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CRYSTALLOGRAPHY ONLINE: WORKSHOP ON THE USE AND APPLICATIONS OF THE BILBAO CRYSTALLOGRAPHIC SERVER

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ECM31
31st European Crystallographic Meeting

CRYSTALLOGRAPHY ONLINE:
BILBAO CRYSTALLOGRAPHIC SERVER

REPRESENTATIONS OF SPACE GROUPS

DATABASES AND TOOLS OF THE BILBAO CRYSTALLOGRAPHIC SERVER

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SPACE GROUPS

Crystal pattern: infinite, idealized crystal structure (without disorder, dislocations, impurities, etc.)

Space group G: The set of all symmetry operations (isometries) of a crystal pattern

Translation subgroup $T_G \lhd G$: 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: $P_G \cong G/H$

SPACE-GROUP REPRESENTATIONS

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

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

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

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 $\{a, a^2, \ldots, a^s\}$

B $\{b, b^2, \ldots, b^r\}$

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

$D^p(a^m), p=0,1,\ldots,s-1$

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

$D^q(b^n)$, $q=0,1,\ldots,r-1$

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

$D^p(a^m) \otimes D^q(b^n)$

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

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

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

$$L: a_1, a_2, a_3 \xleftrightarrow{a_i . a^*_j = 2\pi\delta_{ij}} L^*: a^*_1, a^*_2, a^*_3$$

$$\mathbf{K} = (h_1, h_2, h_3) \begin{vmatrix} \mathbf{a}^*_1 \\ \mathbf{a}^*_2 \\ \mathbf{a}^*_3 \end{vmatrix}$$

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

$k_i = q_i/N_i$

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

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)

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

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

first Brillouin zone (Wigner-Seitz cell)

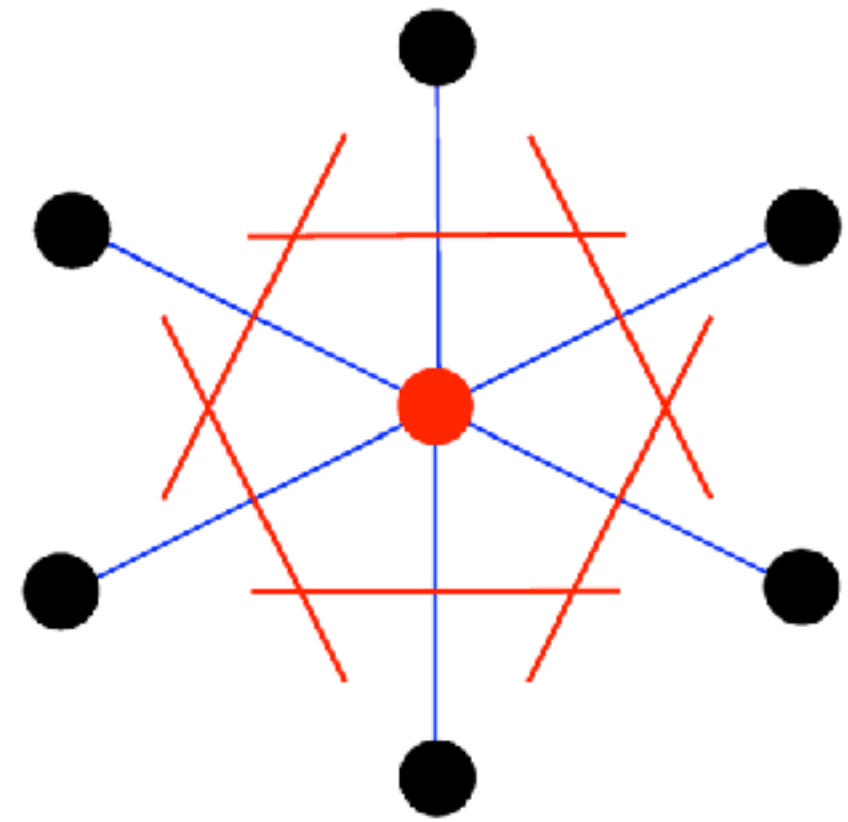
$|\mathbf{k}| \leq |\mathbf{K}-\mathbf{k}|, \ \forall \mathbf{K} \in L^*$

crystallographic unit cell

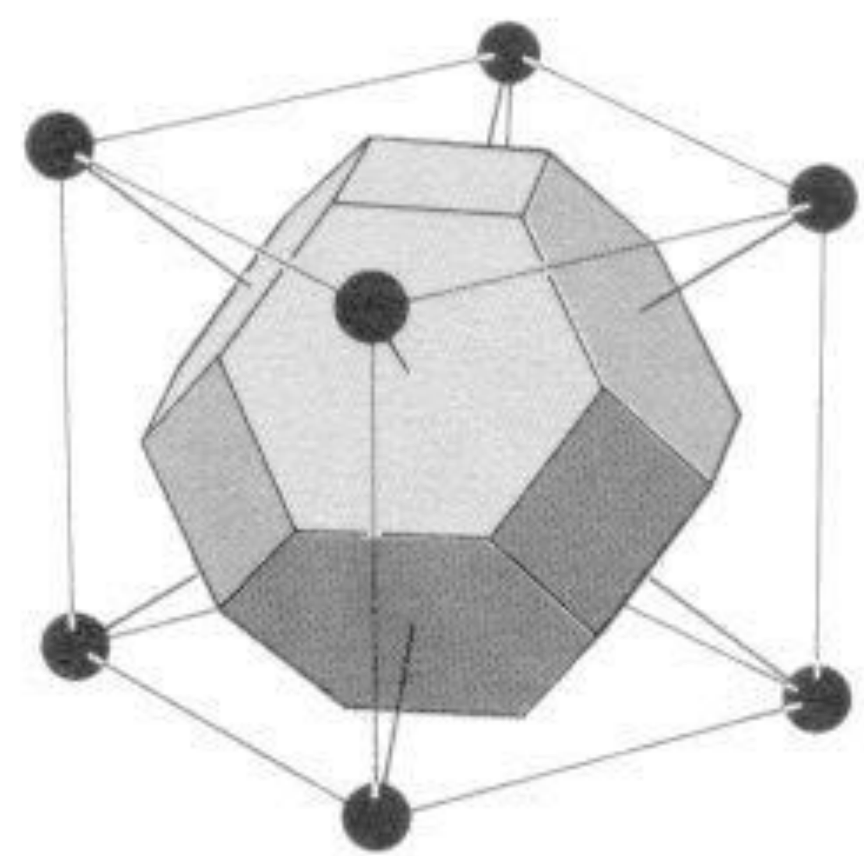
$0 \leq |\mathbf{k}| < 1$

first Brillouin zone
(Wigner-Seitz cell)

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



Wigner-Seitz
construction for
bcc lattice



Step 2.

