Lecture Course
GROUP THEORY AND TOPOLOGY

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APPLICATIONS OF SPACE-GROUP REPRESENTATIONS

COMPUTER TOOLS OF THE BILBAO CRYSTALLOGRAPHIC SERVER

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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

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

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

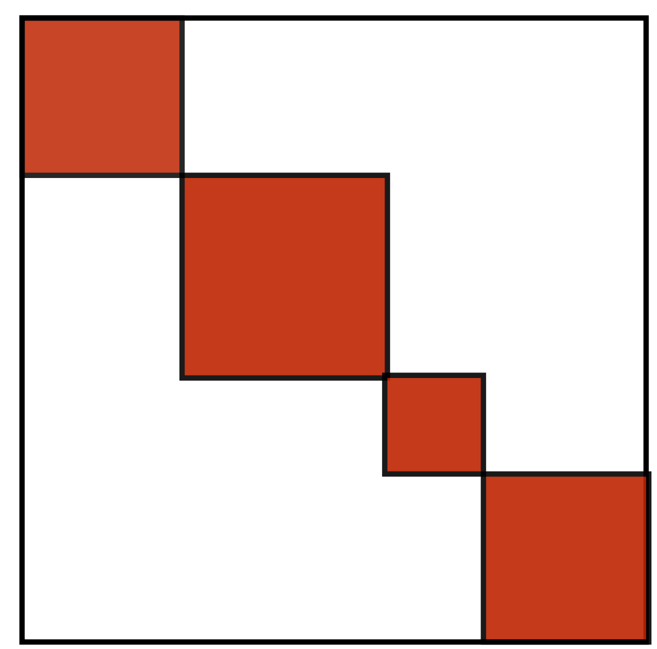
$\{D(G)\downarrow H\}$: subduced rep of H<G

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

Subduction

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

$\bigoplus m_i D_i(H)$



irreps of H

Problem: SUBDUCED space-group representations

Subduction of space group irreps

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

$$m_i = \frac{1}{|H|}\sum_{h} \eta^{*k_G}(h)\,\eta^{*k_{Hi}}(h)^*$$

Step 1. Correlations between wave vectors

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

Step 2. Correlations between characters

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

EXERCISES

Problem 5.1a

The star of the wave vector X(1/2,0,0) in the cubic group Pm-3m (221) consists of three arms:

*X={(1/2,0,0), (01/2,0), (0,0,1/2)}

(i) Determine the wave-vector correlations (spltting) of *X for the group-subgroup chain Pm-3m (a,b,c) > P4mm (a,b,c)

(ii) How the wave-vector correlations of *X change if unit cell of the low-symmetry group is doubled along c axis, i.e. the group-subgroup chain is of the type

Pm-3m (a,b,c) > P4mm (a,b,2c)

Brillouin Zone Database BilbaoCrystServer

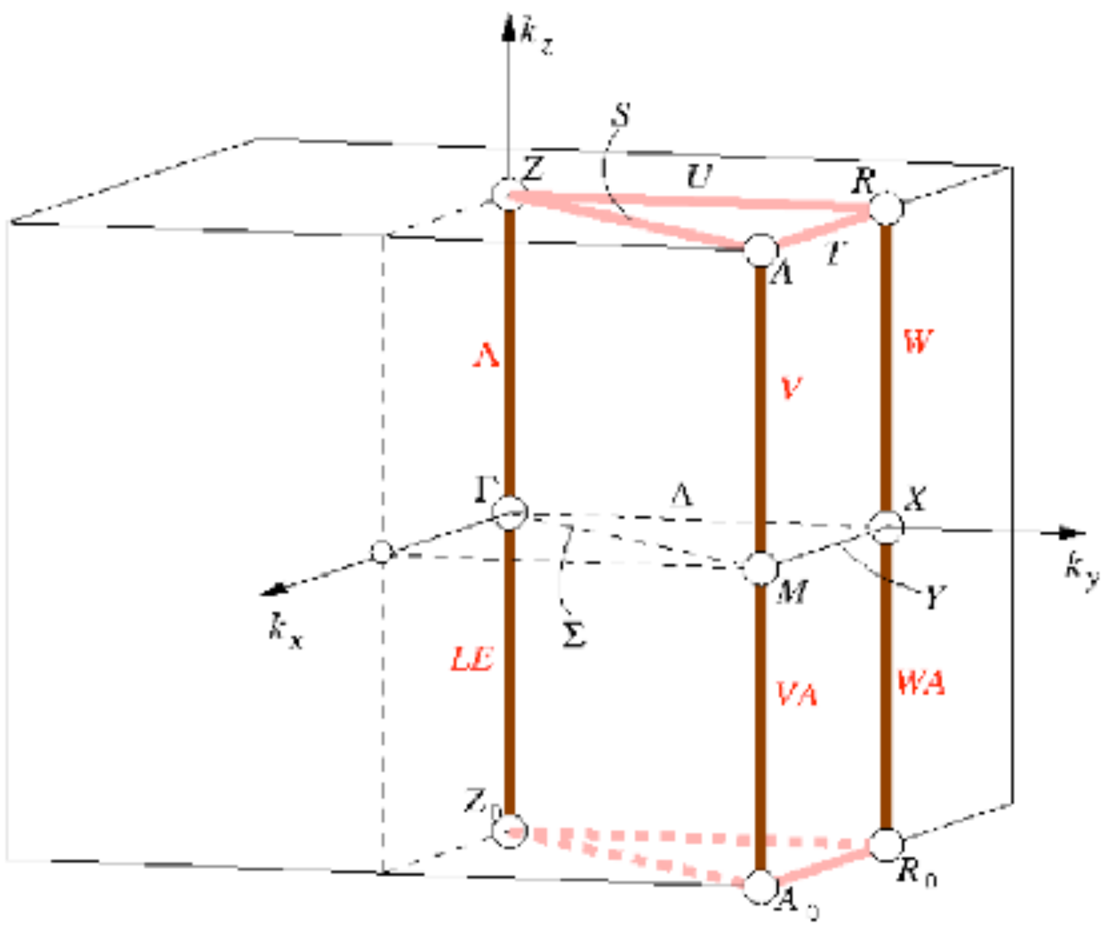
5.5 Crystal class $4mm$

5.5.1 Arithmetic crystal class $4mmP$

Fig. 5.5.1.1 Diagram for arithmetic crystal cl

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

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



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k-vector description		Wyckoff Position		
CDML[1]				
Label	Coefficients			
GM	0,0,0 ex	1	a	4mm
Z	0,0,1/2 ex	1	a	4mm
LD	0,0,u ex	1	a	4mm
LE	0,0,-u ex	1	a	4mm
LE+GM+LD+Z=[Z_0 Z]		1	a	4mm
M	1/2,1/2,0 ex	1	b	4mm
A	1/2,1/2,1/2 ex	1	b	4mm
V	1/2,1/2,u ex	1	b	4mm
VA	1/2,1/2,-u ex	1	b	4mm
VA+M+V+A=[A_0 A]		1	b	4mm
X	0,1/2,0 ex	2	c	2mm.
R	0,1/2,1/2 ex	2	c	2mm.
W	0,1/2,u ex	2	c	2mm.

Problem 5.1a

SOLUTION

Pm-3m: *X={(1/2,0,0), (01/2,0), (0,0,1/2)}

a'=**a**
b'=**b**
c'=**c**

*X={(1/2,0,0), (01/2,0), (0,0,1/2)}

P4mm: *X={(1/2,0,0), (01/2,0)}

*Z={(0,0,1/2)

Problem 5.1a

SOLUTION

Pm-3m: *X={(1/2,0,0), (01/2,0), (0,0,1/2)}

$\downarrow$ **a'**=**a**, **b'**=**b**, **c'**=2**c**

*X={(1/2,0,0), (01/2,0), (0,0,1)}

P4mm: *X={(1/2,0,0), (01/2,0)}

{(0,0,1)} ~ Γ(0,0,0)

Landau theory of phase transitions

Active irrep

the symmetry break taking place in structural phase transitions is due to the condensation (i.e. the change from zero to a non-zero amplitude) of one or a set of collective degrees of freedom that transform according to a single irreducible representation of the space group of the high-symmetry phase (the so-called **active irrep**).

Order parameter

The amplitudes {Qi, i=1,...,n} that become spontaneously non-zero in the low-symmetry phase, constitute the so-called **order parameter,** and the n- dimensional irrep describing its transformation properties is the active irrep of the transition.

Isotropy subgroups

The symmetry group of the low-symmetry phase for which the amplitudes {Qi, i=1,...,n} that become spontaneously non-zero in the low-symmetry phase, is called an **isotropy subgroup** of the corresponding active irrep

Problem: We know the high symmetry and the active irrep or order parameter and we want to know the possible symmetries of the distorted phase

$$G, D(g) \longrightarrow H?$$

possible isotropy subgroups for a given active irrep?

G: space group of the high-symmetry phase

$D=\{D(g), g\in G\}$: matrix irrep of G

$Q=(Q_1, Q_2, \ldots, Q_n)$: order parameter transforming according to D

Transformation of the order-parameter: $D(g)Q=Q', g\in G$

Isotropy subgroup H of **D**: $\mathbf{D(g)Q=Q, g\in H<G}$

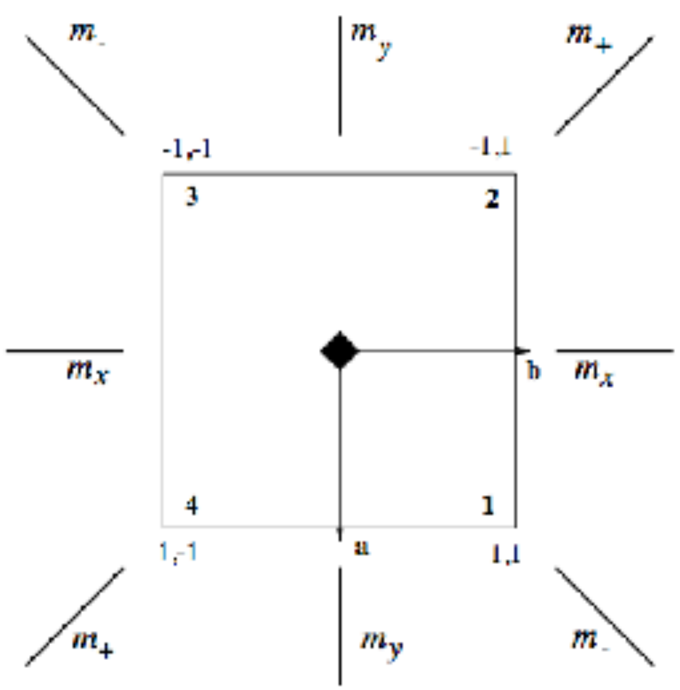
Group-theoretical condition for H to be isotropy subgroup of **D**: $\mathbf{D\downarrow H} \ni \mathbf{\Gamma_1}$

(the identity irrep of H)

