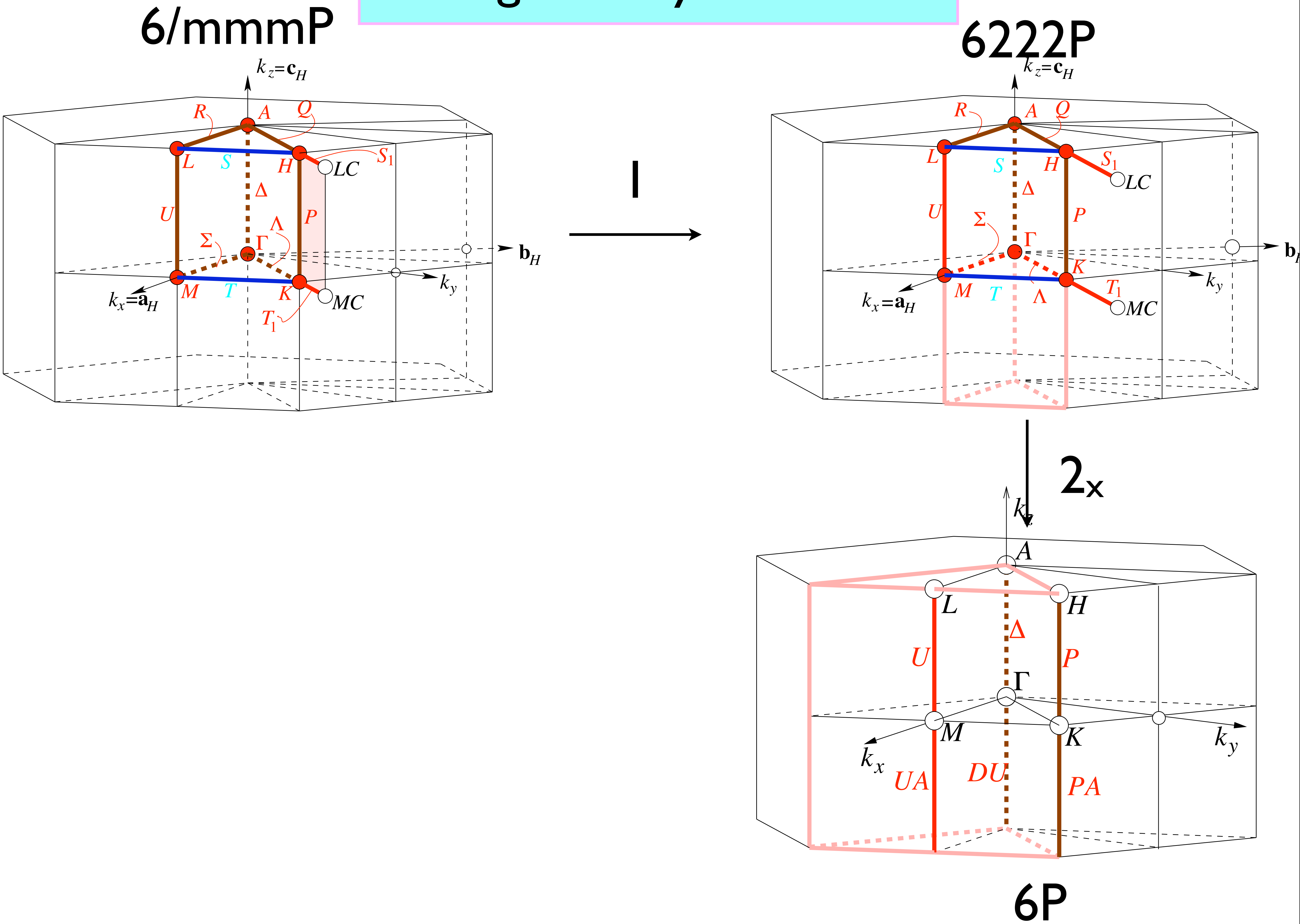
Hexagonal crystal classes



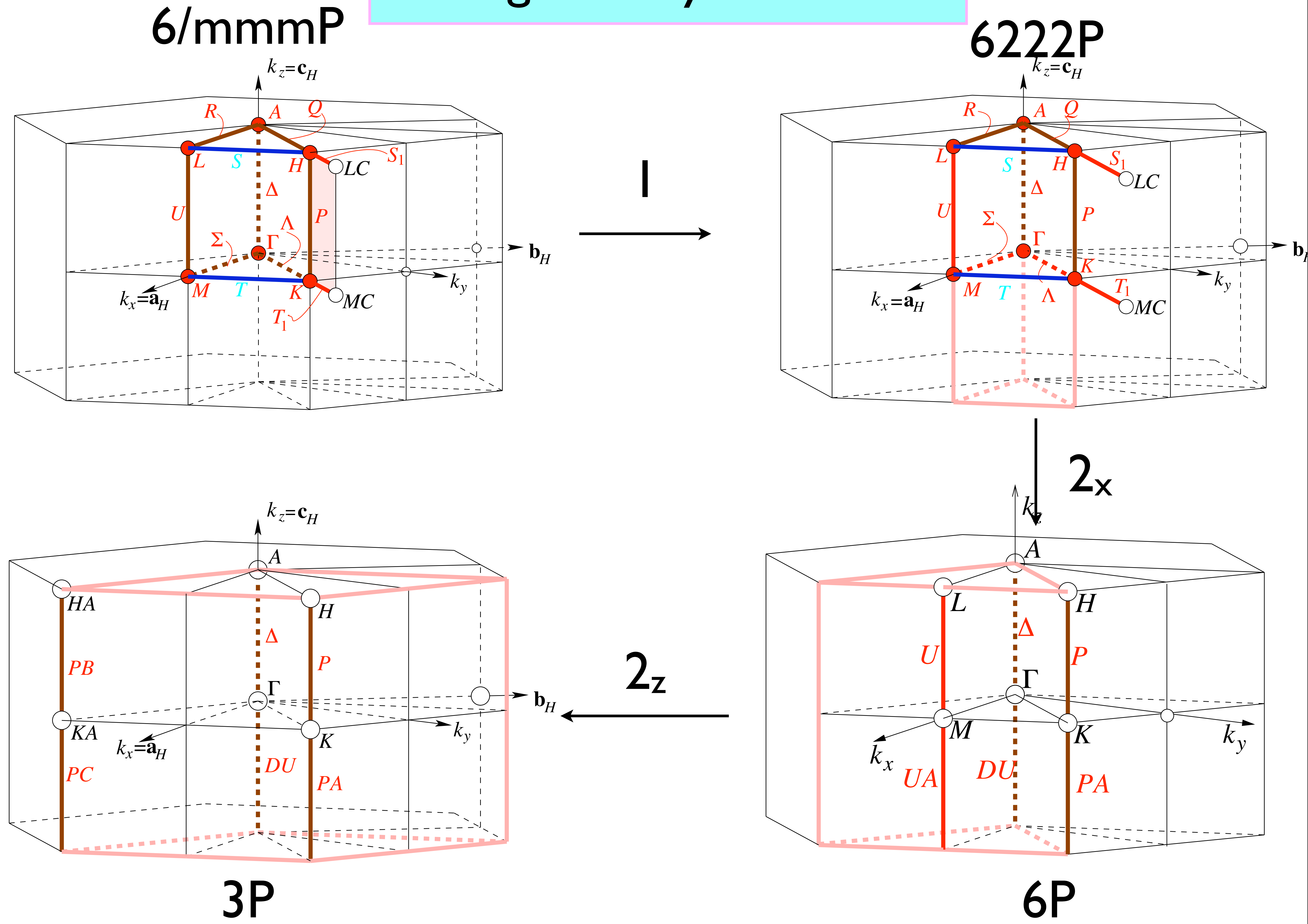




Hexagonal crystal classes



Hexagonal crystal classes



Database on Representations of Point Groups

group-subgroup relations

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

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 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]

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
$[V^2]xV$	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

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

space group

k vector data	Reciprocal basis	primitive (CDML)
	Coordinates	k_x 0 k_y 1/2 k_z 0
	Label	X

k-vector data

Optional: If you wish to see the full-group irreps for the generators check this ☑

Optional: If you wish to change conventional (ITA) basis check this ☐

Rotation	1	0	0
	0	1	0
	0	0	1
Origin Shift	0	0	0

non-conventional setting

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

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

arbitrary element

Space-group data

REPRES: output

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

```
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
```

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

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

Little group G^X

```
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

 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
```

$$G=G^{X}+q_{2}G^{X}+\ldots+q_{k}G^{X}$$

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 3

Obtain the irreps for the space group 4mm for the k-vectors Γ(000) and X(01/20) using the program REPRES. Compare the results with the solutions of Problem 1.

