CRYSTALLOGRAPHY ONLINE Workshop

on the use and applications of the structural and magnetic tools of the

BILBAO CRYSTALLOGRAPHIC SERVER

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REPRESENTATIONS OF CRYSTALLOGRAPHIC GROUPS

SPACE-GROUP REPRESENTATIONS

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SPACE GROUPS

Space group G:

The set of all symmetry operations (isometries) of a crystal pattern

Translation subgroup T:
$T \triangleleft G$

The infinite set of all translations that are symmetry operations of the crystal pattern

Point group of the space groups P_G:

The factor group of the space group G with respect to the translation subgroup T: $P_G \cong G/H$

$$(\boldsymbol{W},\boldsymbol{w}) \longrightarrow \boldsymbol{W} \qquad P_G=\{\boldsymbol{W} | (\boldsymbol{W},\boldsymbol{w}) \in G\}$$

Irreducible representations of a group induced from the irreps of one of its normal subgroups

Method: Consider a group G and its normal subgroup $H \lhd G$ with its all irreps

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

Step 1.

TRANSLATION SUBGROUP IRREPS $T_G \lhd G$

Born-von Karman boundary condition

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

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

homomorphic mapping

infinite T_G: {(I,0), (I,t}, (I,2t),...,(I,Nt),(I,(N+1)t), ...,(I,2Nt), ...}

finite T_G: {(I,0), (I,t}, (I,2t),...,(I,(N-1)t)}

kernel ={(I,0), (I,Nt), (1,2Nt),…}

Irreps of Translation group

Finite Abelian groups $\begin{cases} \text{cyclic groups} \\ \text{direct product of cyclic groups} \end{cases}$

A: $\{a, a^2, \ldots, a^s\}$ → $D^p(a^m)$, $p=0,1,\ldots,s-1$

$$exp(-i2\pi m)\frac{p}{s}$$

B: $\{b, b^2, \ldots, b^r\}$ → $D^q(b^n)$, $q=0,1,\ldots,r-1$

$$exp(-i2\pi n)\frac{q}{r}$$

→ $A \otimes B$: $\{(a^m, b^n)\}$ $m=1,\ldots,s;$ $n=1,\ldots,r$ → $D^p(a^m) \otimes D^q(b^n)$

$$D^{p,q}(a^m, b^n) = exp(-i2\pi m)\frac{p}{s}\; exp(-i2\pi n)\frac{q}{r}$$

$p=0,1,\ldots,s-1 \quad q=0,1,\ldots,r-1$

IRREPS of Translational group

Translational subgroup: T

$$T = T_1 \otimes T_2 \otimes T_3 = \{(t_1^k, t_2^l, t_3^m)\}$$

$$D^{p,q,r}(t_1^k, t_2^l, t_3^m) =$$

$$exp(-i2\pi k)\frac{p}{N_1} \; exp(-i2\pi l)\frac{q}{N_2} \; exp(-i2\pi m)\frac{r}{N_3}$$

number of irreps:

$p = 0, 1, \ldots, N_1 - 1 \quad q = 0, 1, \ldots, N_2 - 1 \quad r = 0, 1, \ldots, N_3 - 1$

$\dim D^{p,q,r}(t_1^k, t_2^l, t_3^m) = 1$

IRREPS of Translational group

reciprocal space

L: a_1, a_2, a_3 ⟷ L*: a^*_1, a^*_2, a^*_3

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

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

$k_i = q_i/N_i$

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

ITA conventions:

$$(\mathbf{k}\ \mathbf{t}) = (k_1, k_2, k_3)\begin{vmatrix}\mathbf{a}^*_1\\ \mathbf{a}^*_2\\ \mathbf{a}^*_3\end{vmatrix}(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)\begin{vmatrix}t_1\\ t_2\\ t_3\end{vmatrix} = 2\pi(k_1, k_2, k_3)\begin{vmatrix}t_1\\ t_2\\ t_3\end{vmatrix}$$

IRREPS of Translational group

unit cell of reciprocal space (fundamental region)

$k' = k + K, \quad K = h_1 \mathbf{a_1}^* + h_2 \mathbf{a_2}^* + h_3 \mathbf{a_3}^*, \; K \in L^*$

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

first Brillouin zone (Wigner-Seitz cell)

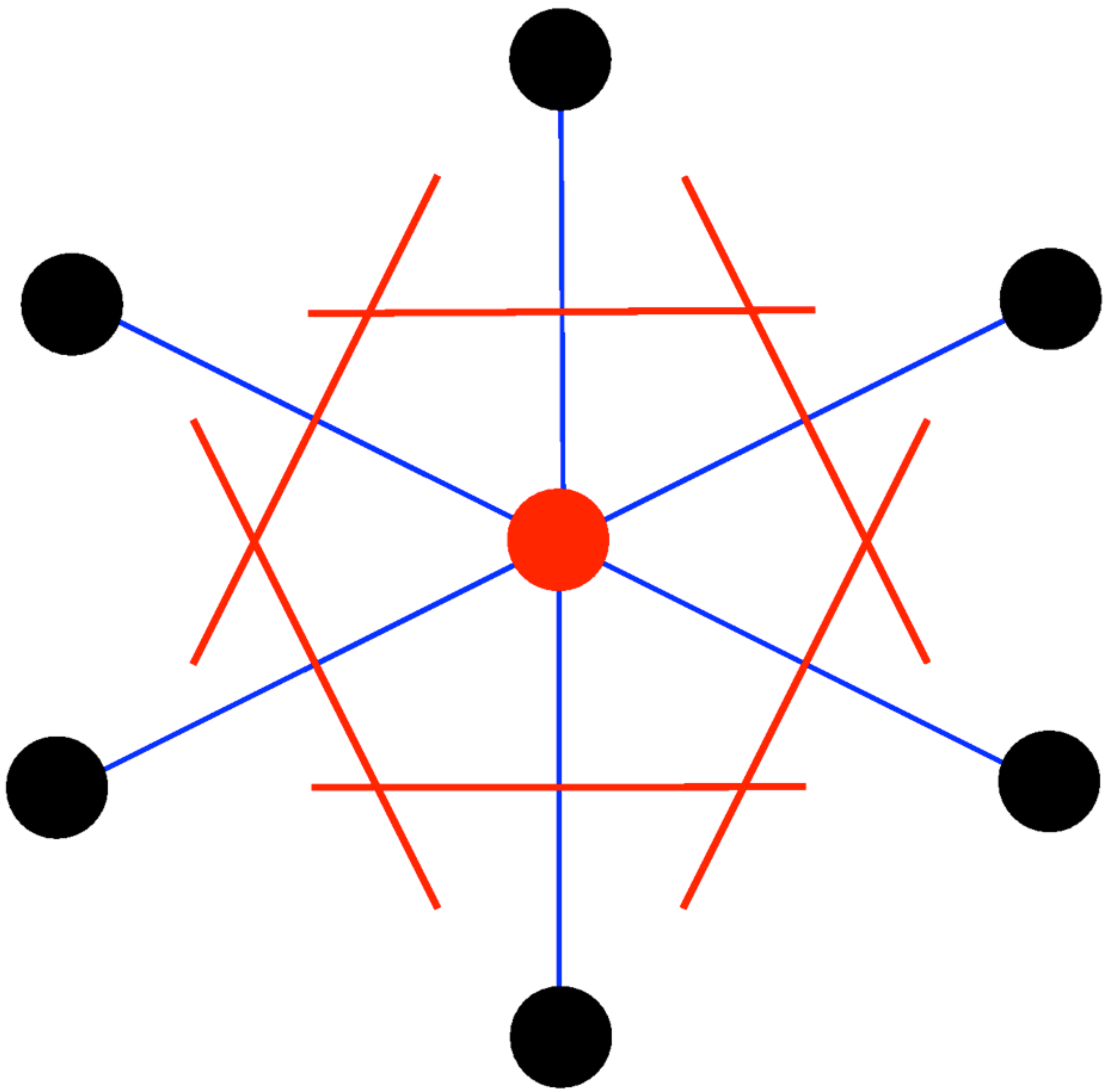
$|k| \leq |K-k|, \; \forall K \in L^*$

crystallographic unit cell

$0 \leq |k| < 1$

first Brillouin zone (Wigner-Seitz cell)