EXERCISES

Problem 5.1b

Determine the isotropy subgroups of the irreps of P4mm with k=0



Character Table of the group C_{4v}(4mm) *

C_{4v}(4mm)	#	1	2	4	m_x	m_d	functions
Mult.	-	1	1	2	2	2	.
A_1	Γ_1	1	1	1	1	1	z, x^2+y^2, z^2
A_2	Γ_2	1	1	1	-1	-1	J_z
B_1	Γ_3	1	1	-1	1	-1	x^2-y^2
B_2	Γ_4	1	1	-1	-1	1	xy
E	Γ_5	2	-2	0	0	0	(x,y),(xz,yz),(J_x,J_y)

$$E(4)=\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \quad E(m_-)=\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

Problem 5.1b

SOLUTION

Irreps of P4mm at k=0 (Γ point)

Character Table of the group C_{4v}(4mm) *

C_{4v}(4mm)	#	1	2	4	m_x	m_d	functions
Mult.	-	1	1	2	2	2	.
A_1	Γ_1	1	1	1	1	1	z, x^2+y^2, z^2
A_2	Γ_2	1	1	1	-1	-1	J_z
B_1	Γ_3	1	1	-1	1	-1	x^2-y^2
B_2	Γ_4	1	1	-1	-1	1	xy
E	Γ_5	2	-2	0	0	0	$(x,y),(xz,yz),(J_x,J_y)$

P4mm
P4
Pmm2
Cmm2

Pm
Cm
P1

for 1-dim irreps rather trivial, for n-dim one must apply the matrix equations or use some group theoretical "tricks"

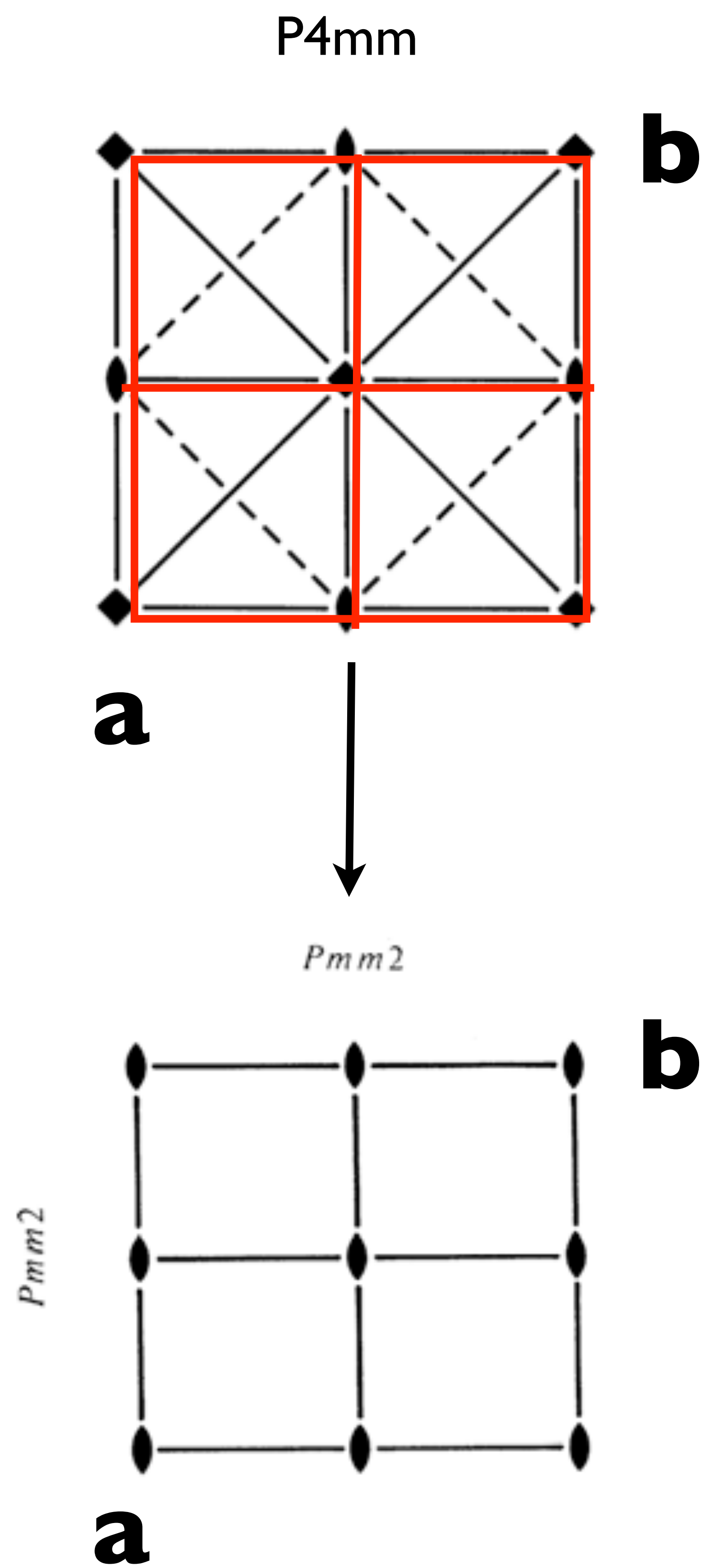
isotropy subgroup depends on the "direction" of the 2-dim order parameter.

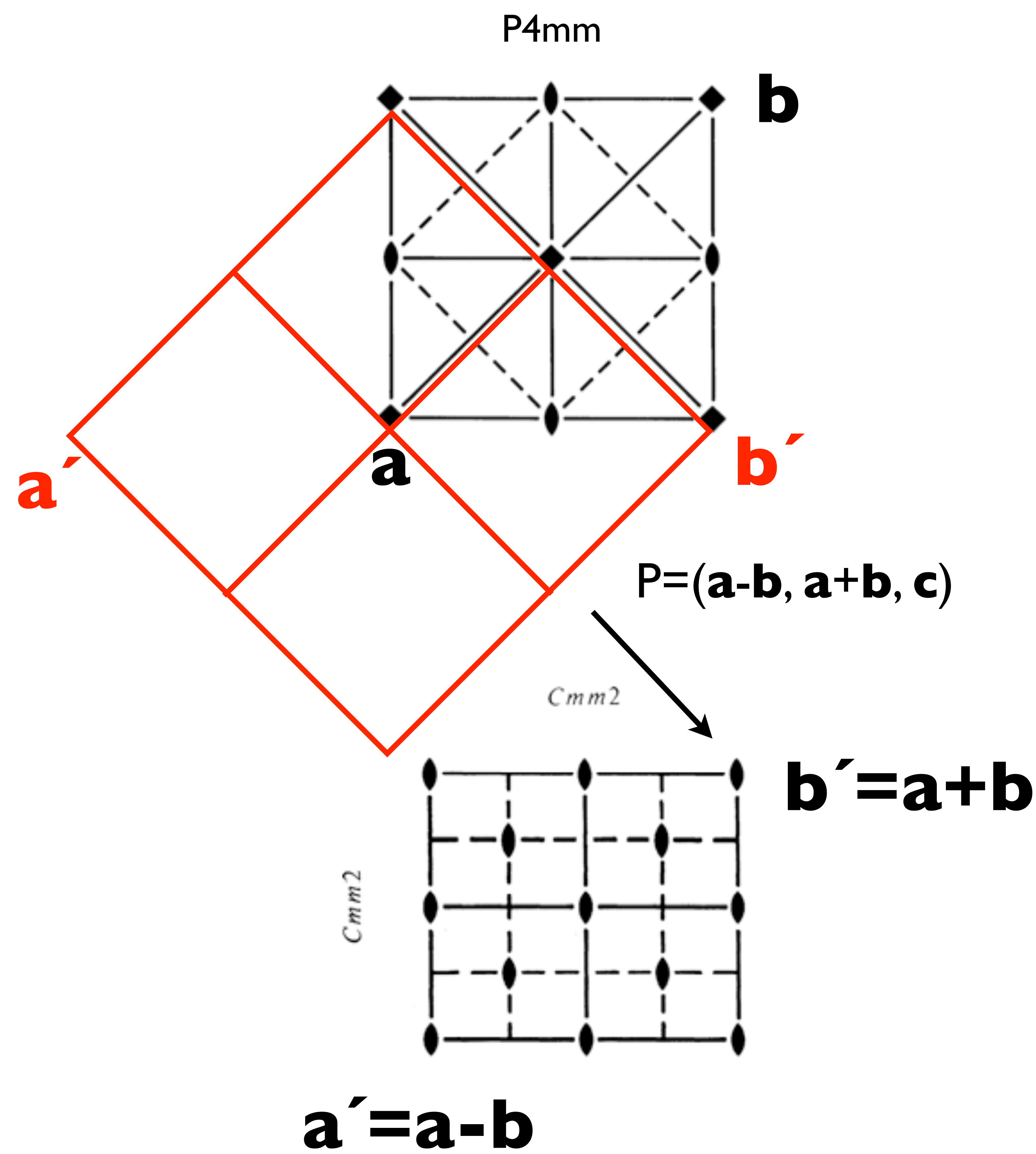
E[g] Q=Q {g}=H

Why Cmm2?
Where the C-centring comes from?

Problem 5.1b

SOLUTION

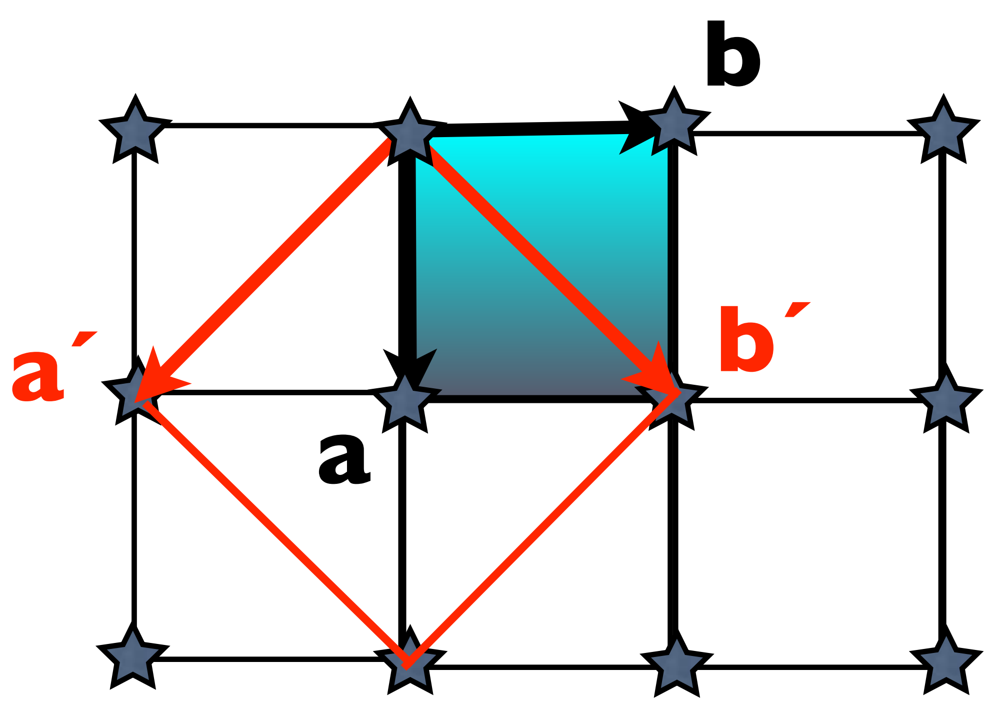




Problem 5.1b

SOLUTION

Remark 1. Due to the convention to choose the basis vectors parallel to the rotation axes, *C*-centered cells appear although the translation lattice has not changed. If the retained twofold axes are diagonal, the conventional basis vectors **a',b',c'** of the subgroup are **a' = a-b, b' = a+b, c' = c** with respect to the basis vectors **a,b,c** of *P*4*mm*. Referred to **a',b',c'** the cell is *C*-centered.