Use the program REPRES for the derivation of the irreps of a general k-vector of the group P4mm and compare the results with the results of Problem 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

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

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

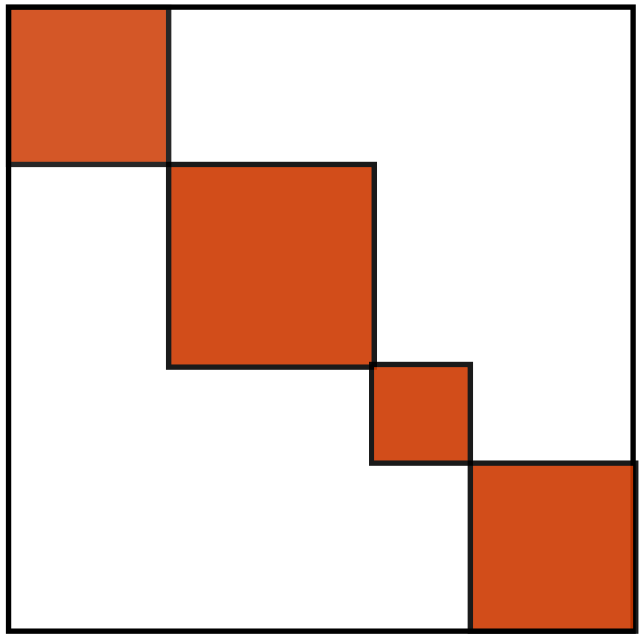
$\{D(G)\downarrow H\}$: subduced rep of H<G

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

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

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

CORREL: INPUT data

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

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

$*k_G = *k_{H,1} + *k_{H,2} + ... + *k_{H,k}$

```
-------------------------------------------------------
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)
```

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

$D_1(G)$: irrep of G

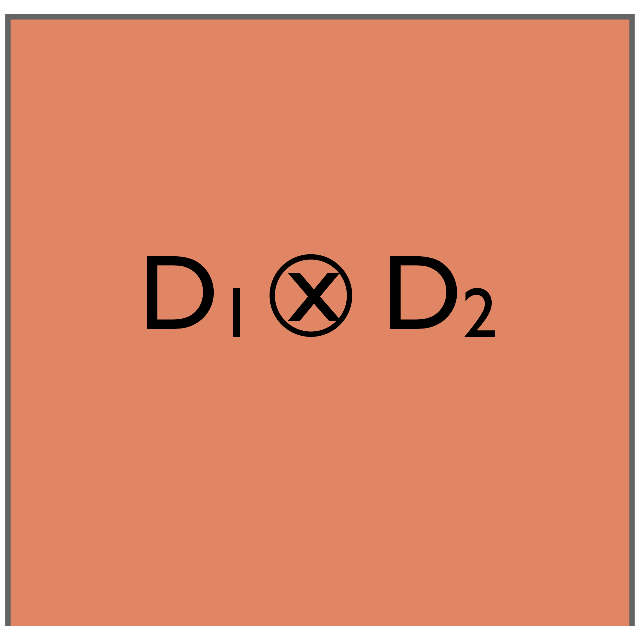
$\{D_1(e), D_1(g_2), \ldots, D_1(g_n)\}$