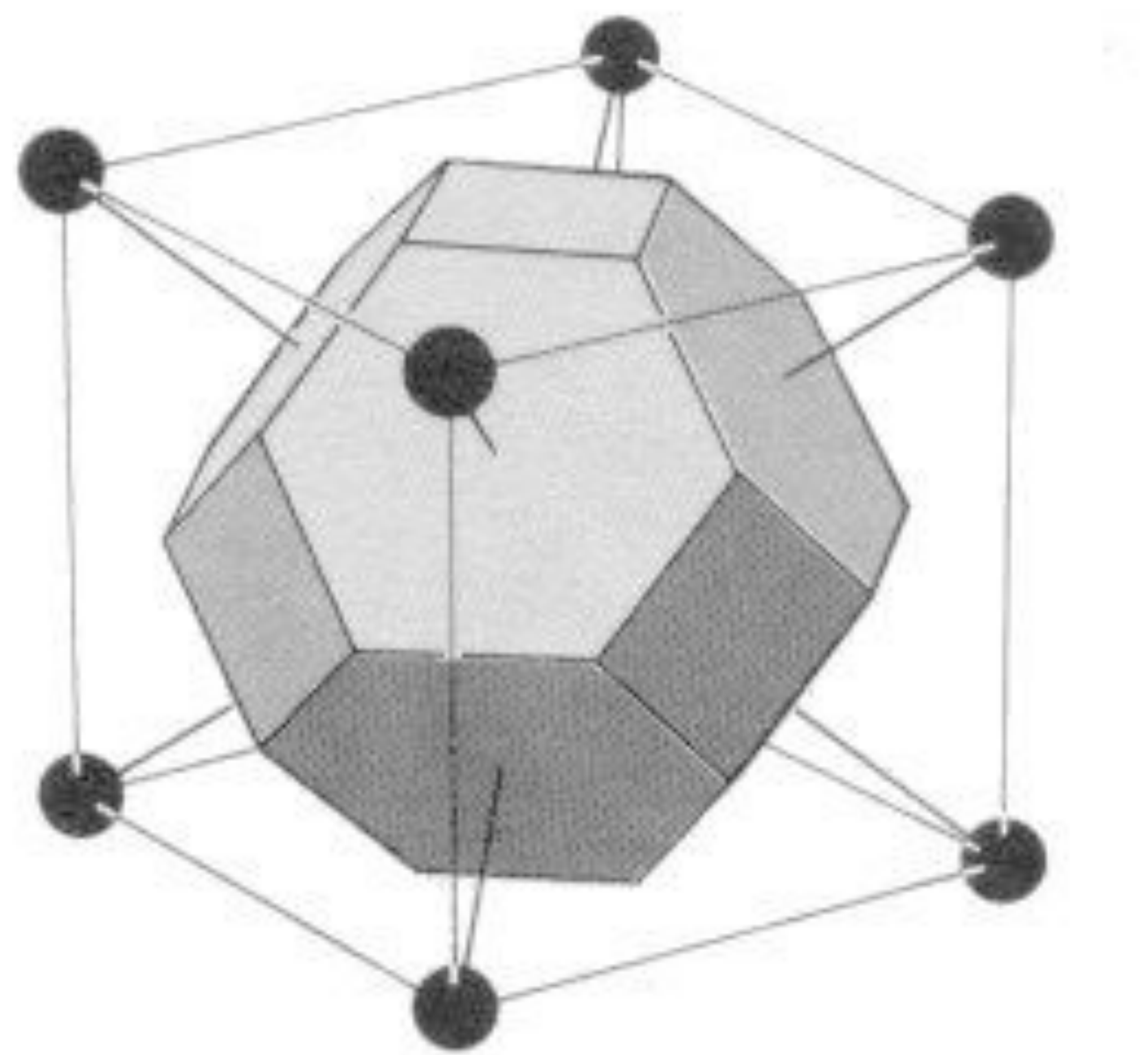
$|k| \leq |K-k|, \forall K \in L^*$



first Brillouin zone (Wigner-Seitz cell)

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

Wigner-Seitz construction for *bcc* lattice

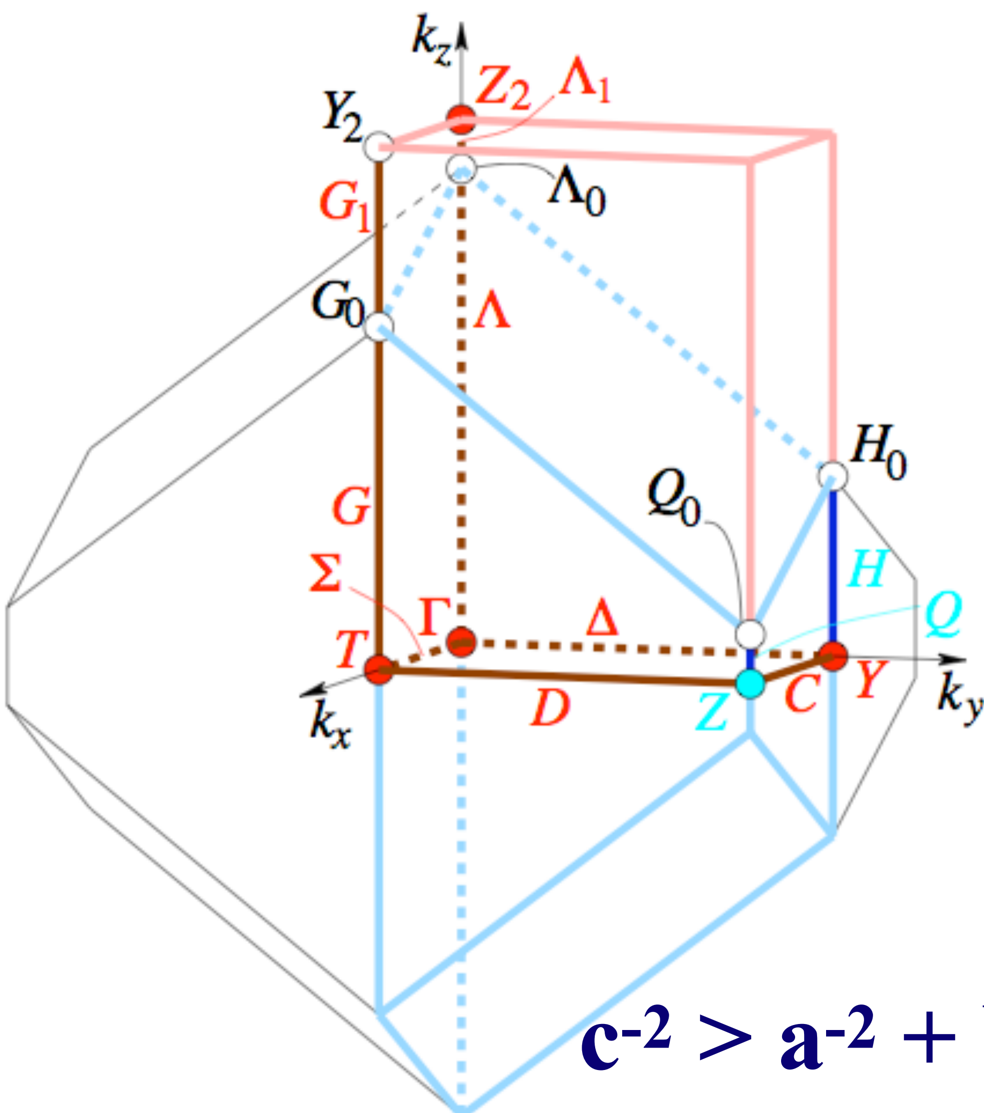


Brillouin Zone Database
Crystallographic Approach

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 [*F222*]