Primitive

a'=a-b

b'=a+b

Centred

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

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

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

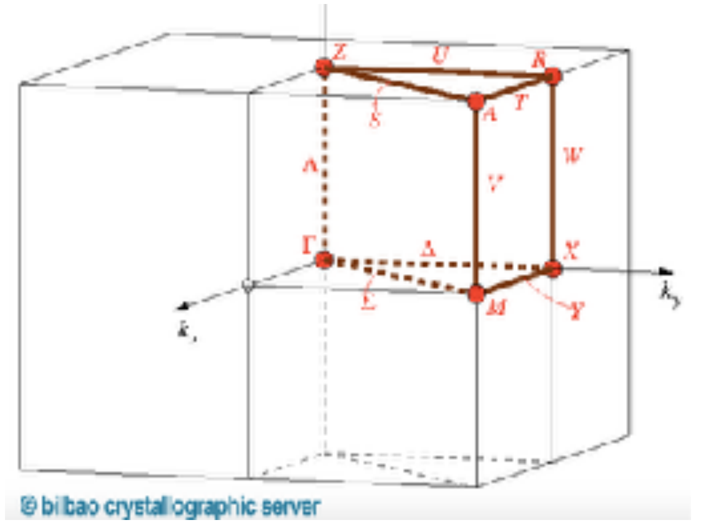
Correlations between representations

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

```
--------------------------------------------------
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: Compatibility relations between little-group representations

in the study of connectivity of energy bands (electronic bands or phonon dispersion curves) as we move in a continuous way from one k-vector point to a neighbouring one with a different symmetry



Group-subgroup little-group pair

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

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

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

'magic' formula

$$m_j = 1/|G^{k'}| \sum_{g^{k'} \in G^{k'}} \eta^{k,i}(g^{k'})\, \eta^{k',j}(g^{k'})^*$$

Problem: Compatibility relations between little-group representations

COMPREL
DCOMPREL

Compatibility Relations between representations of the Double Space Groups

Please, enter the sequential number of group as given in the *International Tables for Crystallography*, Vol. A   [choose it] 130

group G

List of non-equivalent k-vectors of the Space Group *P4/ncc* (No. 130)

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

INPUT data

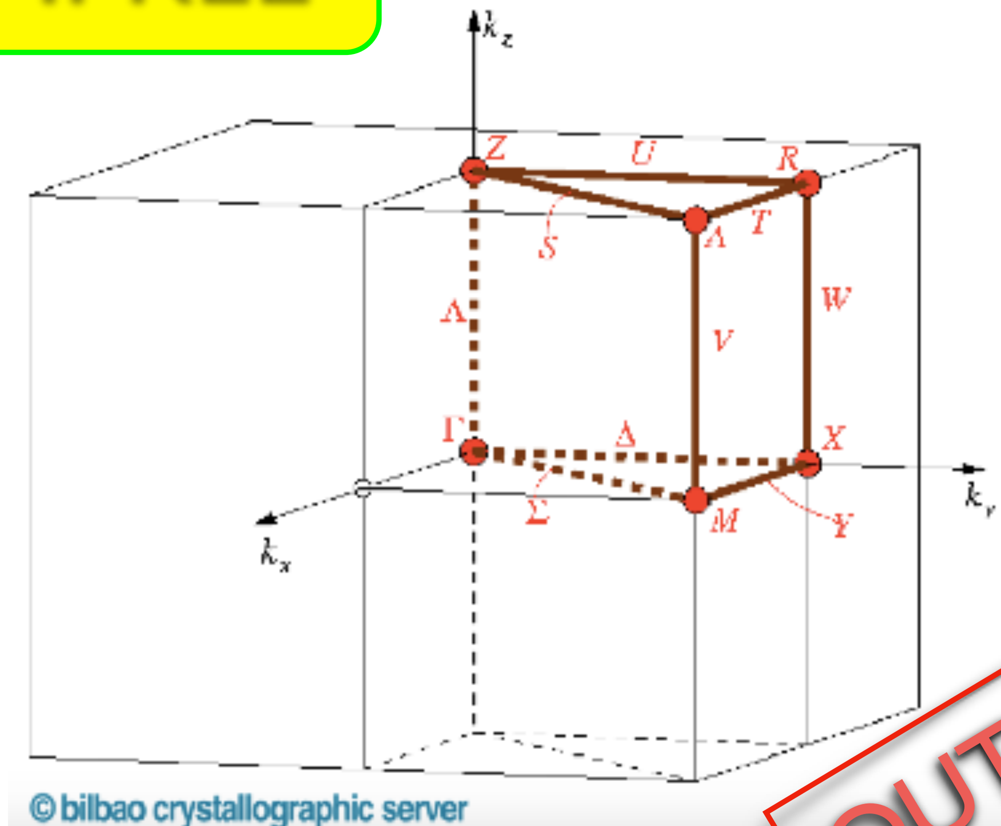
k₁-vector

k₂-vector

Choose the second k-vector.

Choose one	k-vector label	Components in the conventional basis
●	all	
○	B	(0,v,w)
○	F	(u,1/2,w)
○	GP	(u,v,w)
○	R	(0,1/2,1/2)
○	X	(0,1/2,0)

DCOMPREL



P4/ncc (130)

OUTPUT data

Compatibility relations involving the k-vector W:(0,1/2,w).

In parentheses: dimension of the irrep of the little group.

k-vector	Compatibility Relations
B:(0,v,w)	$W_1(1) \rightarrow B_1(1)$ $W_2(1) \rightarrow B_2(1)$ $W_3(1) \rightarrow B_1(1)$ $W_4(1) \rightarrow B_2(1)$ $\overline{W}_5(2) \rightarrow \overline{B}_3(1) \oplus \overline{B}_4(1)$
F:(u,1/2,w)	$W_1(1) \rightarrow F_1(1)$ $W_2(1) \rightarrow F_2(1)$ $W_3(1) \rightarrow F_2(1)$ $W_4(1) \rightarrow F_1(1)$ $\overline{W}_5(2) \rightarrow \overline{F}_3(1) \oplus \overline{F}_4(1)$
GP:(u,v,w)	$W_1(1) \rightarrow GP_1(1)$ $W_2(1) \rightarrow GP_1(1)$ $W_3(1) \rightarrow GP_1(1)$ $W_4(1) \rightarrow GP_1(1)$ $\overline{W}_5(2) \rightarrow 2\overline{GP}_2(1)$
R:(0,1/2,1/2)	$R_1(2) \rightarrow W_1(1) \oplus W_4(1)$ $R_2(2) \rightarrow W_2(1) \oplus W_3(1)$ $\overline{R}_3(2) \rightarrow \overline{W}_5(2)$ $\overline{R}_4(2) \rightarrow \overline{W}_5(2)$
X:(0,1/2,0)	$X_1(2) \rightarrow W_1(1) \oplus W_3(1)$ $X_2(2) \rightarrow W_2(1) \oplus W_4(1)$ $\overline{X}_3(2) \rightarrow \overline{W}_5(2)$ $\overline{X}_4(2) \rightarrow \overline{W}_5(2)$

'magic' formula

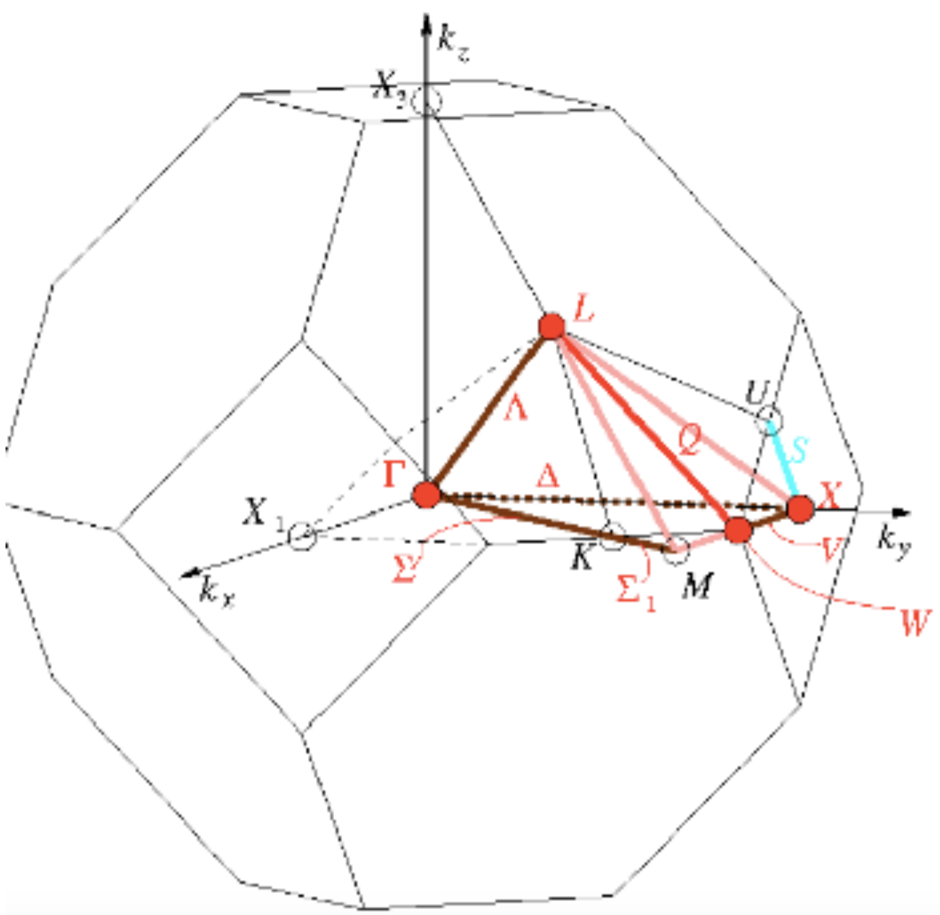
$$m_j = 1/n \sum_{g^{k'}=1}^{n} \eta^{k,i}(g^{k'})\,\eta^{k',j}(g^{k'})^*$$

$g^{k'}$ are the coset representatives of the decomposition of $G^{k'}$ with respect to its translation subgroup

EXERCISES

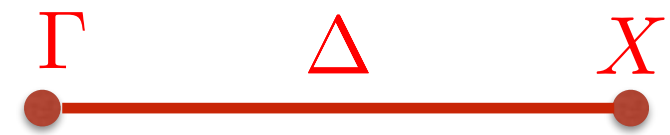
Problem 5.2

Determine the connectivity of the electronic energy bands of Ge, symmetry group Fd-3m (227), between the high symmetry points GM and X over the symmetry line DT

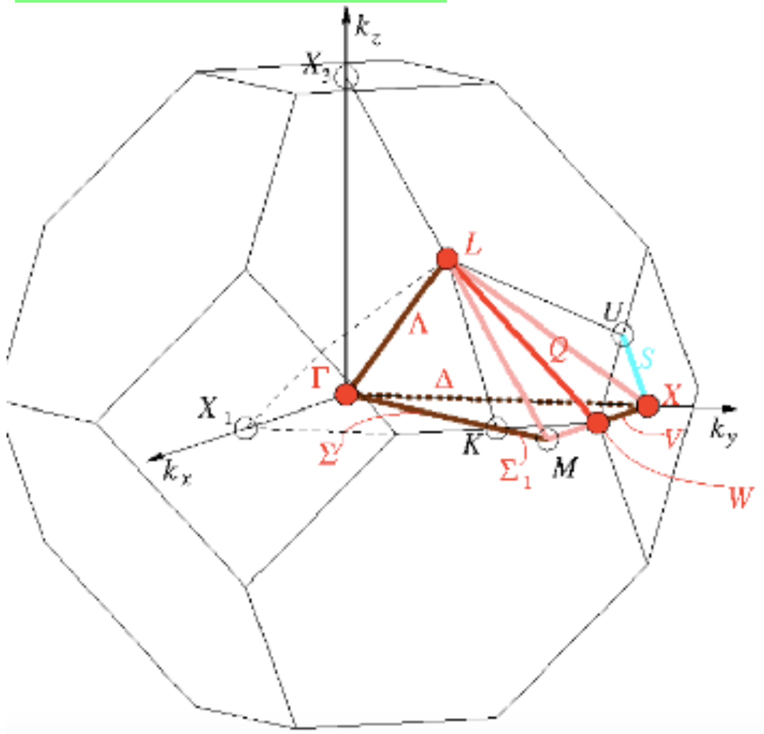


k-vector description			Wyckoff Position		
CDML[1] Label	CDML[1] Primitive basis	Conventional basis			
GM	0,0,0	0,0,0	2	a	m-3m
X	1/2,0,1/2	0,1,0	6	b	4/mm.m
L	1/2,1/2,1/2	1/2,1/2,1/2	8	c	.-3m
W	1/2,1/4,3/4	1/2,1,0	12	d	-4m.2
DT	u,0,u	0,2u,0	12	e	4m.m
LD	u,u,u	u,u,u	16	f	.3m
V	1/2,u,1/2+u	2u,1,0	24	g	mm2..
SM	u,u,2u ex	2u,2u,0	24	h	m.m2
S	1/2+u,2u,1/2+u ex	2u,1,2u	24	h	m.m2

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



SOLUTION



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

$GM_1^+(1) \rightarrow DT_1(1)$

$GM_1^-(1) \rightarrow DT_4(1)$

$GM_2^+(1) \rightarrow DT_2(1)$

$GM_2^-(1) \rightarrow DT_3(1)$

$GM_3^+(2) \rightarrow DT_1(1) \oplus DT_2(1)$

$GM_3^-(2) \rightarrow DT_3(1) \oplus DT_4(1)$

$GM_4^+(3) \rightarrow DT_4(1) \oplus DT_5(2)$

$GM_4^-(3) \rightarrow DT_1(1) \oplus DT_5(2)$

$GM_5^+(3) \rightarrow DT_3(1) \oplus DT_5(2)$

$GM_5^-(3) \rightarrow DT_2(1) \oplus DT_5(2)$

$\overline{GM}_6(2) \rightarrow \overline{DT}_7(2)$

$\overline{GM}_7(2) \rightarrow \overline{DT}_6(2)$

$\overline{GM}_8(2) \rightarrow \overline{DT}_7(2)$

$\overline{GM}_9(2) \rightarrow \overline{DT}_6(2)$

$\overline{GM}_{10}(4) \rightarrow \overline{DT}_6(2) \oplus \overline{DT}_7(2)$

$\overline{GM}_{11}(4) \rightarrow \overline{DT}_6(2) \oplus \overline{DT}_7(2)$