Classification of the irreps of the Translation subgroup.

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

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

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

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

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

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

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

special and general

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

Orbits of irreps of the Translation subgroup.

orbit of **k**

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

star of **k**: **k***

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

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

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

representation domain

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

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

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

special case:

general **k**-vector

star of **k**
little group of **k**
allowed 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 $\mathbf{D}^{\mathbf{k},i}$:

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

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

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

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

$\overline{\mathbf{D}}^{k,i}$ projective (ray) irreps of $\overline{\mathcal{G}}^{k}$

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

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

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

b) 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}	$q_i^{-1}(\boldsymbol{W}_l,\ \boldsymbol{w}_l)$	$q_i^{-1}(\boldsymbol{W}_l,\ \boldsymbol{w}_l)q_j$	$M(\boldsymbol{W}_l,\ \boldsymbol{w}_l)_{ij} \neq 0$
...	...	...	...	...	

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

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

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

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 4.1

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

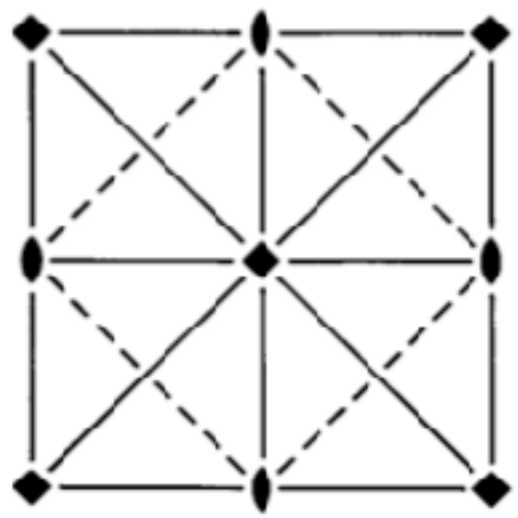
(i) Determine the little groups, the **k**-vector stars, the number and the dimensions of the little-group irreps, the number and the dimensions of the corresponding irreps of the group ***P4mm***

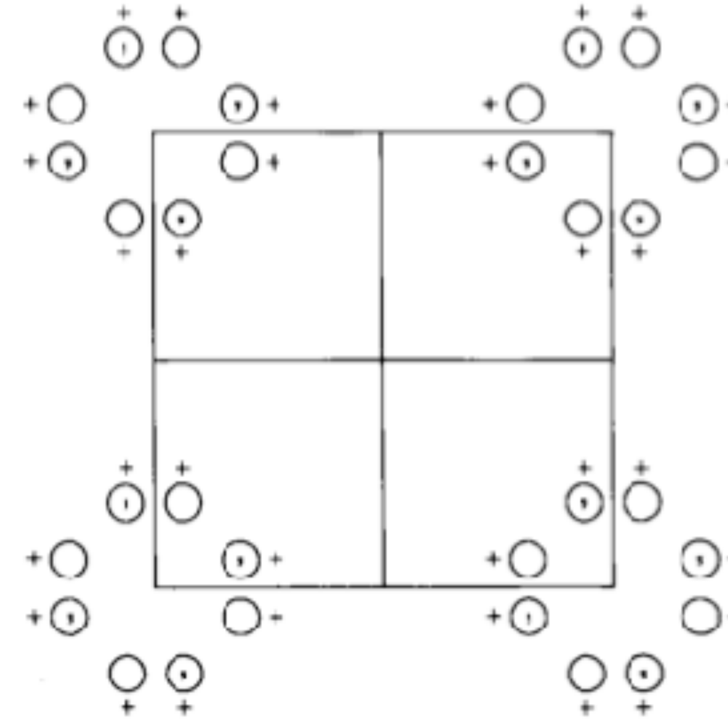
(ii) Calculate a set of coset representatives of the decomposition of the group ***P4mm*** with respect to the little group of the **k**-vectors Γ(000) and **X**, and construct the corresponding full space group irreps of ***P4mm***