$D_2(G)$: irrep of G

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

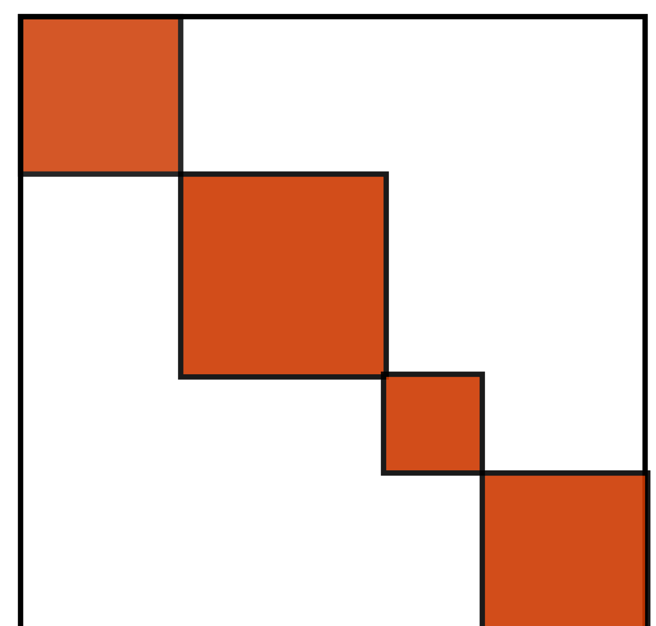
Direct-product representation

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



Reduction

$$D_1 \otimes D_2 \longrightarrow \bigoplus m_i D_i(G)$$



irreps of G

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 P4mm and its k-vector X(01/20). Determine the wave-vector selection rules for the product

$$*X(0\tfrac{1}{2}0) \otimes *X(0\tfrac{1}{2}0).$$

The k-vector Types of Group 99 [*P4mm*]

(Table for arithmetic crystal class 4mmP)

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

Reciprocal-space group (P4mm)*, No. 99

Brillouin zone

k-vector label		Wyckoff position			Parameters
CDML		ITA			ITA
GM	0,0,0	1	a	4mm	0,0,z: z=0
Z	0,0,1/2	1	a	4mm	0,0,z: z=1/2
LD	0,0,u	1	a	4mm	0,0,z: 0<z<1/2
LE	0,0,-u	1	a	4mm	0,0,-z: 0<z<1/2
LE + SM + LD + Z					
[Z_1Z]		1	a	4mm	o,o,z: -1/2<z<=1/2
M	1/2,1/2,0	1	b	4mm	1/2,1/2,z:z=0
A	1/2,1/2,1/2	1	b	4mm	1/2,1/2,z:z=1/2
V	1/2,1/2,u	1	b	4mm	1/2,1/2,z: 0<z<1/2
VA	1/2,1/2,-u	1	b	4mm	1/2,1/2,-z: 0<z<1/2
VA + M + V + A					
[A_1A]		1	b	4mm	0,1/2,z: -1/2<z<=1/2
X	0,1/2,0	2	c	2mm.	0,1/2,z:z=0
R	0,1/2,1/2	2	c	2mm.	0,1/2,z: z=1/2
W	0,1/2,u	2	c	2mm.	0,1/2,z: 0<z<1/2
WA	0,1/2,-u	2	c	2mm.	0,1/2,-z: 0<z<1/2
WA + X + W + R					
[R_2R]		2	c	2mm.	0,1/2,z: -1/2<z<=1/2
SM	u,u,0	4	d	..m	x,x,z: 0=z<x<1/2
S	u,u,1/2	4	d	..m	x,x,z: 0<x<z=1/2
C	u,u,v	4	d	..m	x,x,z: 0<x,z<1/2
CA	u,u,-v	4	d	..m	x,x,-z: 0<x,z<1/2
CA + SM + C + S					
[ZZ_1A_1A]		4	d	..m	x,x,z: 0<x<1/2, -1/2<z<=1/2
DT	0,u,0	4	e	.m.	0,y,z: 0=z<y<1/2
U	0,u,1/2	4	e	.m.	0,y,z: 0<y<z=1/2
B	0,u,v	4	e	.m.	0,y,z: 0<y,z<1/2
BA	0,u,-v	4	e	.m.	0,y,-z: 0<y,z<1/2
BA + DT + B + U					
[ZZ_1R_2R]		4	e	.m.	x,x,z: 0<x<1/2, -1/2<z<=1/2
Y	u,1/2,0	4	f	.m.	x,1/2,z: 0=z<x<1/2
T	u,1/2,1/2	4	f	.m.	x,1/2,z: 0<x<z=1/2
F	u,1/2,v	4	f	.m.	x,1/2,z: 0<x,z<1/2
FA	u,1/2,-v	4	f	.m.	x,1/2,-z: 0<x,z<1/2
FA + Y + F + T					
[AA_1R_2R]		4	f	.m.	x,1/2,z: 0<x<1/2, -1/2<z<=1/2
GP	u,v,w	8	g	1	x,y,z: -1/2<x<y<1/2, -1/2<z<=1/2.