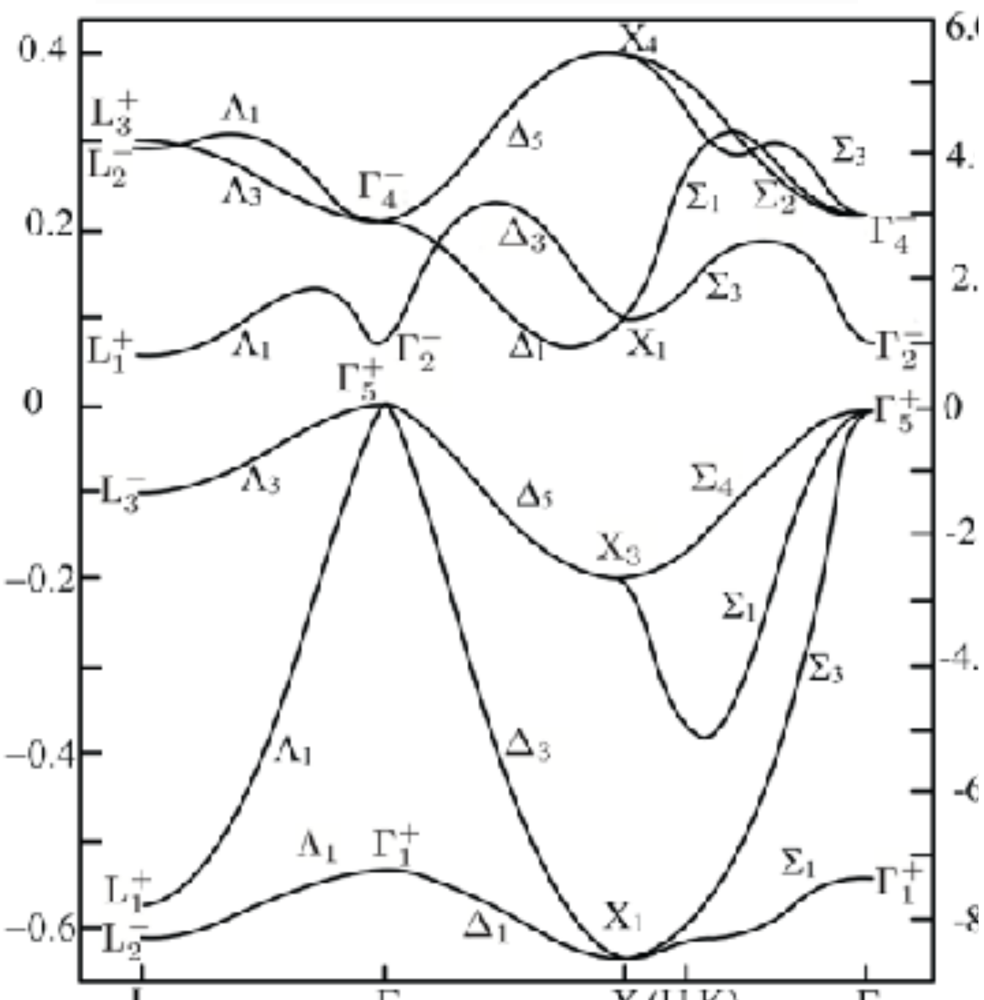
$X_1(2) \rightarrow DT_1(1) \oplus DT_3(1)$

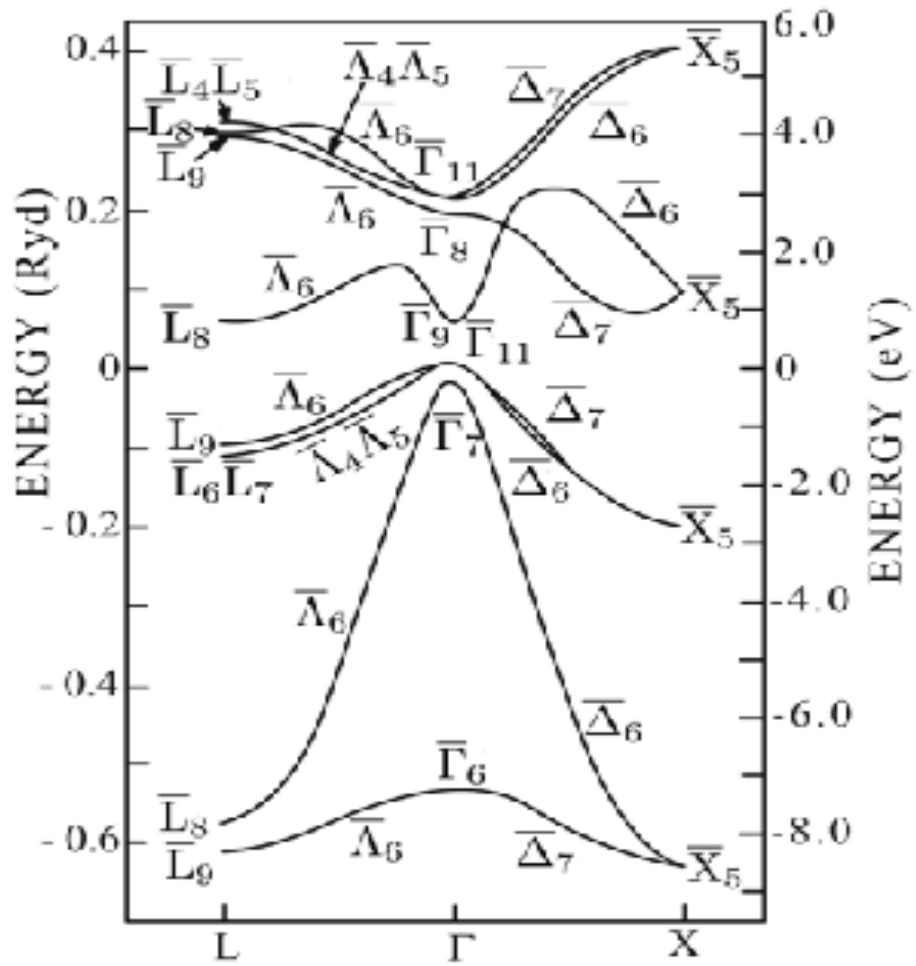
$X_2(2) \rightarrow DT_2(1) \oplus DT_4(1)$

$X_3(2) \rightarrow DT_5(2)$

$X_4(2) \rightarrow DT_5(2)$

$\overline{X}_5(4) \rightarrow \overline{DT}_6(2) \oplus \overline{DT}_7(2)$





DIRECT-PRODUCT SPACE-GROUP REPRESENTATIONS

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

$D_1(G)$: irrep of G

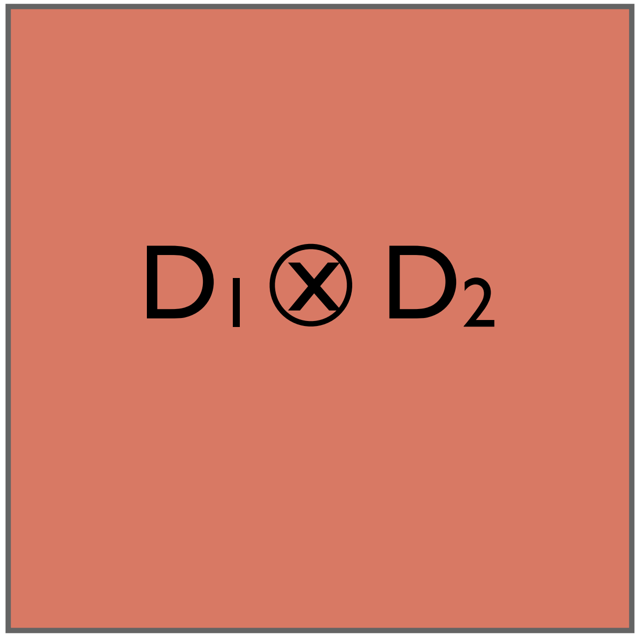
$\{D_1(e), D_1(g_2), \ldots, D_1(g_n)\}$

$D_2(G)$: irrep of G

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

Direct-product representation

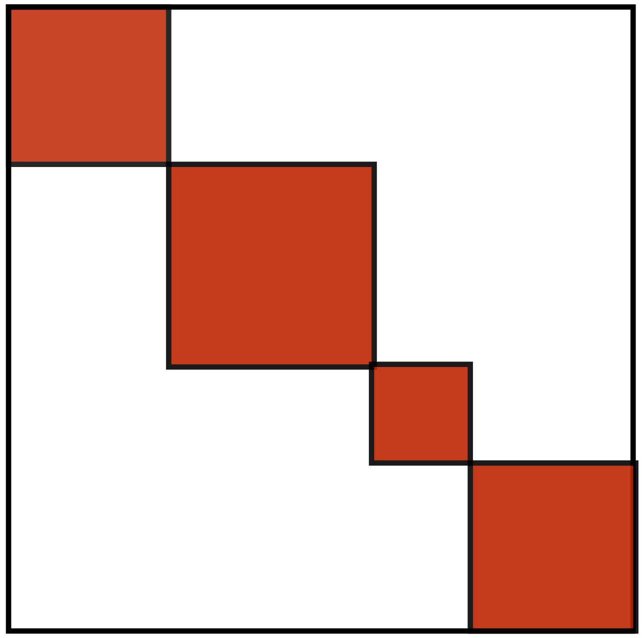
$$D_1 \otimes D_2 = \{D_1(e) \otimes D_2(e), \ldots, D_1(g_i) \otimes D_2(g_i), \ldots\}$$



Reduction

$D_1 \otimes D_2$

$\bigoplus m_i D_i(G)$



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 5.3

(a) Consider the space group P4mm and its **k**-vector X(0,1/2,0). Determine the wave-vector selection rules for the product of the **k**-vector stars:

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

(b) 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

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

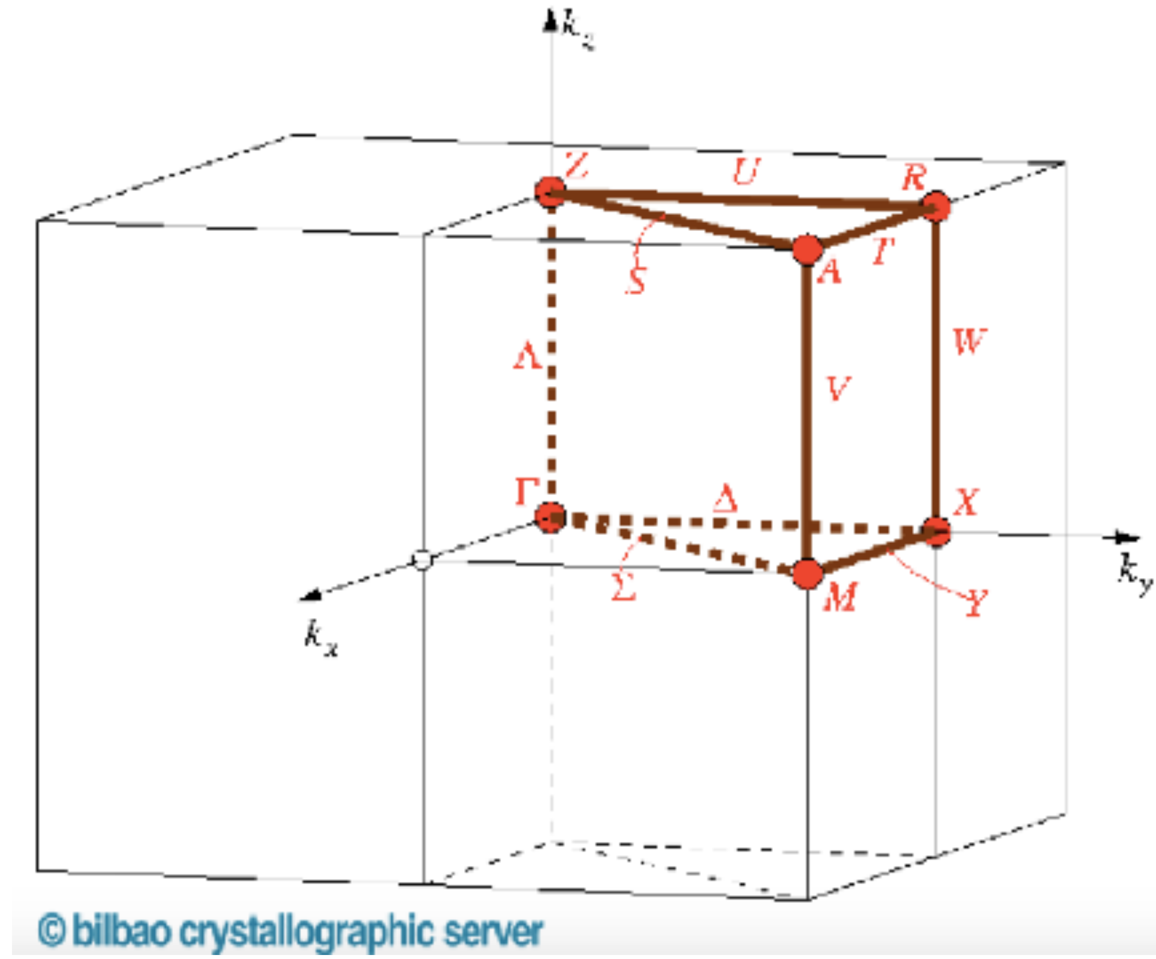
Hints:

The arms of *DT: (0 0.27,0), (0 -0.27,0), (0.27,0,0), (-0.27,0,0)

The arms of *X: ????

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 5.3

SOLUTION

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

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

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

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

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

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

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

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

INPUT data

group G

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

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

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

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

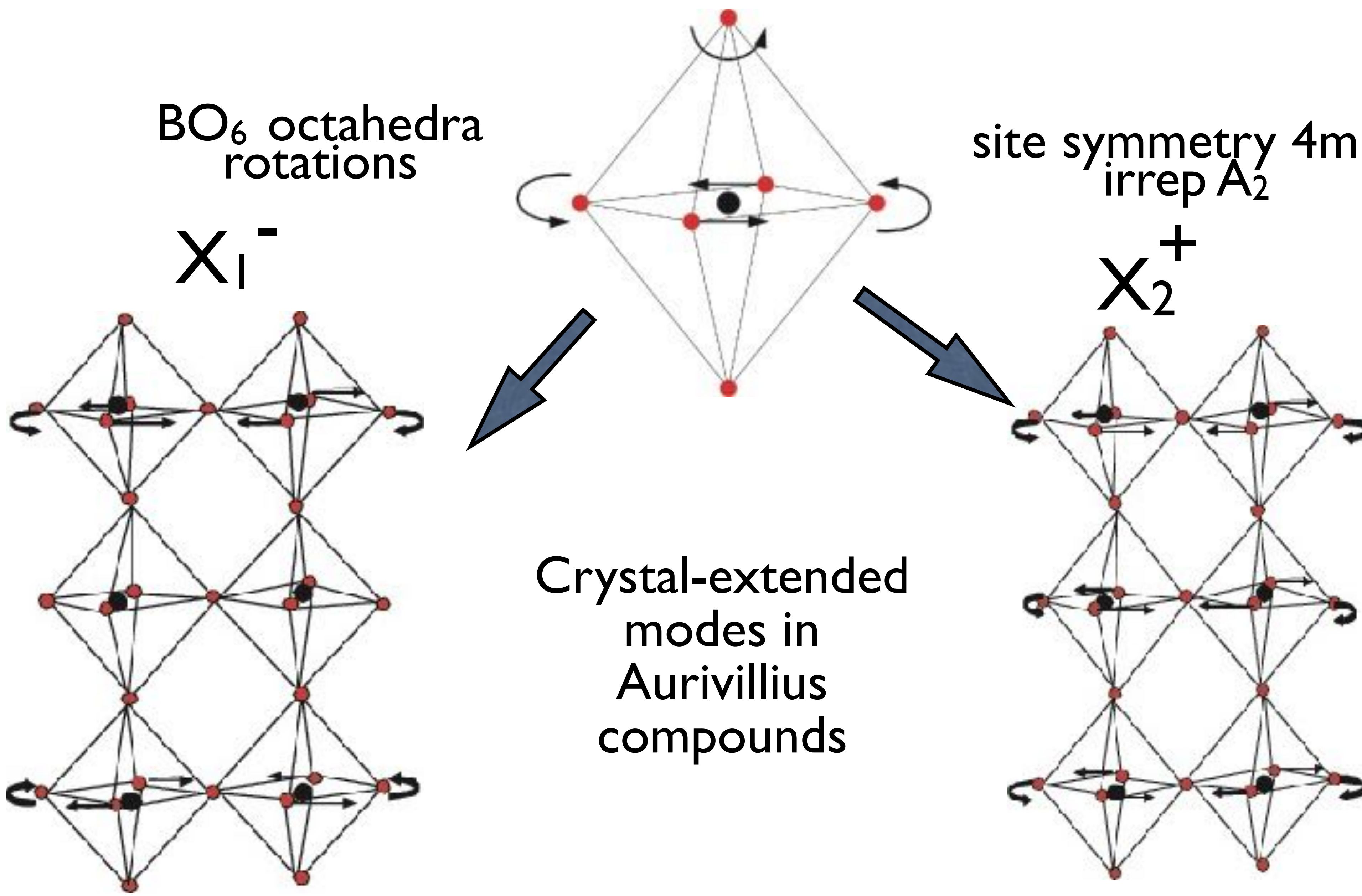
↓

$\bigoplus m_i D_i(G)$

SITE-SYMMETRY APPROACH AND APPLICATIONS

Problem: LOCALIZED and EXTENDED STATES SITE-SYMMETRY APPROACH

symmetry of the extended states (phonons, electronic bands, etc.) of crystal structures over the entire BZ	⟷	symmetry of the localized states (local displacements,, atomic orbitals, etc.) of constituent structural units
irreps of the space group G	⟷	irreps of the local group S



Problem: LOCALIZED and EXTENDED STATES SITE-SYMMETRY APPROACH

the procedure relating localized and extended crystalline states can be described by induction of a representation of a space group $\mathcal{G}$ from a finite subgroup $\mathcal{H}$, followed by a reduction into irreps.

↓

the site-symmetry group $\mathcal{S}$ (isomorphic to a point group) is a subgroup of infinite index of $\mathcal{G}$ implies that the *representation of $\mathcal{G}$* induced by an irrep of $\mathcal{S}$ must be *of infinite dimension*

↓

Frobenius reciprocity theorem, which states that the multiplicities of the irreps of a group $\mathcal{G}$ in the induced representation from an irrep of a subgroup $\mathcal{H}$ of $\mathcal{G}$ can be determined from the multiplicities of the irreps of $\mathcal{H}$ in the representations subduced from $\mathcal{G}$ to $\mathcal{H}$

Site-symmetry approach: although the induced representation has infinite dimension, it is possible to know the part that corresponds to any set of irreps of $\mathcal{G}$ for a given **k**

Evarestov & Smirnov, *Site-symmetry in Crystals* (1997)

Problem: LOCALIZED and EXTENDED STATES

SITESYM DSITESYM

PROCEDURE

(1) Given a space group G and an occupied Wyckoff position, determine its site-symmetry group S (WPOS).

(2) Calculate the irreps of the space group G for the wavevectors k of interest (REPRES or REPRESENTATIONS DSG).

(3) From the obtained space-group irreps of G, calculate the representations subduced to the site-symmetry group S

(4) From the irreps of the site-symmetry group (POINT or REPRESENTATIONS DPG) and making use of the reduction formula, calculate the multiplicities of the site-symmetry irreps in the subduced representations.

(5) Apply the Frobenius reciprocity theorem to obtain the multiplicities of the irreps in the induced representation of G from the multiplicities of irreps of S.

Problem: LOCALIZED and EXTENDED STATES — SITESYM DSITESYM

Site symmetry of the Double Space Groups

Please, enter the sequential number of group as given in the *International Tables for Crystallography*, Vol. A — choose it: 115