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
$T \sim T_2$			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
$Y \sim Y_2$			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
$U \sim SM_1 = [SM_0\ T_2]$			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

Step 2. Distribute the irreps of H into orbits under G and select a representative

Conjugate representations

conjugate representation $G \triangleright H$ **H: normal subgroup**

$$D^S(H)=\{D^S(g^{-1}h_i g),\ h_i\in H,\ g\in G, g\notin H\}$$

$$H=\{e, h_2, h_3, \ldots, h_i, \ldots, h_n\}$$

$$\{D(e), D(h_2), \ldots, D(h_n)\}$$

conjugate irrep

$$\{D(g^{-1}eg), D(g^{-1}h_2 g), \ldots, D(g^{-1}h_n g)\}$$

$$D^S(H)=\{D(e), D(h'_2), \ldots, D(h'_n)\}$$

Conjugate representations

properties

CONJUGATE REPRESENTATION

$$(\mathbf{D}^s(\mathcal{H}))_g = \{\mathbf{D}^s(g^{-1}\, h\, g),\ \ h \in \mathcal{H}\},$$

$$\text{where} g \in \mathcal{G},\ \ g \notin \mathcal{H}$$

1. $dim(\mathbf{D}^s(\mathcal{H})) = dim((\mathbf{D}^s(\mathcal{H}))_g)$;
2. $(\mathbf{D}^s(\mathcal{H}))_g$ is an irrep if $\mathbf{D}^s(\mathcal{H})$ is.
3. Equivalent or nonequivalent conjugate rep

$$(\mathbf{D}^s(\mathcal{H}))_g \begin{cases} \sim \mathbf{D}^s(\mathcal{H}) \\ \not\sim \mathbf{D}^s(\mathcal{H}) \end{cases}$$

Conjugate representations and orbits

Group–normal subgroup pair $\mathcal{G} \triangleright \mathcal{H}$

$\mathcal{G} = \mathcal{H} \cup g_2 \mathcal{H} \cup \ \ldots \ \cup g_r \mathcal{H}$

ORBIT OF CONJUGATE REPS

$O\ (\mathbf{D}^s(\mathcal{H})) = \{\mathbf{D}^s(\mathcal{H}),\ (\mathbf{D}^s(\mathcal{H}))_{g_2}, \ldots,\ (\mathbf{D}^s(\mathcal{H}))_{g_r}\},$

where $g \in \mathcal{G}$

Step 3.

Step 4.

Determination of the **little group** and the **allowed little-group** representations

LITTLE GROUP $\mathcal{G}^s$:

Group-normal subgroup pair $\mathcal{G} \triangleright \mathcal{H}$; Irrep $\mathbf{D}^s(\mathcal{H})$

$$\mathcal{G}^s \equiv \mathcal{G}^s(\mathbf{D}^s(\mathcal{H})) = \{g \in \mathcal{G} : (\mathbf{D}^s(\mathcal{H}))_g \sim \mathbf{D}^s(\mathcal{H})\}$$

$$\mathcal{G} > \mathcal{G}^s \triangleright \mathcal{H}.$$

ALLOWED IRREP OF THE LITTLE GROUP:

$$\mathbf{D}^j(\mathcal{G}^s(\mathbf{D}^s(\mathcal{H}))) \downarrow \mathcal{H} \ni \mathbf{D}^s(\mathcal{H})$$

NOTE: terminology

allowed irrep or ***allowable*** irrep or ***small*** irrep

Step 2.

Classification of the irreps of the Translation subgroup.

orbits of irreps of T (under the action of G)

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

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

$\Gamma^{k'} \sim \Gamma^{k} \quad k'= k\,W + K$

$O(\Gamma^{k})=\{\Gamma^{k}, \Gamma^{k'},\ldots, |k'= k\,W + K, W\in\overline{G}\}$

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

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

special and general

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

space-group irreps

Orbits of irreps of the Translation subgroup.

orbit of k

$$O(\Gamma^k)=\{\Gamma^k, \Gamma^{k'}, \ldots, | k' = k W + K, W \in G\}$$

star of k: k*

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

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

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

representation domain

exactly one k-vector from each star
(one irrep from each orbit of irreps of T)

space-group irreps

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

Step 3.

Little group G^k

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

Step 4.

Allowed irreps of G^k

$$(D^{k,i}\downarrow T) = \exp(-ikt)\boldsymbol{I}$$

special case: general k-vector

star of k
little group of k
allowed irreps

?

space-group irreps

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

Step 4.

Allowed irreps of G^k

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

Case 1.

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 $\overline{\mathcal{G}}^{\mathbf{k}}$,

space-group irreps

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

CASE 2:

1. $\mathbf{k}$ 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 $\mathcal{G}^{\mathbf{k}}$

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

composition series for space groups

space-group irreps

Step 5.

INDUCTION THEOREM

1. Let $\mathbf{D}^j(\mathcal{H})$ be an irrep from the orbit $O(\mathbf{D}^j(\mathcal{H}))$ with the little group $\mathcal{G}^j(\mathbf{D}^j(\mathcal{H}))$ relative to $\mathcal{G}$. Then each allowed irrep $\mathbf{D}^m(\mathcal{G}^j(\mathbf{D}^j(\mathcal{H})))$ of $\mathcal{G}^j(\mathbf{D}^j(\mathcal{H}))$ induces an irrep $\mathbf{D}^{Ind}(\mathcal{G})$, whose subduction to $\mathcal{H}$ yields the orbit $O(\mathbf{D}^j(\mathcal{H}))$.

2. All irreps of $\mathcal{G}$ are obtained exactly once if the procedure described in 1 is applied on one irrep $\mathbf{D}^j(\mathcal{H})$ from each orbit $O(\mathbf{D}^j(\mathcal{H}))$ of irreps of $\mathcal{H}$ relative to $\mathcal{G}$.

Step 5.

Induction procedure

Construction of the irreps of the space group G by induction from the the small (allowed) irreps of the little group G^k<G

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

Decomposition of $\mathcal{G}$ relative to $\mathcal{G}^{\mathsf{k}}$

An obvious choice of coset representatives of $\mathcal{G}$ relative to $\mathcal{G}^{\mathsf{k}}$ 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 $\overline{\mathcal{G}}^{\mathsf{k}}$

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

a) Construction of the induction matrix

The elements of the little group $\mathcal{G}^{\mathbf{k}}$ and the coset representatives $\{q_1, q_2, ..., q_s\}$ 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	I	0	0
0	0	I	0
I	0	0	0
0	0	0	I

All irreps of the space group $\mathcal{G}$ for a given $\mathbf{k}$ 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 3.5.1.1

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***

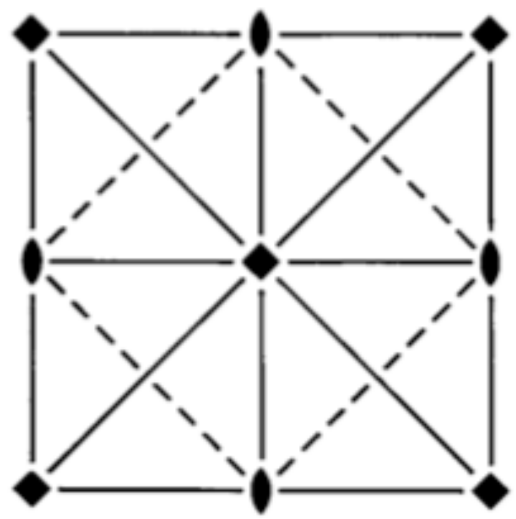
(ii) Calculate a set of coset representatives of the decomposition of the group ***P4mm*** with respect to the little groups of the **k**-vectors Γ(000) and **X**, and construct the corresponding full space group irreps of ***P4mm***