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

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

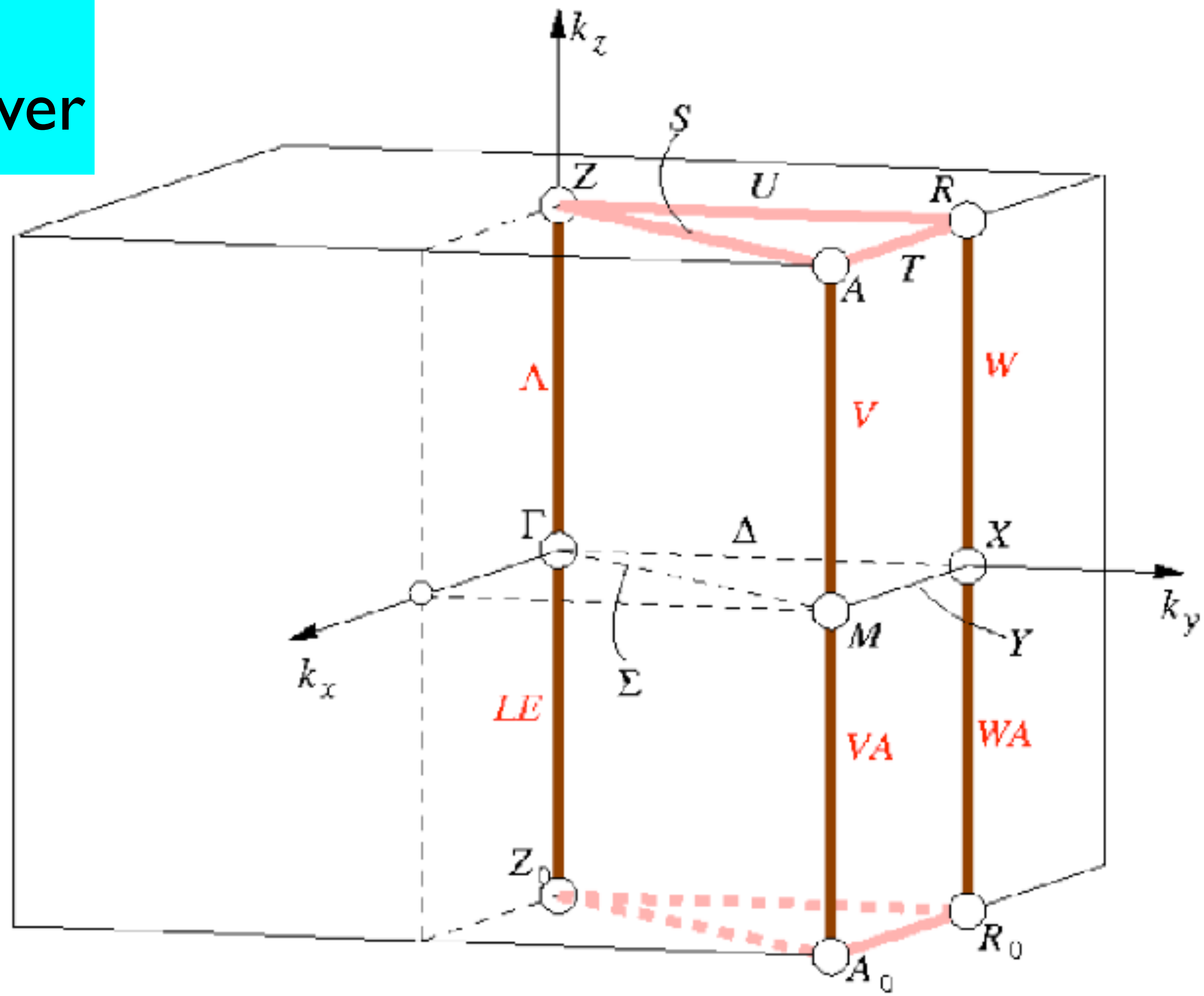
5.5 Crystal class $4mm$

5.5.1 Arithmetic crystal class $4mmP$

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

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

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



EXERCISES

Problem 4.2

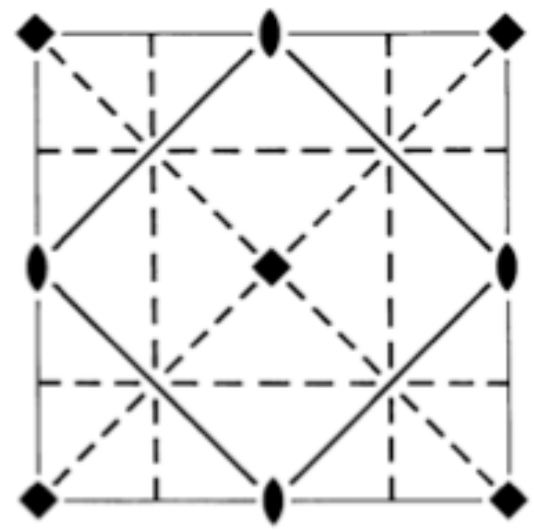
Consider the **k**-vectors Γ(000) and **X** (0½0) of the group ***P4bm***

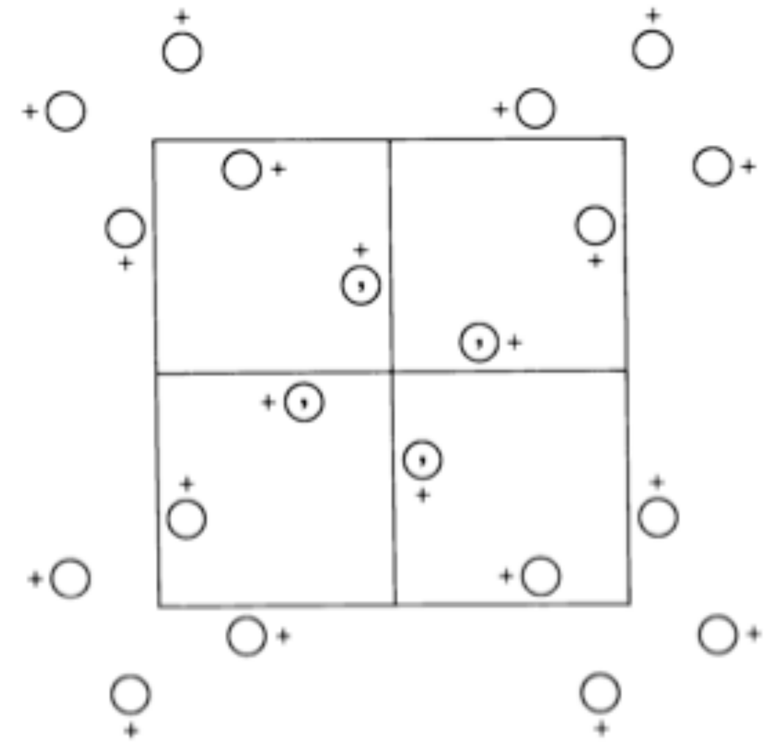
(i) Determine the little groups, the **k**-vector stars, the number and the dimensions of the little-group irreps, the number and the dimensions of the corresponding irreps of the group ***P4bm***

(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 sy





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

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) $y+\frac{1}{2},x+\frac{1}{2},z$