group G

List of non-equivalent k-vectors of the Space Group $P\bar{4}m2$ (No. 115)

The components are referred to the conventional basis

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

k-vector

INPUT data

Choose a Wyckoff position

	Multiplicity	Wyckoff letter	Coordinates
○	8	l	(x,y,z),(-x,-y,z),(y,x,-z),(-y,-x,-z) (y,-x,-z),(-y,x,-z),(-x,y,z),(x,-y,z)
○	4	k	(x,1/2,z),(-x,1/2,z),(1/2,x,-z),(1/2,-x,-z)
○	4	j	(x,0,z),(-x,0,z),(0,x,-z),(0,-x,-z)
○	4	i	(x,x,1/2),(-x,-x,1/2),(x,-x,1/2),(-x,x,1/2)
○	4	h	(x,x,0),(-x,-x,0),(x,-x,0),(-x,x,0)
●	2	g	(0,1/2,z),(1/2,0,-z)
○	2	f	(1/2,1/2,z),(1/2,1/2,-z)
○	2	e	(0,0,z),(0,0,-z)
○	1	d	(0,0,1/2)
○	1	c	(1/2,1/2,1/2)
○	1	b	(1/2,1/2,0)
○	1	a	(0,0,0)

Wyckoff position

Induced site-symmetry representations of the double space group *P*-4*m*2 (No. 115)

k-vector: M: (1/2,1/2,0) and Wyckoff position 2g: (0,1/2,z)

Site symmetry group for 2g: (0,1/2,z)

	Shorthand notation	Matrix presentation	
g_1	x,y,z s^+,s^-	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$
g_2	-x,1-y,z $-is^+,is^-$	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix}$
g_3	x,1-y,z $-s^-,s^+$	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$
g_4	-x,y,z $-is^-,-is^+$	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix}$
g_5	x,y,z $-s^+,-s^-$	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$
g_6	-x,1-y,z $is^+,-is^-$	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}$
g_7	x,1-y,z $+s^-,-s^+$	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$
g_8	-x,y,z $+is^-,is^+$	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}$

DSITESYM

OUTPUT data

Irreducible representations

Character table for *mm*2

*mm*2	#	1	2_{001}	m_{010}	m_{100}	$^d1$	$^d2_{001}$	$^dm_{010}$	$^dm_{100}$
A_1	Γ_1	1	1	1	1	1	1	1	1
A_2	Γ_2	1	1	-1	-1	1	1	-1	-1
B_2	Γ_3	1	-1	-1	1	1	-1	-1	1
B_1	Γ_4	1	-1	1	-1	1	-1	1	-1
$\bar{E}$	$\bar{\Gamma}_5$	2	0	0	0	-2	0	0	0

Subduced representations

Character table for the subduced representations (*M↓*mm*2) for Wyckoff position 2g

Reps\Irreps	g_1	g_2	g_3	g_4	g_5	g_6	g_7	g_8
M_1	1	-1	-1	1	1	-1	-1	1
M_2	1	-1	-1	1	1	-1	-1	1
M_3	1	-1	1	-1	1	-1	1	-1
M_4	1	-1	1	-1	1	-1	1	-1
M_5	2	2	0	0	2	2	0	0
$\bar{M}_6$	2	0	0	0	-2	0	0	0
$\bar{M}_7$	2	0	0	0	-2	0	0	0

DSITESYM

Decomposition of (*M↓*mm*2)
into irreducible
representations of *mm*2

Reps\Irreps	A_1	A_2	B_2	B_1	$\bar{E}$
M_1	.	.	1	.	.
M_2	.	.	1	.	.
M_3	.	.	.	1	.
M_4	.	.	.	1	.
M_5	1	1	.	.	.
$\bar{M}_6$	.	.	.	.	1
$\bar{M}_7$	.	.	.	.	1

Induced representations

Induced representations for the point M of *P*-4*m*2

Reps\Irreps	M_1	M_2	M_3	M_4	M_5	$\bar{M}_6$	$\bar{M}_7$
A_1	.	.	.	.	1	.	.
A_2	.	.	.	.	1	.	.
B_2	1	1	.	.	.	.	.
B_1	.	.	1	1	.	.	.
$\bar{E}$	.	.	.	.	.	1	1

OUTPUT data

$$A_1 \uparrow P4m2 \sim M_5 \oplus \cdots$$
$$A_2 \uparrow P\bar{4}m2 \sim M_5 \oplus \cdots$$
$$B_2 \uparrow P\bar{4}m2 \sim M_1 \oplus M_2 \oplus \cdots$$
$$B_1 \uparrow P\bar{4}m2 \sim M_3 \oplus M_4 \oplus \cdots$$
$$\bar{E} \uparrow P\bar{4}m2 \sim \bar{M}_6 \oplus \bar{M}_7 \oplus \cdots$$

BAND REPRESENTATIONS

Zak (1982)

A set of extended energy states over the entire reciprocal space $E_n(\mathbf{k})$, related to the symmetry of (exponentially) localized states (Wannier orbitals)

The localized states (the atomic orbitals, for example) of an atom that occupy a given Wyckoff position of $\mathcal{G}$ transform according to a representation $\mathbf{d}_\alpha$ of its site-symmetry group (or double site-symmetry group, if spin-orbit coupling is considered). A **band representation** can be defined as the induced representation $\mathbf{d}_\alpha \uparrow \mathcal{G}$, being a particular case of the site-symmetry approach

Necessary to calculate only BRs induced from the **irreps** of its site-symmetry group

$$\mathbf{d}_\alpha = \bigoplus_\beta n_\beta^{(\alpha)} \mathbf{d}_\beta \qquad \mathbf{d}_\alpha \uparrow \mathcal{G} = \bigoplus_\beta n_\beta^{(\alpha)} (\mathbf{d}_\beta \uparrow \mathcal{G})$$

The BRs induced from different irreps of the same site-symmetry group are not equivalent, but BRs induced from different Wyckoff positions could be equivalent.

Equivalence of Band Representations ?

BAND REPRESENTATIONS

Equivalence of Band Representations:

the definition of equivalence of BRs is different from the definition of equivalence of representations

two BRs $\rho_{\mathcal{G}}^{\mathbf{k}}$ and $\sigma_{\mathcal{G}}^{\mathbf{k}}$ are **equivalent** if subduce into the same little-group representations at **all** points in the Brillouin zone

Consider the Wyckoff positions Q and Q' with site symmetry groups $\mathcal{S}_Q$ and $\mathcal{S}_{Q'}$