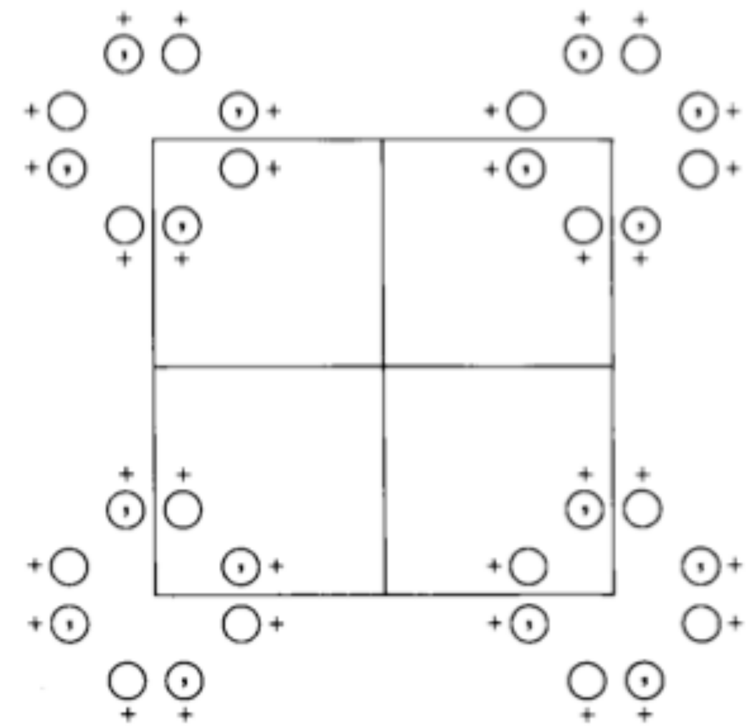
International Tables for Crystallography (2006). Vol. A, Space group 99, pp. 382–383.

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

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

ITA space-group data (selection)





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) $m \ \ x,x,z$

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

Brillouin Zone Database BilbaoCrystServer

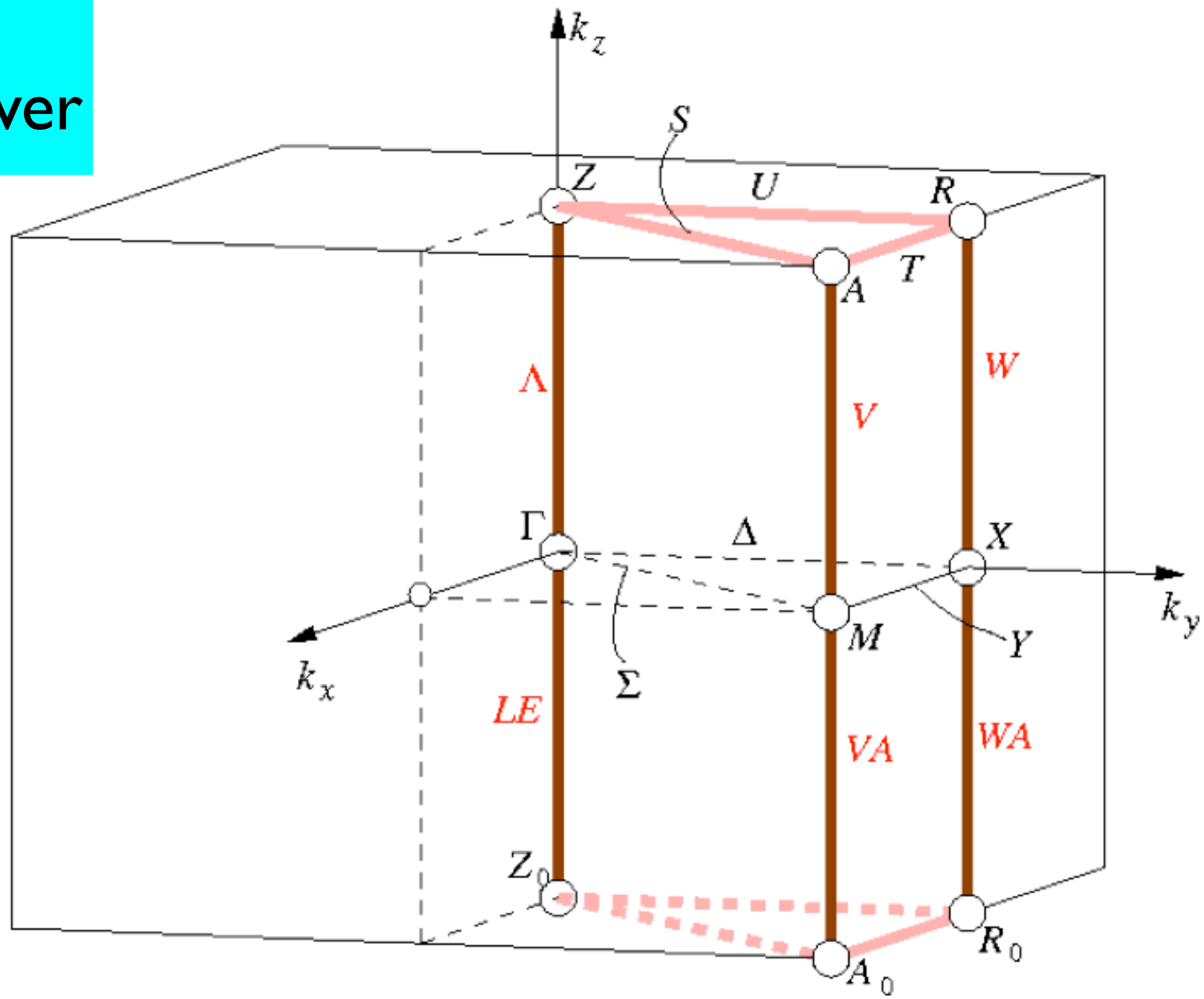
5.5 Crystal class $4mm$

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 3.5.1.2

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

(i) Determine the full irreps of space group **P4bm**, **k**-vector Γ(000). Is there a difference to the irreps of space group **P4mm**, **k**= Γ(000)?

(ii) Determine the allowed little-group irreps of the space group **P4bm**, for **k**-vector **X** (0½0). Compare the obtained results with those obtained for the space group **P4mm**, **k**= **X** (0½0).

EXERCISES

Problem 3.5.1.3

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.

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BASIC DATABASES AND PROGRAMS OF REPRESENTATIONS OF CRYSTALLOGRAPHIC GROUPS

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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
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 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