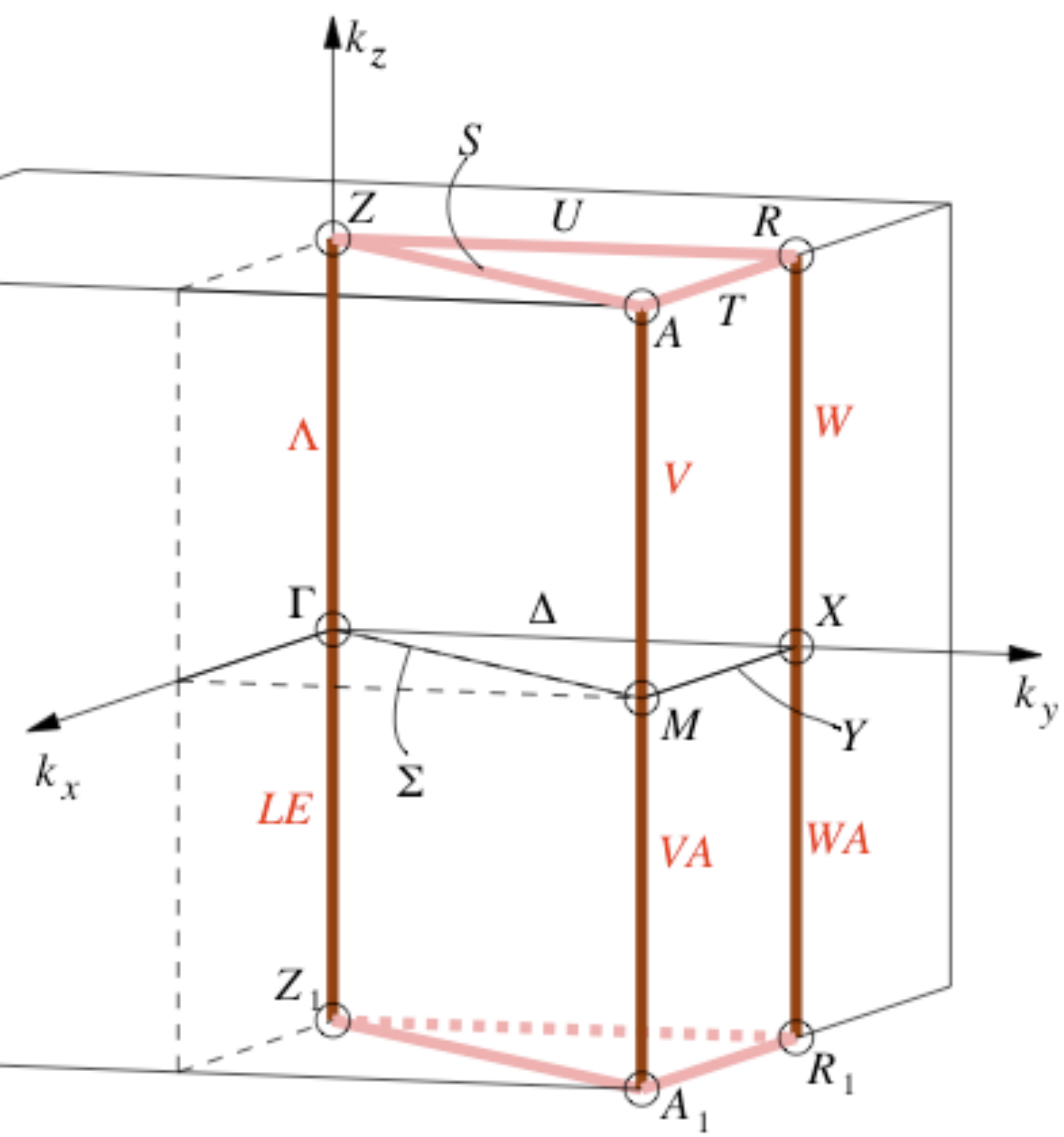
5.5 Crystal class $4mm$

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 4.3

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.

REPRESENTATIONS OF CRYSTALLOGRAPHIC GROUPS

DATABASES AND TOOLS OF THE BILBAO CRYSTALLOGRAPHIC SERVER

REPRESENTATIONS OF CRYSTALLOGRAPHIC GROUPS

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Space-group symmetry

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20-21 August 20

News:

- New Article in Nature
  07/2017: Bradlyn *et al.* "Topolo
  chemistry" *Nature* (2017). 547
- New program: BANDRE
  04/2017: Band representations
  Band representations of Doubl
- New section: Double po
  groups
  - New program: DGE
    04/2017: General positi
    Space Groups
  - New program:
    REPRESENTATIONS DPG

Representations and 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
MECHANICAL REP. ⚠	Decomposition of the mechanical representation into irreps
MAGNETIC REP. ⚠	Decomposition of the magnetic representation into irreps
BANDREP ⚠	Band representations and Elementary Band representations of Double Space Groups

Bilbao Crystallographic Server

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 of Representations of Point Groups

Bilbao Crystallographic Server

POINT

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]

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

character tables
matrix representations
basis functions

Database of Representations of Point Groups

Bilbao Crystallographic Server

REPRESENTATIONS PG

Irreducible representations of the Point Group 4 (No. 9)

Matrices of the representations of the group

er the label of the irrep indicates the "reality" of the irrep: (1) for real, (-1) for pseudoreal and (0

N	Matrix presentation	Seitz Symbol	$GM_1(1)$	$GM_2(1)$	$GM_3(0)$	$GM_4(0)$
1	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	1	1	1	1	1
2	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	2_{001}	1	1	-1	-1
3	$\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	4^+_{001}	1	-1	i	-i
4	$\begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	4^-_{001}	1	-1	-i	i