ρ of $\mathcal{S}_{\mathbf{Q}}$, σ of $\mathcal{S}_{\mathbf{Q}'}$, τ of $\mathcal{S}_o = \mathcal{S}_{\mathbf{Q}} \cap \mathcal{S}_{\mathbf{Q}'}$

if $\tau \uparrow S_{\mathbf{Q}} = \rho$ and $\tau \uparrow S_{\mathbf{Q}'} = \sigma$ then the two BR $\begin{matrix}(\sigma \uparrow \mathcal{G}) \downarrow \mathcal{G}^{\mathbf{k}} = \sigma_{\mathcal{G}}^{\mathbf{k}} \\ (\rho \uparrow \mathcal{G}) \downarrow \mathcal{G}^{\mathbf{k}} = \rho_{\mathcal{G}}^{\mathbf{k}}\end{matrix}$ are equivalent

Composite and Elementary Band Representations:

A band representation is called **composite** if it is equivalent to the direct sum of other band representations. A band representation that is not composite is called **elementary**.

All elementary band representations (EBRs) are induced from the **Wyckoff positions of maximal symmetry**, but the opposite is not true

Wyckoff positions of maximal symmetry

A Wyckoff position Q with a site-symmetry group S_Q has maximal symmetry if it is not connected to another Wyckoff position Q' whose site-symmetry group $S_{Q'}$ is a supergroup of S_Q

Wyckoff positions are **connected** if (i) the coordinate triplet of at least one of them depends on one or more variable parameters, and (ii) for specific values of the variable parameters, the coordinate triplets of the two Wyckoff positions coincide.

Wyckoff positions of the double space group P4/ncc

Wyckoff position	Site-symmetry group	Coordinate triplet	Maximal symmetry
4*a*	$222(D_2)$	(3/4, 1/4, 1/4)	Yes
4*b*	$\bar{4}(S_4)$	(3/4, 1/4, 0)	Yes
4*c*	$4(C_4)$	(1/4, 1/4, *z*)	Yes
8*d*	$\bar{1}(C_i)$	(0, 0, 0)	Yes
8*e*	$2(C_2)$	(3/4, 1/4, *z*)	No $z = 1/4 \rightarrow 4a$
8*f*	$2(C_2)$	$(x + 1/2, x, 1/4)$	No $x = 1/4 \rightarrow 4a$
16*g*	$1(C_1)$	(*x*, *y*, *z*)	No $x = y = z = 0 \rightarrow 8d$

k-vectors of maximal symmetry

k- vector of maximal symmetry: if its little co-group **is not a subgroup** of the little co-group of another $\mathbf{k}_0$-vector type connected to **k**

connected k-vector types: if (i) the coefficient triplet of at least one of them depends on one or more variable parameters, and (ii) for specific values of the variable parameters, the coefficient triplets of the two k-vector types coincide.

non-centrosymmetric groups: modification of the set of maximal-symmetry **k** vectors (splitting of the **k**-vector types) under time-reversal symmetry

TRIM points: Time Reversal Invariant Momentum points:

k-vector types of of maximal symmetry the double space group P4 (No.75)

Label	Little co-group	Coefficients
Λ	$4(C_4)$	$(0, 0, w)$
W	$4(C_4)$	$(0, 1/2, w)$
V	$4(C_4)$	$(1/2, 1/2, w)$

NO time-reversal symmetry

Label	Little co-group	Coefficients
Γ	$4(C_4)$	$(0, 0, 0)$
Z	$4(C_4)$	$(0, 0, 1/2)$
X	$4(C_4)$	$(0, 1/2, 0)$
R	$4(C_4)$	$(0, 1/2, 1/2)$
M	$4(C_4)$	$(1/2, 1/2, 0)$
A	$4(C_4)$	$(1/2, 1/2, 1/2)$

WITH time-reversal symmetry

Problem: BAND REPRESENTATIONS BANDREP

PROCEDURE

(i) Site-symmetry approach

- given a space group G, a BR is fully identified by a Wyckoff position, an irrep of its site-symmetry group and the irreps of the little groups of any **k** vector of the reciprocal space: the irrep multiplicities of BRs are determined by applying the site-symmetry approach.

- it is only necessary to consider **k** vectors of maximal symmetry: compatibility relations for the irrep multiplicities of any other k vector

(ii) Elementary or composite BR

- BRs induced from Wyckoff positions of maximal symmetry

- Each BR is characterized by a set of multiplicities of the little-group irreps but only for **k** vectors of maximal symmetry

- candidate to be a composite BR: check if decomposes at every **k** as the direct sum of two or more BR (induced of different Wyckoff position Q')

- equivalence check with the irreps τ of the intersection group $\mathcal{S}_o = \mathcal{S}_{\mathbf{Q}} \cap \mathcal{S}_{\mathbf{Q}'}$

if the candidate-for-composite BR $(\rho \uparrow \mathcal{G}) \downarrow \mathcal{G}^{\mathbf{k}} = \rho^{\mathbf{k}}_{\mathcal{G}}$ induced from ρ of $\mathcal{S}_{\mathbf{Q}}$ is equivalent to a band representation $(\sigma \uparrow \mathcal{G}) \downarrow \mathcal{G}^{\mathbf{k}} = \sigma^{\mathbf{k}}_{\mathcal{G}}$ induced from a **reaucible** representation σ of $\mathcal{S}_{\mathbf{Q}'}$ with $\tau \uparrow S_{\mathbf{Q}} = \rho$ and $\tau \uparrow S_{\mathbf{Q}'} = \sigma$

Problem: BAND REPRESENTATIONS BANDREP

group G

Band representations of the Double Space Groups

Band Representations

This program calculates the band representations (BR) induced from the irreps of the site-symmetry group of a given Wyckoff position.
Alternatively, it gives the set of elementary BRs of a Double Space Group.