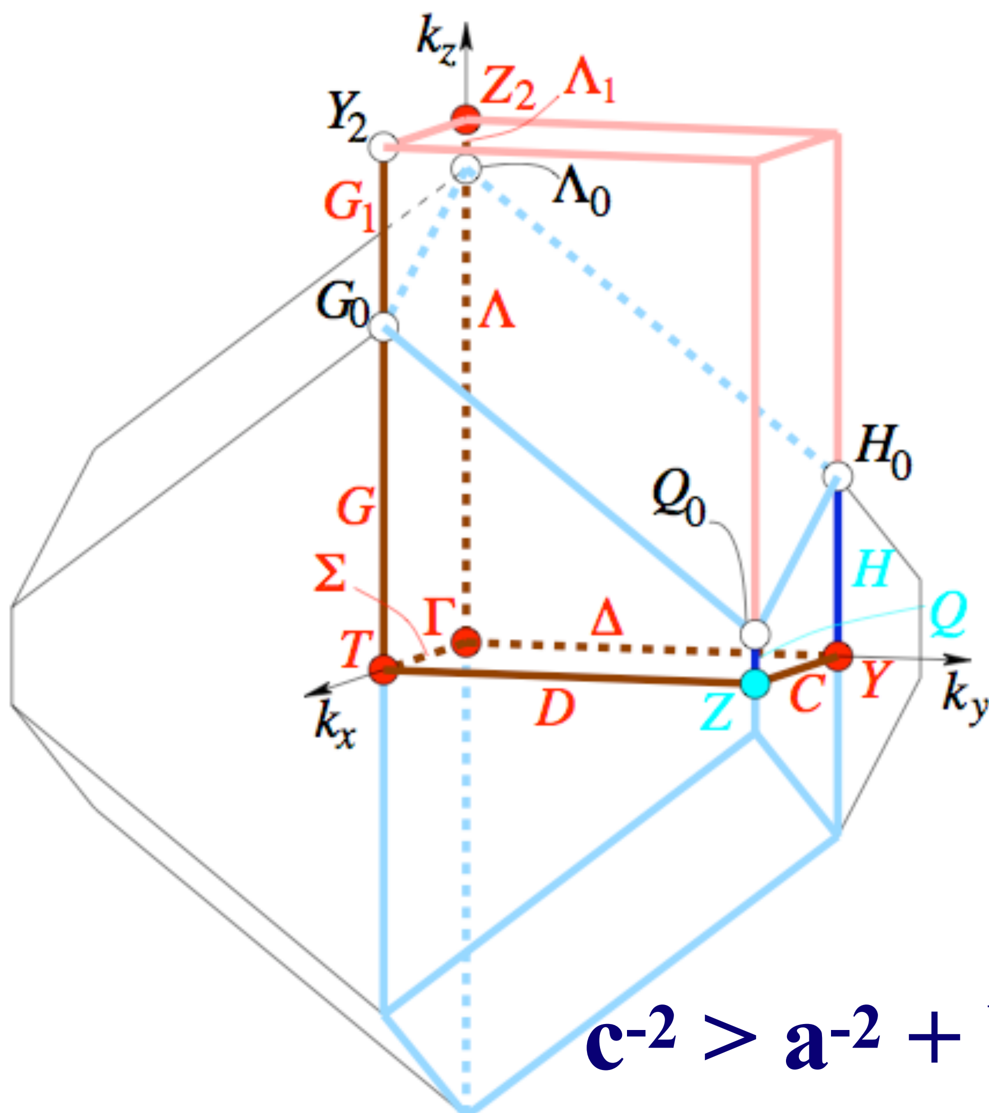
C_{6v}(6mm)	A_1	A_2	B_1	B_2	E_2	E_1
V	1	·	·	·	·	1
$[V^2]$	2	·	·	·	1	1
$[V^3]$	2	·	1	1	1	2
$[V^4]$	3	·	1	1	3	2
A	·	1	·	·	·	1
$[A^2]$	2	·	·	·	1	1
$[A^3]$	·	2	1	1	1	2
$[A^4]$	3	·	1	1	3	2
$[V^2]\times V$	3	1	1	1	2	4
$[[V^2]^2]$	5	·	1	1	4	3
$\{V^2\}$	·	1	·	·	·	1
$\{A^2\}$	·	1	·	·	·	1
$\{[V^2]^2\}$	1	2	1	1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

Brillouin Zone Database Crystallographic Approach

Reciprocal space groups
- 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 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
$T \sim T_2$			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
$Y \sim Y_2$			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
$U \sim SM_1=[SM_0\ T_2]$			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

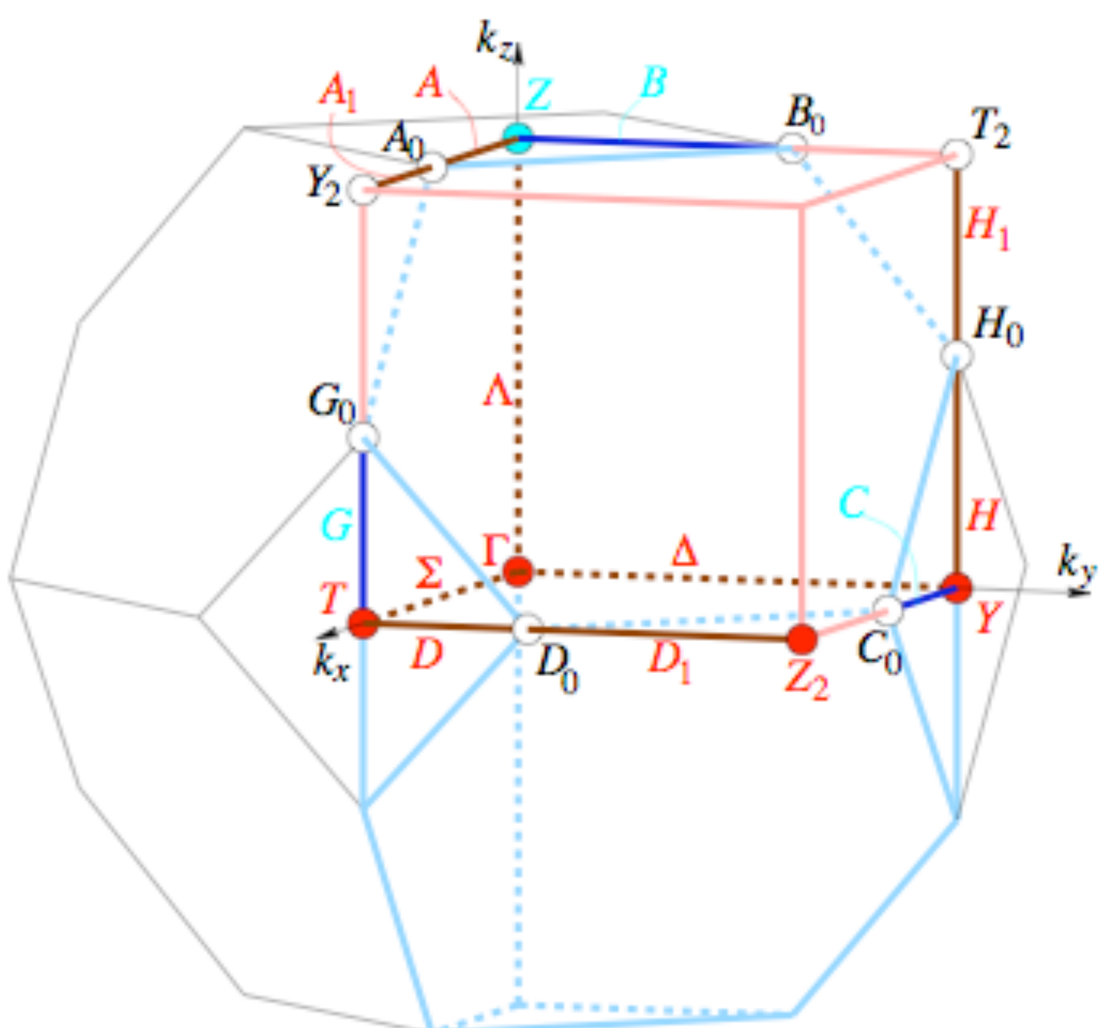
Example:

Brillouin zone Database

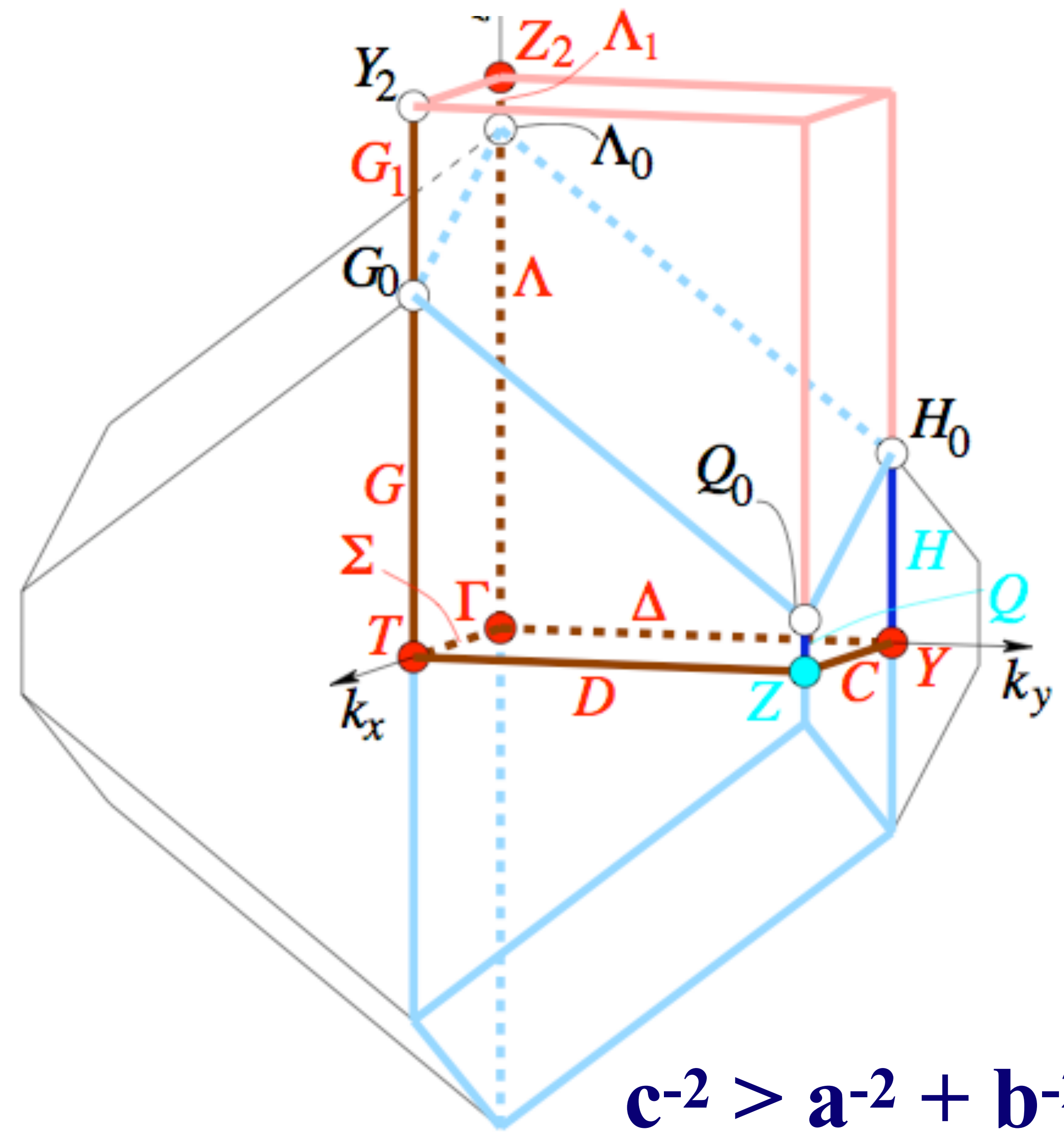
The k-vector Types of Group 22 [*F*222]

Brillouin zone

(Diagram for arithmetic crystal class 222F)



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



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

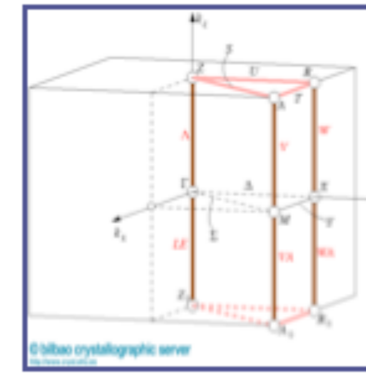
Problem: Representations of space groups REPRES

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

```
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
```

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

```
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
```

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

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   0   1       0       0   0   1       0
```

$$G=G^X+q_2G^X+\ldots+q_kG^X$$

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
```

$$G = G^X + q_2 G^X + \ldots + q_k G^X$$

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

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

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

Problem:

BILBAO CRYSTALLOGRAPHIC SERVER

Representations of space groups

Representations SG

Bilbao Crystallographic Server → Representations

Irreducible representations of the Space Groups

Representations: Get the irreducible representations of the Space Groups

Representations provides a set of irreducible representations (or physically irreducible representations in a real basis) of a given Space Group and a wave vector.

Reference. For more information about this program see the following article:

- Elcoro *et al.* "Double crystallographic groups and their representations on the Bilbao Crystallographic Server" *J. of Appl. Cryst.* (2017). **50**, 1457-1477. doi:10.1107/S1600576717011712

If you are using this program in the preparation of an article, please cite the above reference.

Enter the label of the space group: choose it

Irreducible representations Submit

Physically irreducible representations given in a real basis Submit

INPUT

REPRESENTATIONS SG

Irreducible representations of the Space Groups

Representations: Get the irreducible representations of the Space Groups

Representations provides a set of irreducible representations of a given Space Group and a wave vector.

k-vector data

List of non-equivalent k-vectors of the Space Group *P4mm* (N. 99)

The components are referred to the conventional basis

Choose one	k-vector label	Components in the conventional basis
○	**W**,X,R	(0,1/2,w)
○	**LD**,Z,GM	(0,0,w)
○	**V**,M,A	(1/2,1/2,w)
○	**C**,SM,S	(u,u,w)
○	**B**,U,DT	(0,v,w)
○	**F**,Y,T	(u,1/2,w)
○	**GP**,E,D	(u,v,w)

Submit

List of non-equivalent k-vectors of the Space Group *P4mm* (No. 99)

The components are referred to the conventional basis

Choose one	k-vector label	Components in the conventional basis
●	W	(0,1/2,w)
○	X	(0,1/2,0)
○	R	(0,1/2,1/2)

OUTPUT

REPRESENTATIONS SG

Irreducible representations of the Space Group *P4mm* (No. 99)

and wave vector k_1=(0,1/2,0).

The matrices of the representations (the whole representation and the representation of the little group) with dimension smaller than 5 are given explicitly. When the representation is larger than 5, only the non-zero elements are given using the following notation: (i;j)=x means that the (i,j) element of the matrix is x.

Matrices of the representations of the little group

Little group G^X

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

Matrix presentation	Seitz Symbol	X_1	X_2	X_3	X_4
$\begin{pmatrix} 1 & 0 & 0 & t_1 \\ 0 & 1 & 0 & t_2 \\ 0 & 0 & 1 & t_3 \end{pmatrix}$	$\{1\|t_1,t_2,t_3\}$	$e^{i\pi t_2}$	$e^{i\pi t_2}$	$e^{i\pi t_2}$	$e^{i\pi t_2}$
$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	$\{2_{001}\|0,0,0\}$	1	1	-1	-1
$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	$\{m_{010}\|0,0,0\}$	1	-1	-1	1
$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	$\{m_{100}\|0,0,0\}$	1	-1	1	-1

Vectors of the star

k-vector and its star *k

k_1=(0,1/2,0), k_2=(1/2,0,0)

OUTPUT

REPRESENTATIONS SG

Matrices of the representations of the group

The number in parentheses after the label of the irrep indicates the "reality" of the irrep: (1) for real, (-1) for pseudoreal and (0) for complex representations.