Table of characters

(1)	(2)	(3)	C_1	C_2	C_3	C_4
GM_1	A	GM_1	1	1	1	1
GM_2	B	GM_2	1	1	-1	-1
GM_3	^2E	GM_3	1	-1	i	-i
GM_4	^1E	GM_4	1	-1	-i	i

conjugacy classes

C_1: 1

C_2: 2_{001}

C_3: 4^+_{001}

C_4: 4^-_{001}

character tables

matrix representations

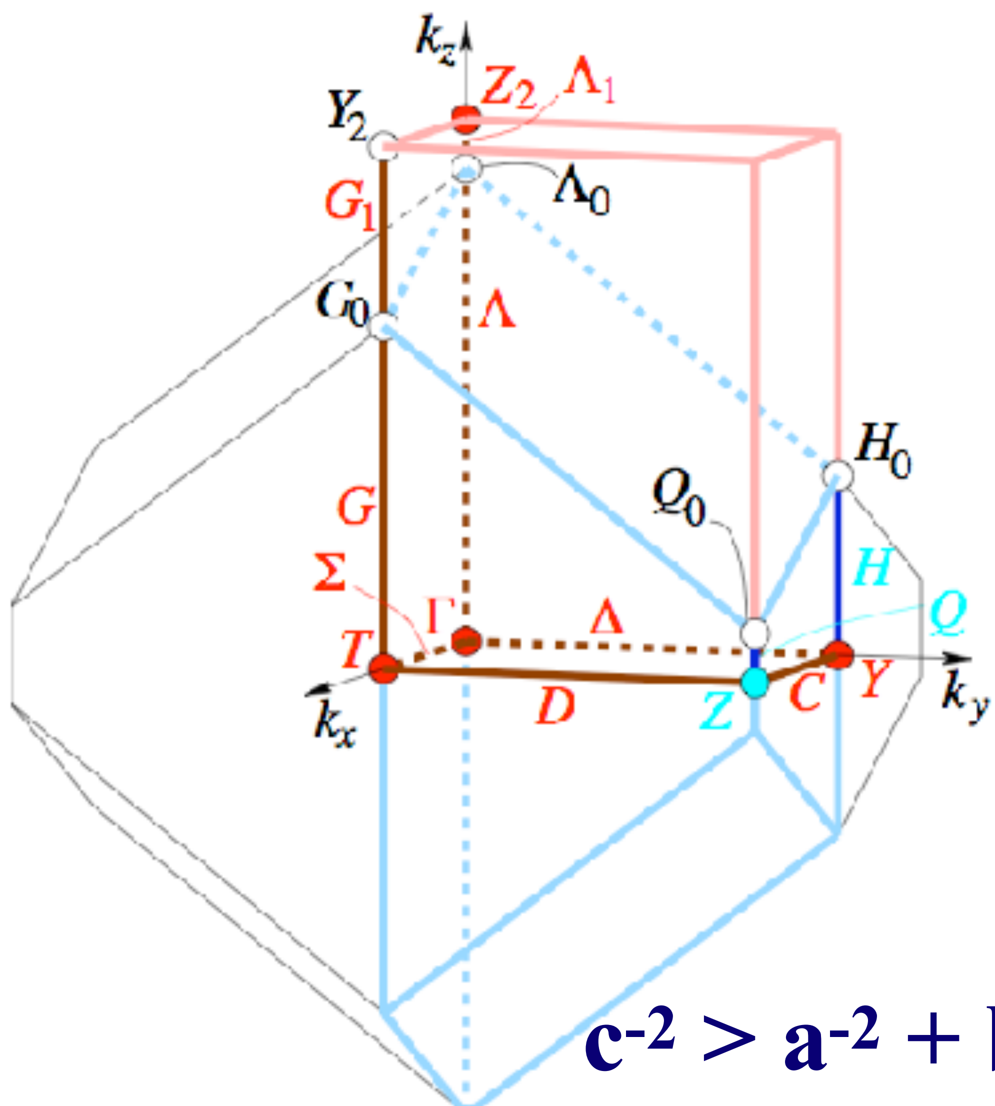
'reality' of irreps

pairs of conjugated irreps

GM_3+GM_4

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
$T \sim T_2$			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

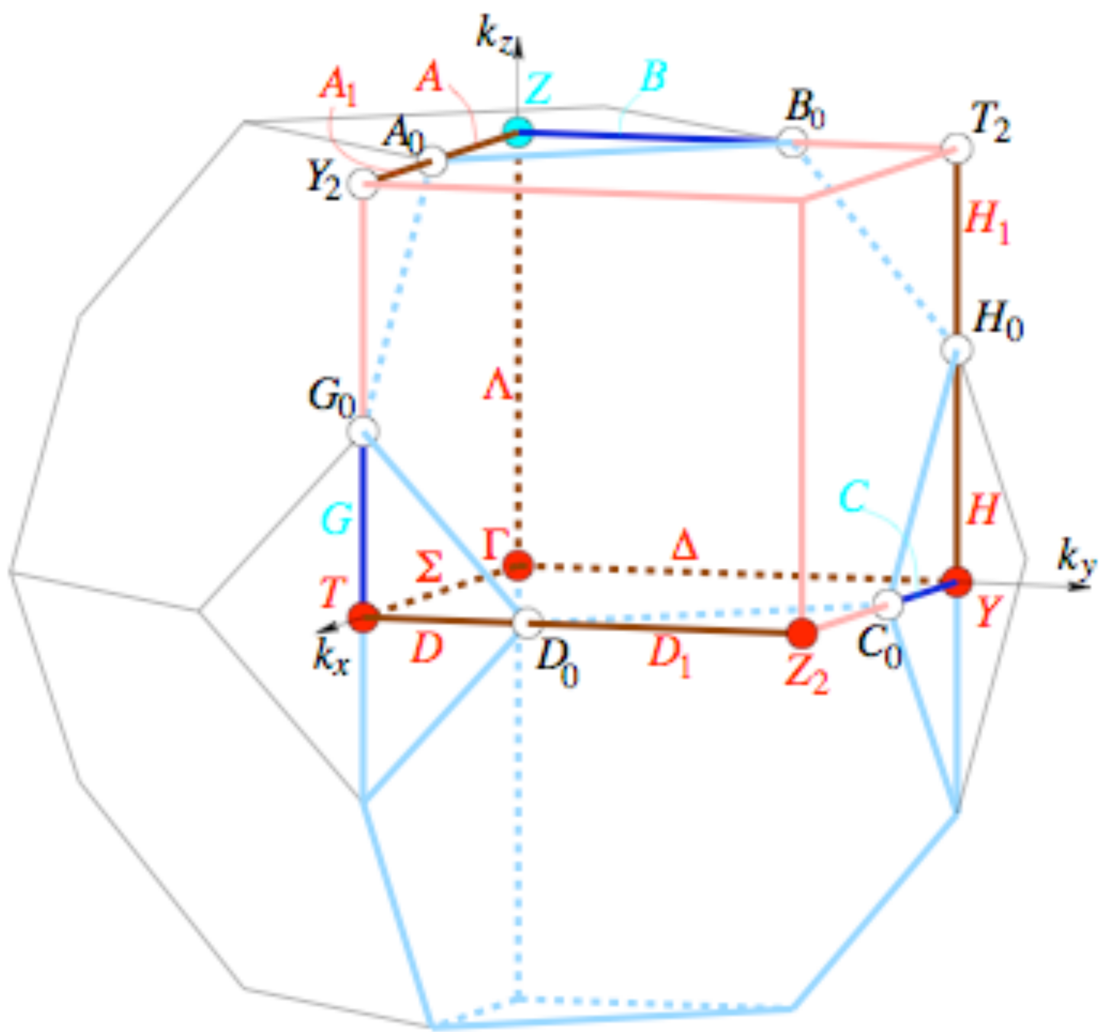
Example:

Brillouin zone Database

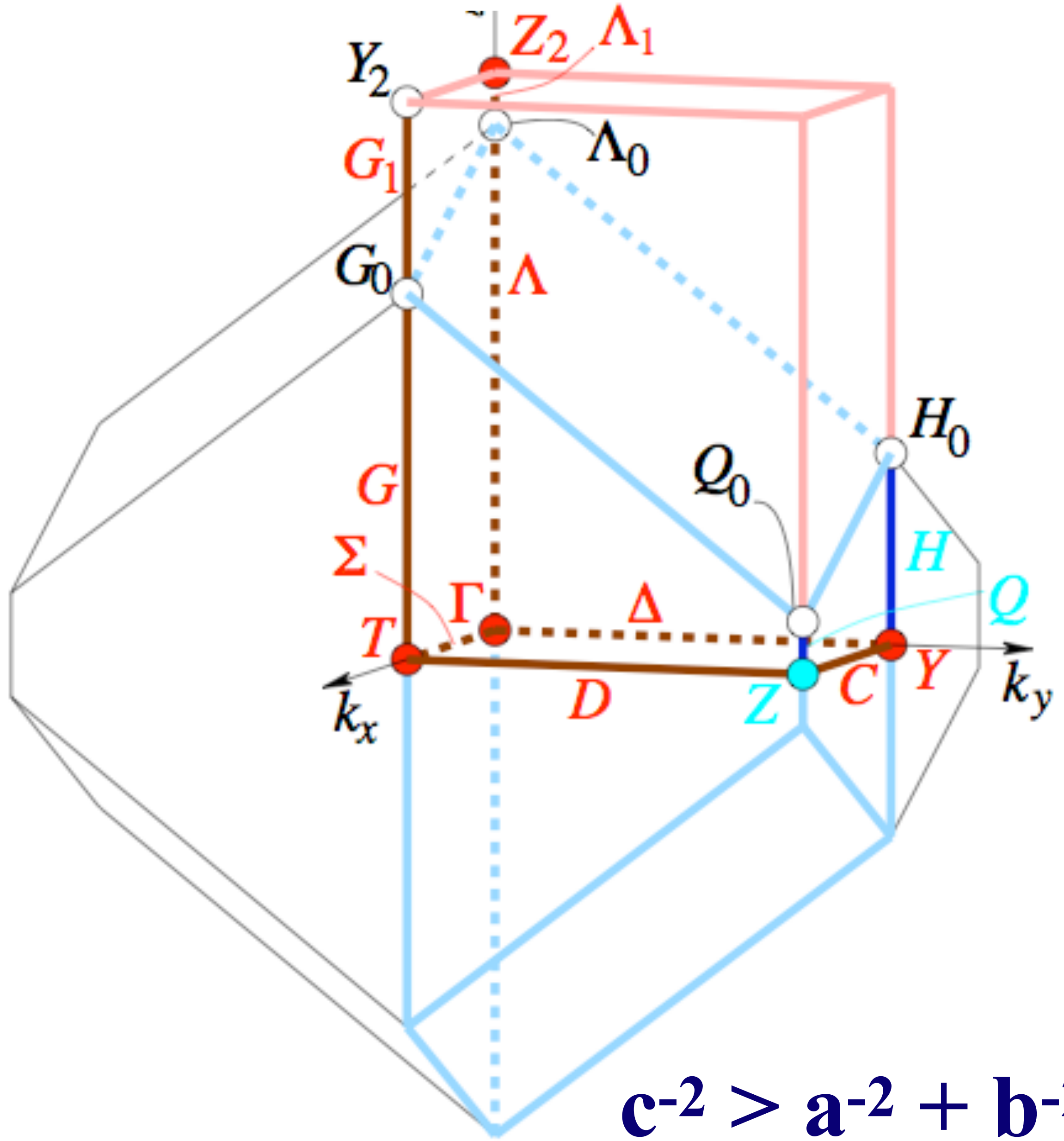
The k-vector Types of Group 22 [*F*222]

Brillouin zone

(Diagram for arithmetic crystal class 222F)



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



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

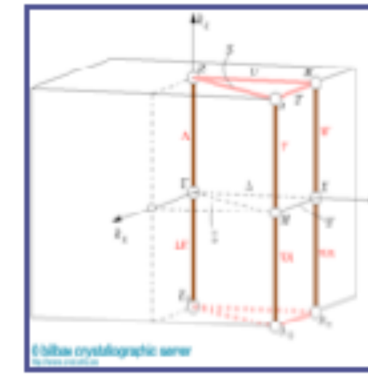
Problem: Representations of space groups REPRES

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
```

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

```
          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
```

```
Number of elements : 8
```

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

```
          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
```

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

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
```

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

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 4.4

(a) Obtain the irreps for the space group *P4mm* for the **k**-vectors Γ(000) and X(01/20) using the program REPRES. Compare the results with the solutions of Problem 4.1.

(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 6.3.

EXERCISES

Problem 4.5

Obtain the irreps for the space group *P4bm* for the **k**-vectors Γ(000) and X(01/20) using the program REPRES. Compare the results with the solutions of Problem 4.2.

Problem: Representations of space groups REPRESENTATIONS SG

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

Matrices of the full-group irreps

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

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

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

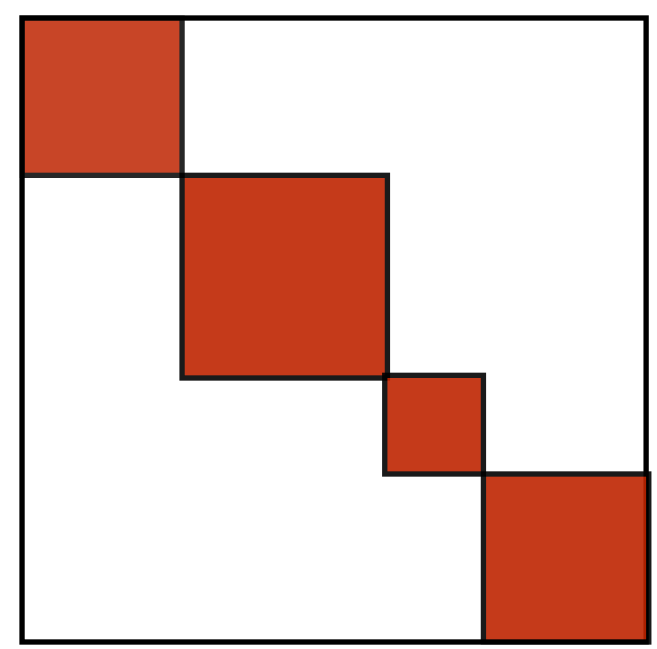
$\{D(G)\downarrow H\}$: subduced rep of H<G

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

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 $\begin{cases} k,\ G^{k},\ D^{k,i} \\ k',\ G^{k'}, D^{k',j} \end{cases}$ such that $k'=k+\delta$