In both cases, it can be chosen to get the BRs with or without time-reversal symmetry.
The program also indicates if the elementary BRs are decomposable or indecomposable. If it is decomposable, the program gives all the possible ways to decompose it.

Please, enter the sequential number of group as given in the *International Tables for Crystallography*, Vol. A [choose it] 130

1. Get the elementary BRs without time-reversal symmetry [Elementary]
2. Get the elementary BRs with time-reversal symmetry [Elementary TR]
3. Get the BRs without time-reversal symmetry from a Wyckoff position [Wyckoff]
4. Get the BRs with time-reversal symmetry from a Wyckoff position [Wyckoff TR]

Band-representations of the Double Space Group *P4/ncc* (No. 130)

Choose a Wyckoff position

INPUT data

Wyckoff positions of maximal symmetry

	Multiplicity	Wyckoff letter	Coordinates
◉	4	a	(3/4,1/4,1/4),(1/4,3/4,1/4),(1/4,3/4,3/4),(3/4,1/4,3/4)
○	4	b	(3/4,1/4,0),(1/4,3/4,0),(1/4,3/4,1/2),(3/4,1/4,1/2)
○	4	c	(1/4,1/4,z),(3/4,3/4,1/2-z),(3/4,3/4,-z),(1/4,1/4,1/2+z)
○	8	d	(0,0,0),(1/2,0,0),(0,1/2,0),(1/2,0,1/2) (0,1/2,1/2),(1/2,1/2,0),(1/2,1/2,1/2),(0,0,1/2)

Wyckoff positions of non-maximal symmetry

	Multiplicity	Wyckoff letter	Coordinates
○	8	e	(3/4,1/4,z),(1/4,3/4,z),(1/4,3/4,1/2-z),(3/4,1/4,1/2-z) (1/4,3/4,-z),(3/4,1/4,-z),(3/4,1/4,1/2+z),(1/4,3/4,1/2+z)
○	8	f	(x,-x,1/4),(1/2+x,x,1/4),(-x,1/2-x,1/4),(1/2-x,1/2+x,1/4) (-x,x,3/4),(1/2-x,-x,3/4),(x,1/2+x,3/4),(1/2+x,1/2-x,3/4)
○	16	g	(x,y,z),(1/2-y,x,z),(y,1/2-x,z),(1/2+x,-y,1/2-z) (-x,1/2+y,1/2-z),(1/2-x,1/2-y,z),(1/2+y,1/2+x,1/2-z),(-y,-x,1/2-z) (-x,-y,-z),(1/2+y,-x,-z),(-y,1/2+x,-z),(1/2-x,y,1/2+z) (x,1/2-y,1/2+z),(1/2+x,1/2+y,-z),(1/2-y,1/2-x,1/2+z),(y,x,1/2+z)

OPTION I

BANDREP

Elementary band-representations without time-reversal symmetry of the Double Space Group *P4/ncc* (No. 130)

The first row shows the Wyckoff position from which the band representation is induced.
In parenthesis, the symbol of the point group isomorphic to the site-symmetry group.

The second row gives the symbol ρ↑G, where ρ is the irrep of the site-symmetry group.
In parenthesis, the dimension of the representation.

The output shows the decomposition of the band representations into irreps of the little groups of the given k-vectors in the first column.
In parenthesis, the dimensions of the representations.

Minimal set of paths and compatibility relations to analyse the connectivity

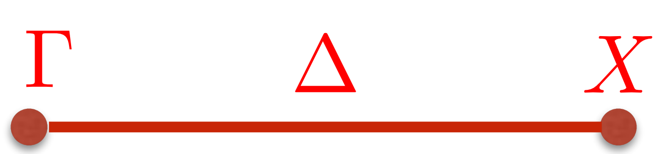
Show all types of k-vectors

Wyckoff pos.	4a(222)	4a(222)	4a(222)	4a(222)	4b($\bar{4}$)	4b($\bar{4}$)	
Band-Rep.	A_1↑G(4)	B_1↑G(4)	B_2↑G(4)	B_3↑G(4)	A↑G(4)	B↑G(4)	
Decomposable\ Indecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposable	Inde
A:(1/2,1/2,1/2)	$A_1(2) \oplus A_2(2)$	$A_1(2) \oplus A_2(2)$	$A_3(2) \oplus A_4(2)$	$A_3(2) \oplus A_4(2)$	$A_1(2) \oplus A_2(2)$	$A_1(2) \oplus A_2(2)$	A_3(
Γ:(0,0,0)	$\Gamma_1^+(1) \oplus \Gamma_1^-(1) \oplus \Gamma_4^+(1) \oplus \Gamma_4^-(1)$	$\Gamma_2^+(1) \oplus \Gamma_2^-(1) \oplus \Gamma_3^+(1) \oplus \Gamma_3^-(1)$	$\Gamma_5^+(2) \oplus \Gamma_5^-(2)$	$\Gamma_5^+(2) \oplus \Gamma_5^-(2)$	$\Gamma_1^+(1) \oplus \Gamma_2^-(1) \oplus \Gamma_3^+(1) \oplus \Gamma_4^-(1)$	$\Gamma_1^-(1) \oplus \Gamma_2^+(1) \oplus \Gamma_3^-(1) \oplus \Gamma_4^+(1)$	Γ_5^+(
M:(1/2,1/2,0)	$2\ M_2(2)$	$2\ M_1(2)$	$M_3(2) \oplus M_4(2)$	$M_3(2) \oplus M_4(2)$	$M_1(2) \oplus M_2(2)$	$M_1(2) \oplus M_2(2)$	M_3(
R:(0,1/2,1/2)	$R_1(2) \oplus R_2(2)$	$R_1(2) \oplus R_2(2)$	$R_1(2) \oplus R_2(2)$	$R_1(2) \oplus R_2(2)$	$R_1(2) \oplus R_2(2)$	$R_1(2) \oplus R_2(2)$	R_1(
X:(0,1/2,0)	$X_1(2) \oplus X_2(2)$	$X_1(2) \oplus X_2(2)$	$X_1(2) \oplus X_2(2)$	$X_1(2) \oplus X_2(2)$	$X_1(2) \oplus X_2(2)$	$X_1(2) \oplus X_2(2)$	X_1(
Z:(0,0,1/2)	$Z_1(2) \oplus Z_2(2)$	$Z_1(2) \oplus Z_2(2)$	$Z_3(2) \oplus Z_4(2)$	$Z_3(2) \oplus Z_4(2)$	$Z_1(2) \oplus Z_2(2)$	$Z_1(2) \oplus Z_2(2)$	

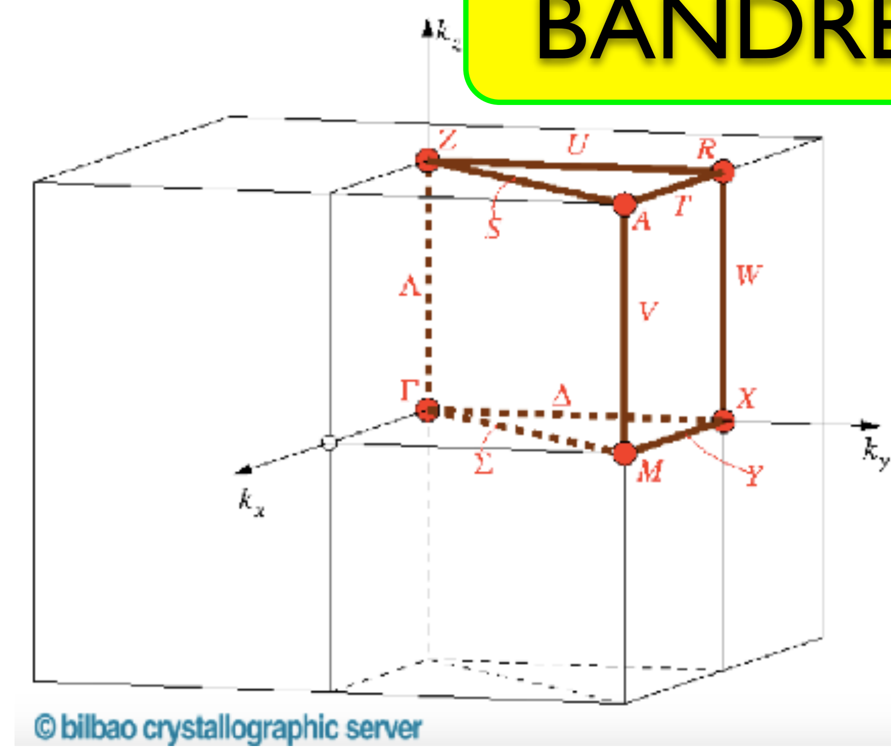
OUTPUT data

Independent paths between k-vectors of maximal symmetry in the space group *P4/ncc* (No. 130).

Maximal k-vector	Intermediate path	Maximal k-vector
Γ:(0,0,0)	Δ:(0,v,0)	X:(0,1/2,0)
Γ:(0,0,0)	Λ:(0,0,w)	Z:(0,0,1/2)
A:(1/2,1/2,1/2)	S:(u,u,1/2)	Z:(0,0,1/2)
Γ:(0,0,0)	Σ:(u,u,0)	M:(1/2,1/2,0)
A:(1/2,1/2,1/2)	T:(u,1/2,1/2)	R:(0,1/2,1/2)
R:(0,1/2,1/2)	U:(0,v,1/2)	Z:(0,0,1/2)
A:(1/2,1/2,1/2)	V:(1/2,1/2,w)	M:(1/2,1/2,0)
R:(0,1/2,1/2)	W:(0,1/2,w)	X:(0,1/2,0)
M:(1/2,1/2,0)	Y:(u,1/2,0)	X:(0,1/2,0)



BANDREP



Independent sets of compatibility relations along the independent paths, necessary for the analysis of connectivities of the elementary band representations (band graphs).