DIRPRO: INPUT data

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)

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

```
------------------------------------------------------------------------------
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 $D^{DT,1}$

DIRPRO: output

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)
```

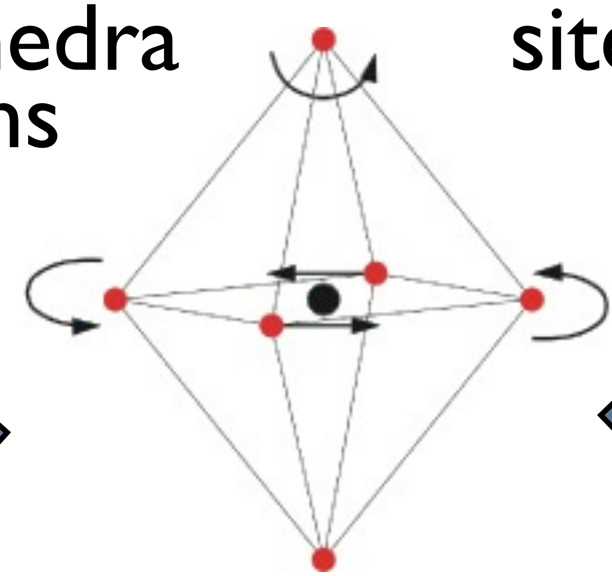
$$D_1(G) \otimes D_2(G)$$

$$\bigoplus \; m_i D_i(G)$$

Problem: LOCALIZED and EXTENDED STATES — SITESYM

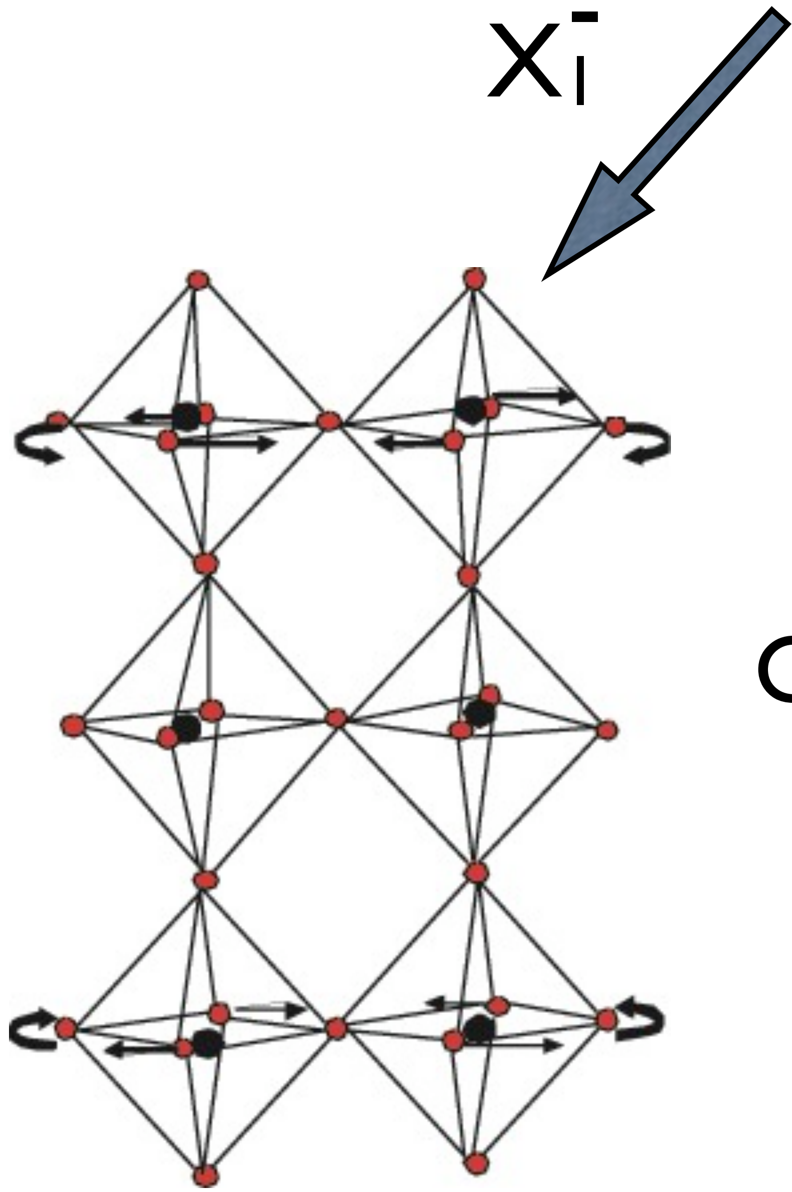
BO_6 octahedra rotations

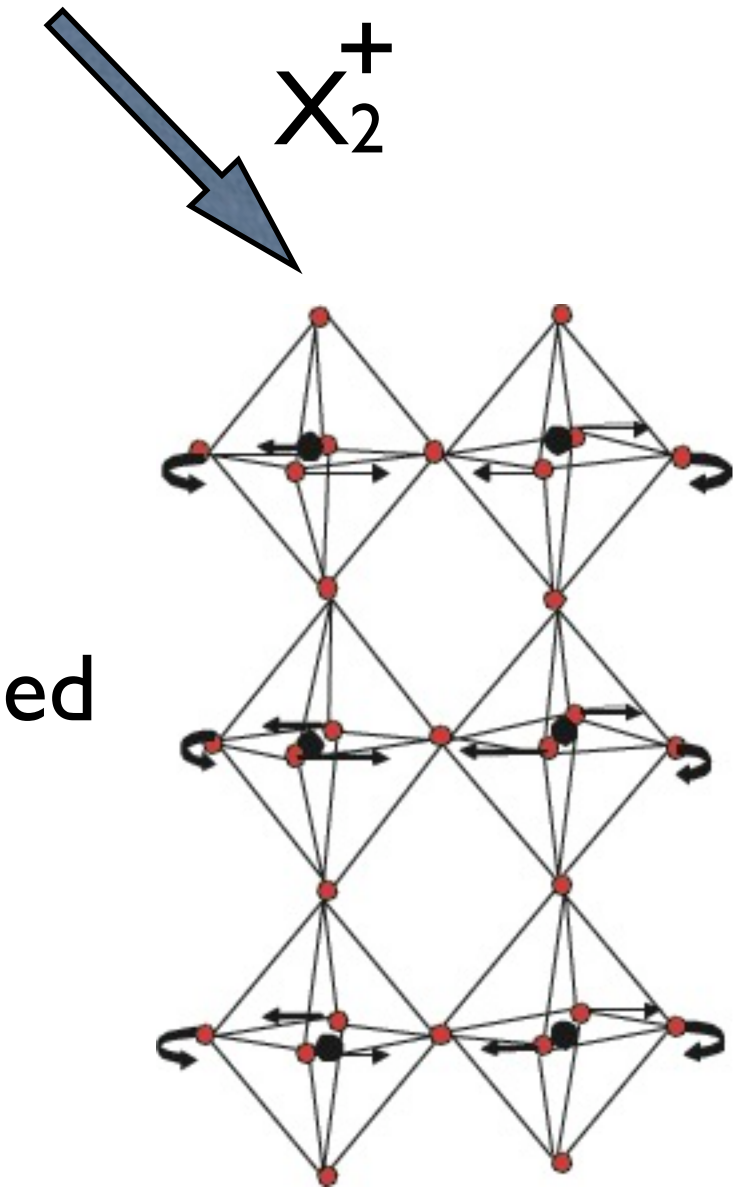
site symmetry 4mm irrep A_2



X_1^-

X_2^+





Crystal-extended modes in Aurivillius compounds