Matrix presentation	Seitz Symbol	$X_1(1)$	$X_2(1)$	$X_3(1)$	$X_4(1)$
$\begin{pmatrix} 1 & 0 & 0 & t_1 \\ 0 & 1 & 0 & t_2 \\ 0 & 0 & 1 & t_3 \end{pmatrix}$	$\{1\|t_1,t_2,t_3\}$	$\begin{pmatrix} e^{i\pi t_2} & 0 \\ 0 & e^{i\pi t_1} \end{pmatrix}$	$\begin{pmatrix} e^{i\pi t_2} & 0 \\ 0 & e^{i\pi t_1} \end{pmatrix}$	$\begin{pmatrix} e^{i\pi t_2} & 0 \\ 0 & e^{i\pi t_1} \end{pmatrix}$	$\begin{pmatrix} e^{i\pi t_2} & 0 \\ 0 & e^{i\pi t_1} \end{pmatrix}$
$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	$\{2_{001}\|0,0,0\}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	-1 0 [illegible]	$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$
$\begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	$\{4^{+}_{001}\|0,0,0\}$	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	[illegible]	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$
$\begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	[illegible]	[illegible] 1 0	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$
$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	$\{m_{010}\|0,0,0\}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$
$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	$\{m_{100}\|0,0,0\}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$

Matrices of the full-group irreps

EXERCISES

Problem 3.5.2.1

(a) Obtain the irreps for the space group *P4mm* for the **k**-vectors Γ(0,0,0) and X(0,1/2,0) using the program REPRES. Compare the results with the solutions of Problem 3.5.1.1.

(b) 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 3.5.1.3.

EXERCISES

Problem 3.5.2.2

Obtain the irreps for the space group *P4bm* for the **k**-vectors Γ(0,0,0) and X(0,1/2,0) using the program REPRES. Compare the results with the solutions of Problem 3.5.1.2.

EXERCISES

Problem 3.5.2.3

Consider the **k**-vectors **Γ**(000), **R** (½½½) and **M**(½½0) of the group ***Pm-3m*** (221). Using the tools of the Bilbao Crystallographic Server:

(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 ***Pm-3m***

(ii) Calculate a set of coset representatives of the decomposition of the group ***Pm-3m*** with respect to the little group of the **k**-vectors **R** and **M**, and construct the corresponding full space group irreps of ***Pm-3m***

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

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

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

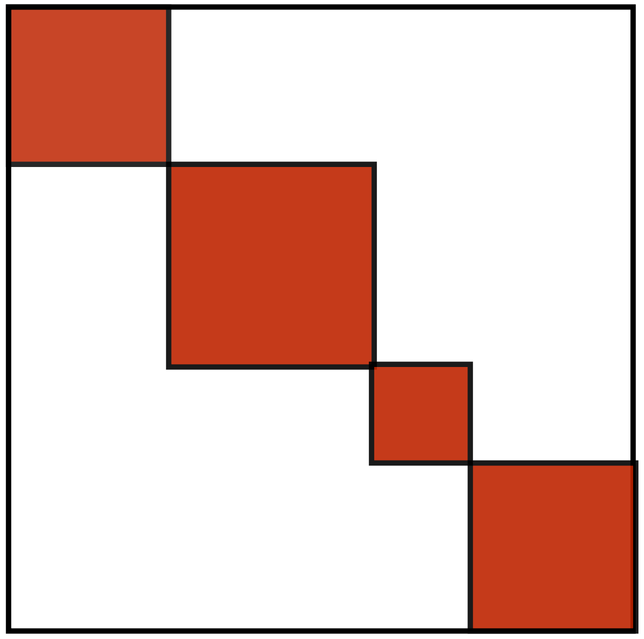
$\{D(G)\downarrow H\}$: subduced rep of H<G

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

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 $\delta \longrightarrow 0$

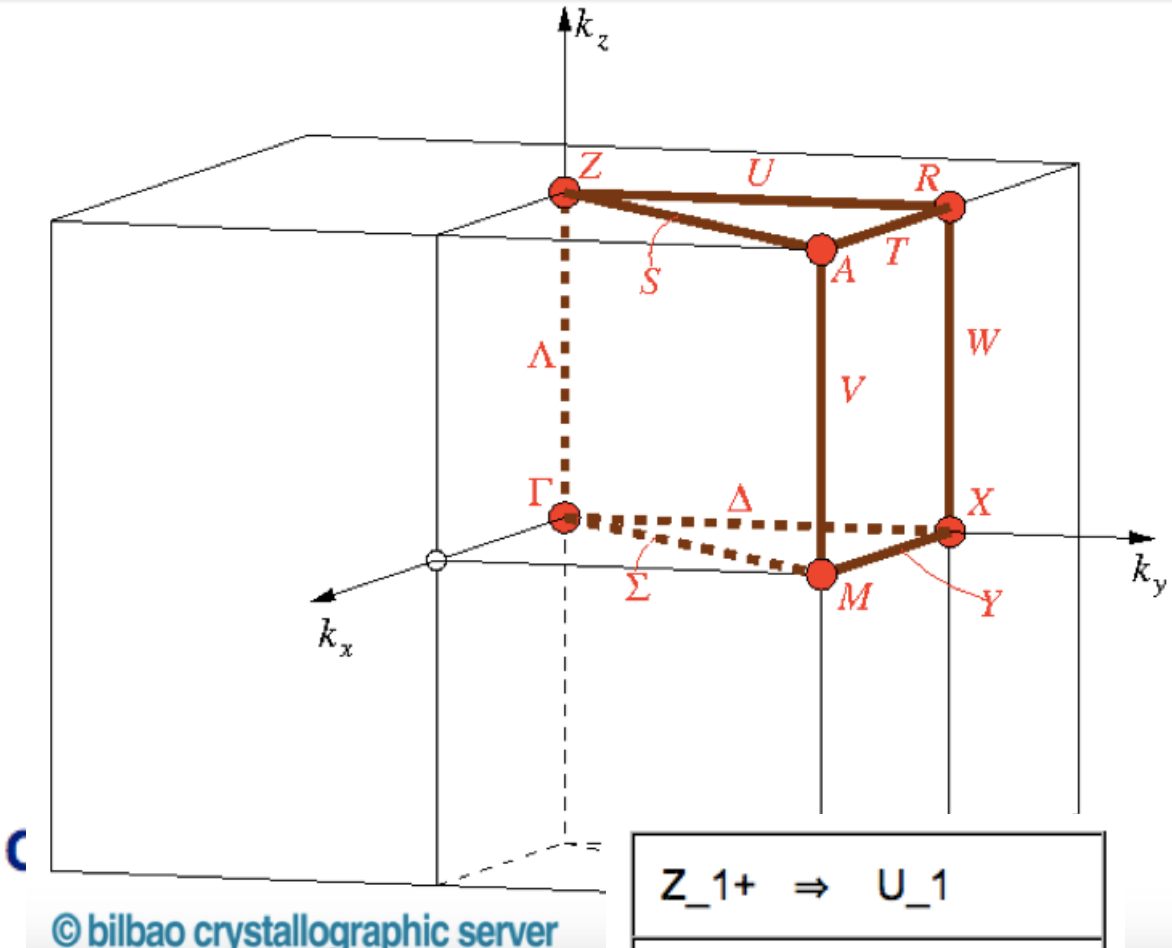
$$D^{k,i}(G^{k}) \downarrow G^{k'} \sim \bigoplus m_j D^{k'j}(G^{k'})$$

Correlations between characters

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

EXAMPLE

k-vector description		ITA description	
k-vector label	Conventional basis	Wyckoff position	
		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



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

EXERCISES

Problem 3.5.2.4

Using the program COMPATIBILITY RELATIONS determine the connectivity of the electronic energy bands of Ge, symmetry group Fd-3m (227) between the high-symmetry points Γ(0,0,0) and X(1/2,0,1/2) over the symmetry line DT (u,0,u) (cf. BZ data of Fd-3m provided by the program KVEC).