Subduction of little group irreps

in the limit $\delta \longrightarrow 0$

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

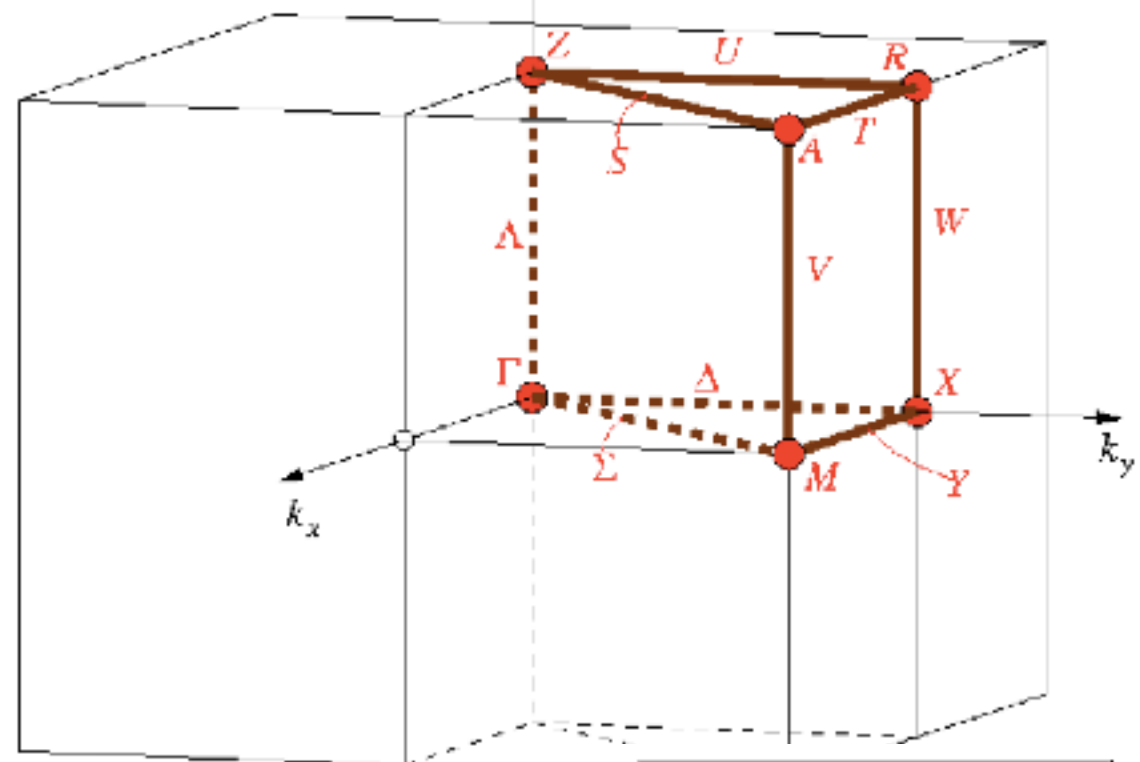
Correlations between characters

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

EXAMPLE P4/mmm

BILBAO CRYSTALLOGRAPHIC SERVER

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

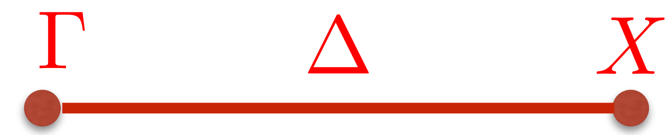


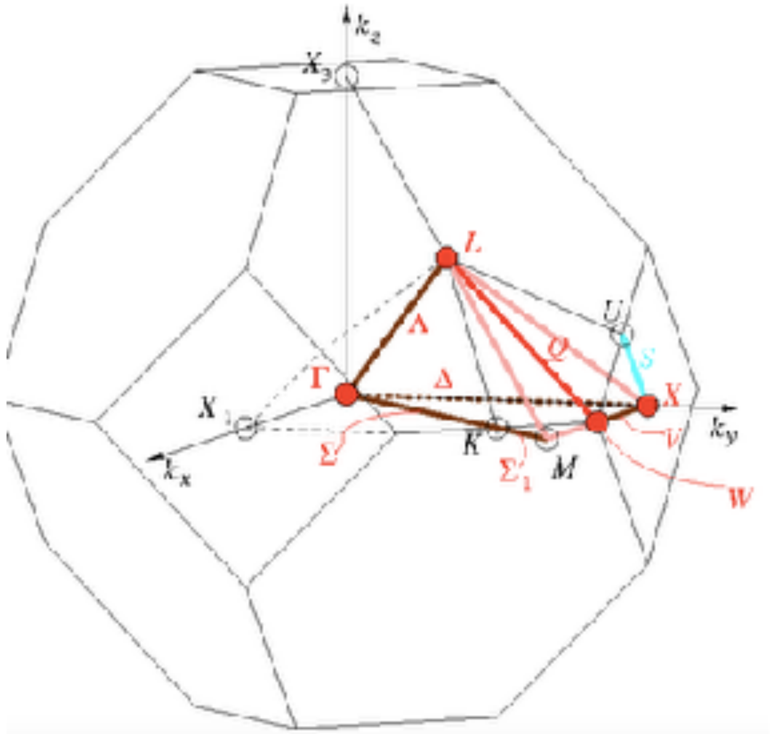
© bilbao crystallographic server

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)