(In parenthesis, the dimension of the representations)

The two different sets of compatibility relations for some pairs of k vecs are due to a non-symmorphic symmetry element (helicoidal axis or a glide-plane). The two sets have been calculated at two different k-vecs of maximal symmetry related by a translation of the reciprocal lattice

Maximal k-vec	Compatibility relations		Intermediate path	Compatibility relations		Maximal k-ve
Γ:(0,0,0)	$\Gamma_1^+(1) \to \Delta_1(1)$ $\Gamma_1^-(1) \to \Delta_2(1)$ $\Gamma_2^+(1) \to \Lambda_1(1)$ $\Gamma_2^-(1) \to \Delta_2(1)$ $\Gamma_3^+(1) \to \Delta_4(1)$ $\Gamma_3^-(1) \to \Delta_3(1)$ $\Gamma_4^+(1) \to \Delta_4(1)$ $\Gamma_4^-(1) \to \Delta_3(1)$ $\Gamma_5^+(2) \to \Delta_2(1) \oplus \Delta_3(1)$ $\Gamma_5^-(2) \to \Delta_1(1) \oplus \Delta_4(1)$ $\overline{\Gamma}_6(2) \to \overline{\Delta}_5(2)$ $\overline{\Gamma}_7(2) \to \overline{\Delta}_5(2)$ $\overline{\Gamma}_8(2) \to \overline{\Delta}_5(2)$ $\overline{\Gamma}_9(2) \to \overline{\Delta}_5(2)$		Δ:(0,v,0)		$X_1(2) \to \Delta_1(1) \oplus \Delta_3(1)$ $X_2(2) \to \Delta_2(1) \oplus \Delta_4(1)$ $\overline{X}_3(2) \to \overline{\Delta}_5(2)$ $\overline{X}_4(2) \to \overline{\Delta}_5(2)$	X:(0,1/2,0)
	$\Gamma_1^+(1) \to \Lambda_1(1)$ $\Gamma_1^-(1) \to \Lambda_4(1)$ $\Gamma_2^+(1) \to \Lambda_2(1)$ $\Gamma_2^-(1) \to \Lambda_3(1)$ [illegible]	$\Gamma_1^+(1) \to \Lambda_4(1)$ $\Gamma_1^-(1) \to \Lambda_1(1)$ $\Gamma_2^+(1) \to \Lambda_3(1)$ $\Gamma_2^-(1) \to \Lambda_2(1)$ [illegible]			$Z_1(2) \to \Lambda_2(1) \oplus \Lambda_3(1)$ [illegible]	

OUTPUT data

OPTION 3

BANDREP

Band-representations without time-reversal symmetry of the Double Space Group *P4/ncc* (No. 130) and Wyckoff position 8d:(0,0,0)

Induced band representations from the irreps of the site-ymmetry group isomorphic to the point group overbarini1overbarfin
In parenthesis, the dimension of the representation.

The output shows the decomposition of the band representations into irreps of the little groups of the given k-vectors in the first column.
In parenthesis, the dimensions of the representations.

Minimal set of paths and compatibility relations to analyse the connectivity

Show all types of k-vectors

Band-Rep.	$A^g \uparrow G(8)$	$A^u \uparrow G(8)$	$\bar{A}^g \uparrow G(8)$	$\bar{A}^u \uparrow G(8)$
Band-type	Elementary	Elementary	Elementary	Elementary
Decomposable\ Indecomposable	Decomposable	Decomposable	Decomposable	Decomposable
A:(1/2,1/2,1/2)	$A_1(2) \oplus A_2(2) \oplus A_3(2) \oplus A_4(2)$	$A_1(2) \oplus A_2(2) \oplus A_3(2) \oplus A_4(2)$	$2\,\bar{A}_5(4)$	$2\,\bar{A}_5(4)$
Γ:(0,0,0)	$\Gamma_1^+(1) \oplus \Gamma_2^+(1) \oplus \Gamma_3^+(1) \oplus \Gamma_4^+(1) \oplus 2\,\Gamma_5^+(2)$	$\Gamma_1^-(1) \oplus \Gamma_2^-(1) \oplus \Gamma_3^-(1) \oplus \Gamma_4^-(1) \oplus 2\,\Gamma_5^-(2)$	$2\,\bar{\Gamma}_6(2) \oplus 2\,\bar{\Gamma}_7(2)$	$2\,\bar{\Gamma}_8(2) \oplus 2\,\bar{\Gamma}_9(2)$
M:(1/2,1/2,0)	$M_1(2) \oplus M_2(2) \oplus M_3(2) \oplus M_4(2)$	$M_1(2) \oplus M_2(2) \oplus M_3(2) \oplus M_4(2)$	$2\,\bar{M}_5(4)$	$2\,\bar{M}_5(4)$
R:(0,1/2,1/2)	$2\,R_1(2) \oplus 2\,R_2(2)$	$2\,R_1(2) \oplus 2\,R_2(2)$	$2\,\bar{R}_3(2) \oplus 2\,\bar{R}_4(2)$	$2\,\bar{R}_3(2) \oplus 2\,\bar{R}_4(2)$
X:(0,1/2,0)	$2\,X_1(2) \oplus 2\,X_2(2)$	$2\,X_1(2) \oplus 2\,X_2(2)$	$2\,\bar{X}_3(2) \oplus 2\,\bar{X}_4(2)$	$2\,\bar{X}_3(2) \oplus 2\,\bar{X}_4(2)$
Z:(0,0,1/2)	$Z_1(2) \oplus Z_2(2) \oplus Z_3(2) \oplus Z_4(2)$	$Z_1(2) \oplus Z_2(2) \oplus Z_3(2) \oplus Z_4(2)$	$\bar{Z}_5(2) \oplus \bar{Z}_6(2) \oplus \bar{Z}_7(2) \oplus \bar{Z}_8(2)$	$\bar{Z}_5(2) \oplus \bar{Z}_6(2) \oplus \bar{Z}_7(2) \oplus \bar{Z}_8(2)$

OUTPUT data

Possible decompositions of elementary band representations

BANDREP

OUTPUT data

Possible decompositions of the elementary band representation induced from the irreducible representation A_g (without time-reversal symmetry) of the space group *P4/ncc* (No. 130) of the point group $\bar{1}$, isomorphic to the site-symmetry group of the Wyckoff position 8d.

	branch 1	branch 2
1	$A_1,A_2,\Gamma_1^+,\Gamma_3^+,\Gamma_5^+,M_1,M_2,R_1,R_2,X_1,X_2,Z_2,Z_3$	$A_3,A_4,\Gamma_2^+,\Gamma_4^+,\Gamma_5^+,M_3,M_4,R_1,R_2,X_1,X_2,Z_1,Z_4$
2	$A_1,A_2,\Gamma_1^+,\Gamma_3^+,\Gamma_5^+,M_1,M_2,R_1,R_2,X_1,X_2,Z_2,Z_4$	$A_3,A_4,\Gamma_2^+,\Gamma_4^+,\Gamma_5^+,M_3,M_4,R_1,R_2,X_1,X_2,Z_1,Z_3$
3	$A_1,A_2,\Gamma_2^+,\Gamma_4^+,\Gamma_5^+,M_1,M_2,R_1,R_2,X_1,X_2,Z_1,Z_3$	$A_3,A_4,\Gamma_1^+,\Gamma_3^+,\Gamma_5^+,M_3,M_4,R_1,R_2,X_1,X_2,Z_2,Z_4$
4	$A_1,A_2,\Gamma_2^+,\Gamma_4^+,\Gamma_5^+,M_1,M_2,R_1,R_2,X_1,X_2,Z_1,Z_4$	$A_3,A_4,\Gamma_1^+,\Gamma_3^+,\Gamma_5^+,M_3,M_4,R_1,R_2,X_1,X_2,Z_2,Z_3$