Problem: **Correlations between representations of space groups** **CORREL**

group G

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

$\downarrow$

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

subgroup H<G

D(G): irrep of G

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

$\downarrow$

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

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

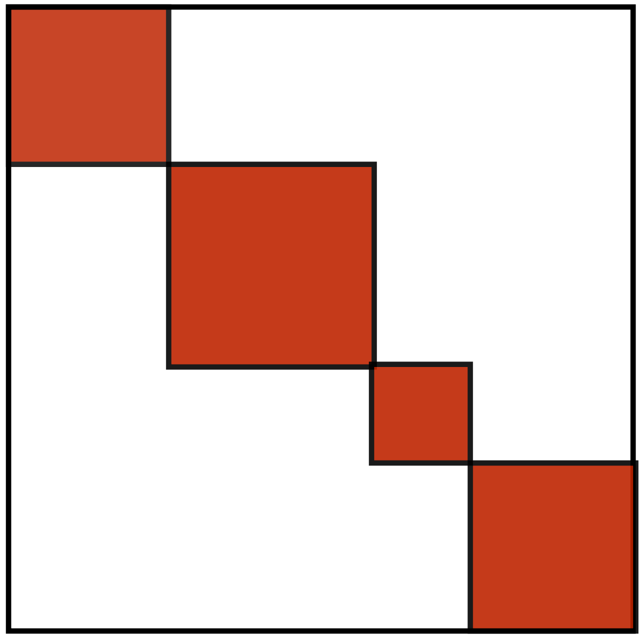
$\{D(G)\downarrow H\}$

Subduction

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

$\longrightarrow$

$\bigoplus m_i D_i(H)$



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 OF SPACE-GROUP REPRESENTATIONS

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

$D_1(G)$: irrep of G

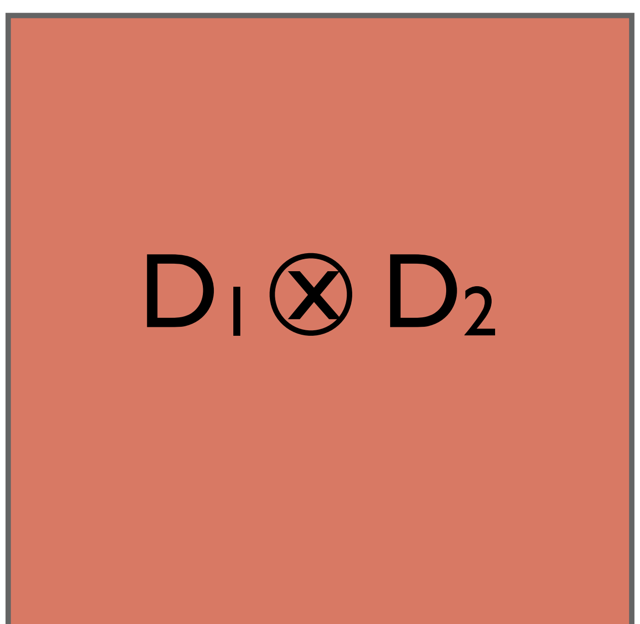
$\{D_1(e), D_1(g_2), \ldots, D_1(g_n)\}$

$D_2(G)$: irrep of G

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

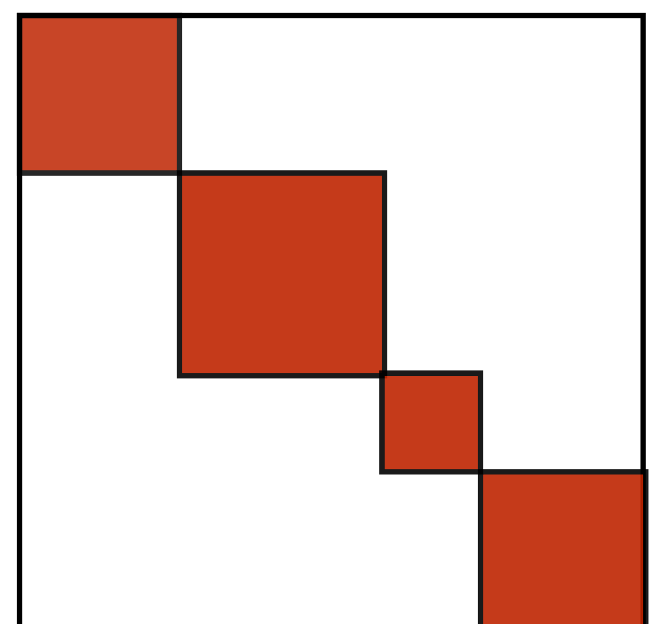
Direct-product representation

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



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

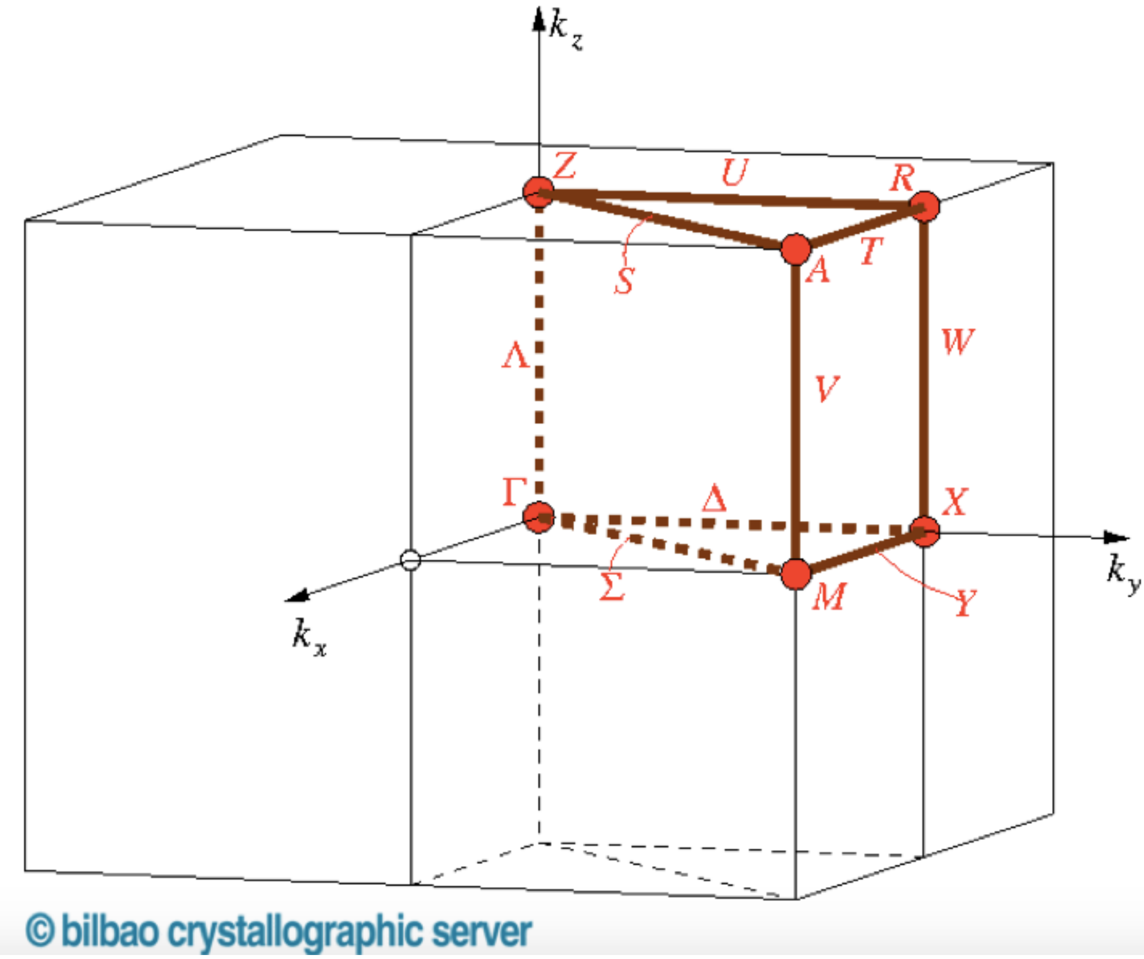
Problem 3.5.2.5

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

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

BILBAO CRYSTALLOGRAPHIC SERVER

KVEC database



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: 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)
```

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

↓

$$\bigoplus m_i D_i(G)$$