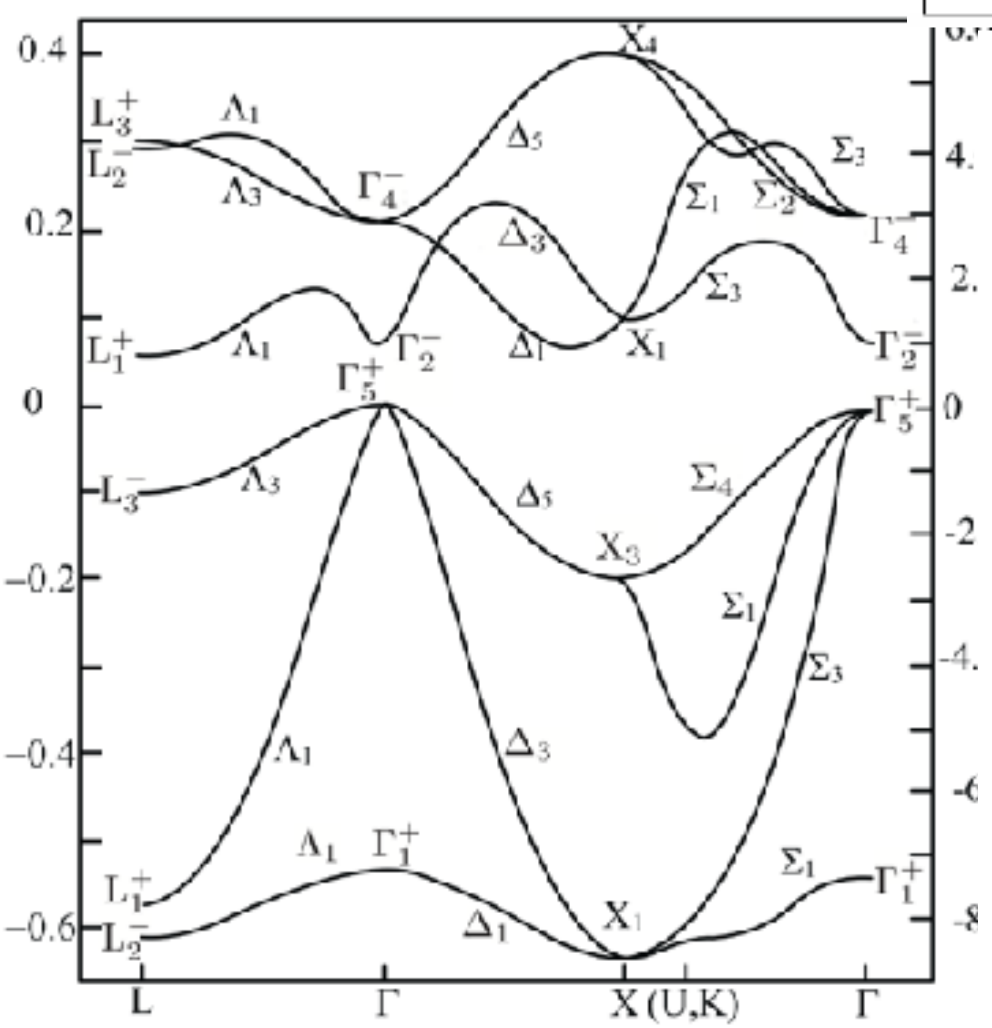


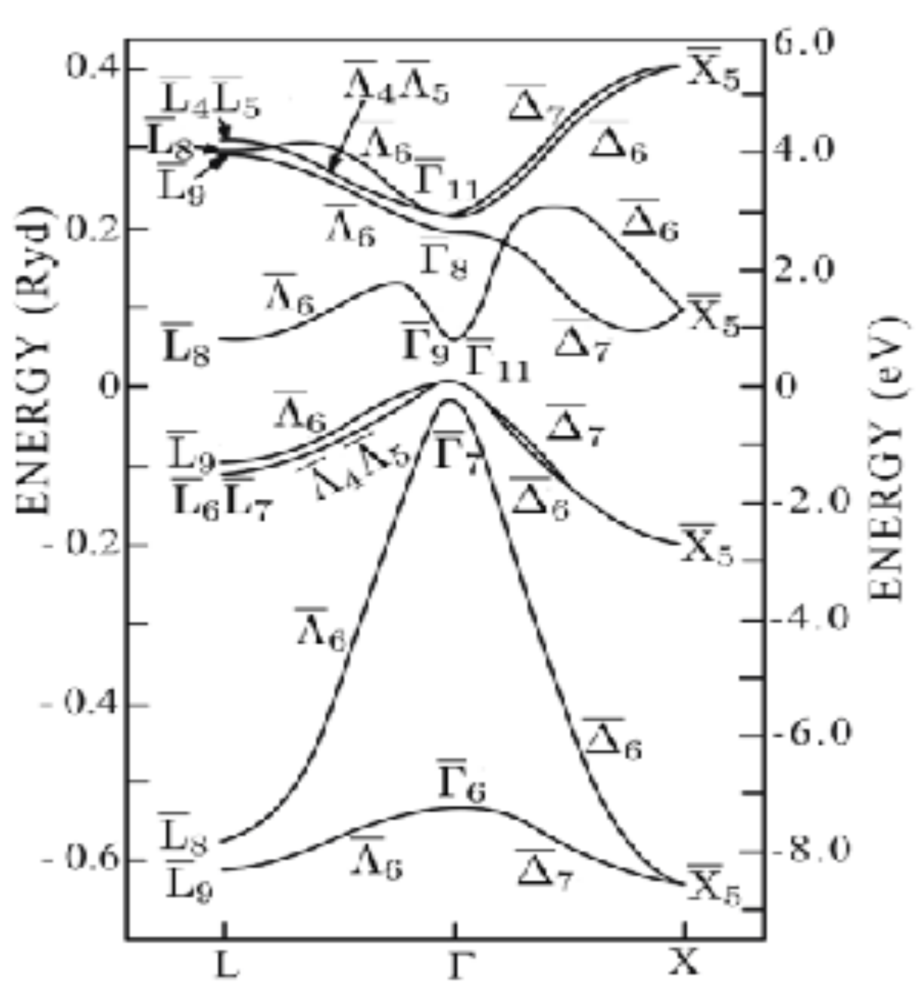
k-vector description		ITA description	
		Wyckoff position	
k-vector label	Conventional basis	Multiplicity	Letter
GM	0,0,0	2	a
X	0,1,0	6	b
L	1/2,1/2,1/2	8	c
W	1/2,1,0	12	d
DT	0,u,0	12	e
LD	u,u,u	16	f
V	u,1,0	24	g
SM (S)	u,u,0	24	h
Q	1/2,1-u,u	48	i
A (B)	v,u,0	48	j
C (J)	v,v,-u	48	k
GP	u,v,w	96	l

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

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

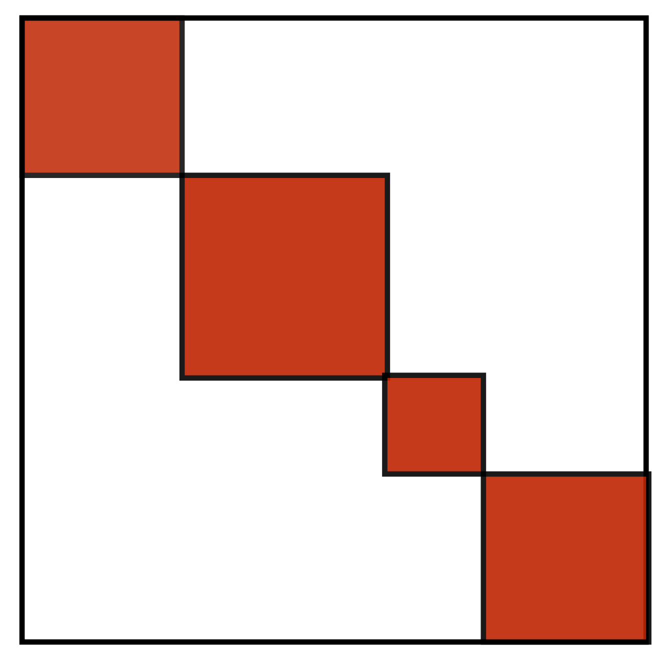
$\{D(e), D(h_2), D(h_3), \ldots, D(h_m)\}$

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

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

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

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

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

Enter the transformation matrix below:

INPUT data

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)
```

CORREL: OUTPUT data

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)
```