

**The program NEUTRON: Phonon Selection Rules for  
neutron and X-ray Inelastic Scattering**

**J. Manuel Perez-Mato, Mois I. Aroyo, A. Kirov**

**Universidad del País Vasco  
Bilbao**

# SAM: Modes and selection rules for Infrared and Raman Spectroscopy

## NEUTRON: Phonon selection rules for neutron and X-ray inelastic scattering

The screenshot shows a web browser window titled "Bilbao Crystallographic Server" with the URL "http://www.cryst.ehu.es/". The page content is organized into two main sections: "Representation Theory Applications" and "Solid State Theory Applications".

**Representation Theory Applications**

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

**Solid State Theory Applications**

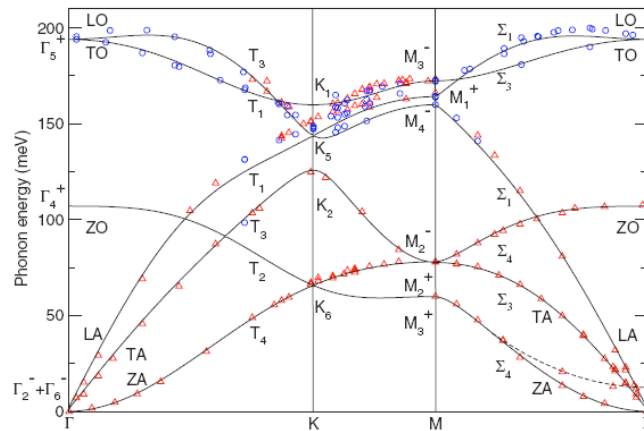
SAM	Spectral Active Modes (IR and RAMAN Selection Rules)
NEUTRON	Neutron Scattering Selection Rules
SYMMODES	Primary and Secondary Modes for a Group - Subgroup pair
AMPLIMODES	Symmetry Mode Analysis
PSEUDO	Pseudosymmetry Search in a Structure
DOPE	Degree of Pseudosymmetry Estimation
BPLOT	Pseudosymmetry Search with KPLOT
TRANPATH	Transition Paths (Group not subgroup relations)

On the left side of the page, there is a list of software tools with brief descriptions and dates:

- **AMPLIMODES for FullProf**  
10-2008: Refine your structures with FullProf using symmetry modes.
- **TRANSTRU**  
5-2008: Transform structures to lower symmetry Space Group basis.
- **AMPLIMODES**  
2-2008: Symmetry Mode Analysis of Structural Phase Transitions.
- **CELLSUPER**  
10-2007: New version of program CELLSUPER.
- **TRANPATH**  
7-2007: Minor update and fixes.
- **SUPERGROUPS**  
6-2007: Added link to Wyckoff Positions splitting.
- **SERIES**

At the bottom left, the word "Terminado" is partially visible.

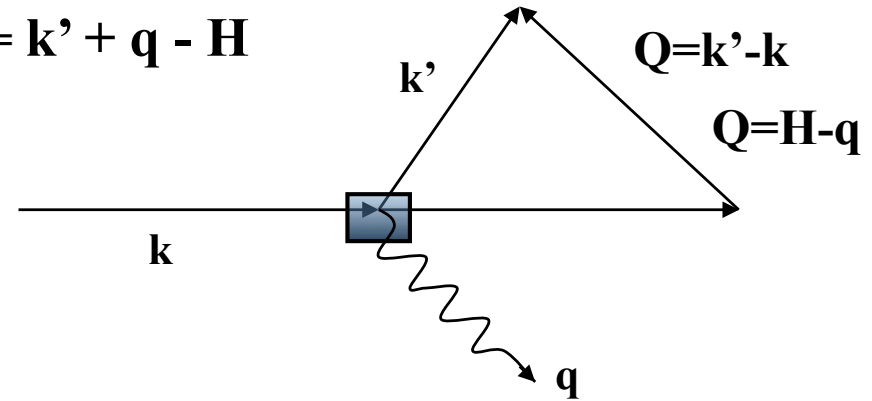
# Phonon selection rules for neutron and X-ray inelastic scattering



(Mohr et al. PRB 2007)

**H:** reciprocal lattice vector

$$\mathbf{k} = \mathbf{k}' + \mathbf{q} - \mathbf{H}$$



**normal mode:**

$$\mathbf{u}(\mu, \mathbf{T}) = A (m_\mu)^{-1/2} \mathbf{e}(\mu | \mathbf{q}, j) e^{i\mathbf{q} \cdot (\mathbf{r}_\mu + \mathbf{T})} + c.c. = A \boldsymbol{\varepsilon}(\mu, \mathbf{T} | \mathbf{q}, j) + c.c.$$

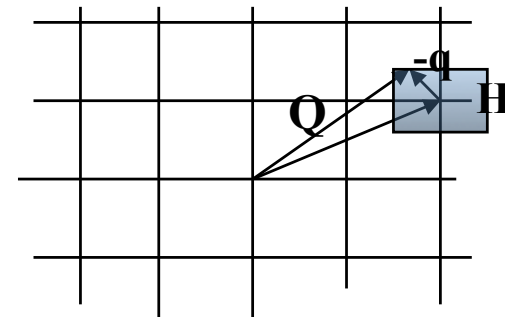
( $\mu$ : atoms within cell,  $\mathbf{T}$ : lattice translation,  $j$ : degeneracy index)

**Dynamic structure factor of the mode:**

$$F_j(\mathbf{Q}) = (1/N) \sum_{\mu, \mathbf{T}} b_\mu [\boldsymbol{\varepsilon}(\mu, \mathbf{T} | \mathbf{q}, j) \cdot \mathbf{Q}] e^{i\mathbf{Q} \cdot (\mathbf{r}_\mu + \mathbf{T})}$$

**Intensity from all degenerate modes :**

$$I(\mathbf{Q}) \sim \sum_j |F_j(\mathbf{Q})|^2 \quad \mathbf{Q} = \mathbf{H} - \mathbf{q}$$



# Phonon selection rules for neutron and X-ray inelastic scattering

(PRL 81 (1998) 2462)

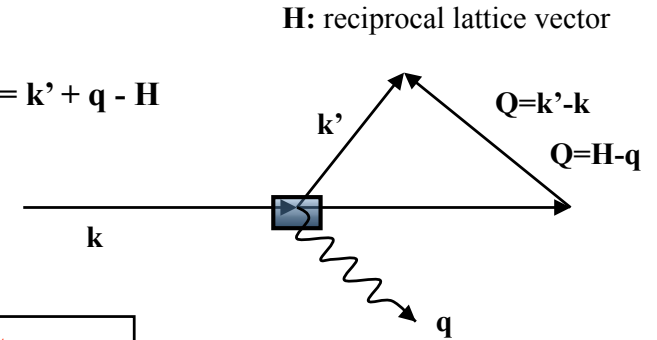
$$\mathbf{u}(\mu, \mathbf{T}) = A \boldsymbol{\varepsilon}(\mu, \mathbf{T} | \mathbf{q}, j) + \text{c.c.}$$

irrep mode:  $D^{q,\tau}$

space group transformation:  $(\mathbf{R} | \mathbf{t})$

$$\boldsymbol{\varepsilon}^{\text{tr}}(\mu, \mathbf{T} | \mathbf{q}, j) = \sum_i D^{q,\tau}(\mathbf{R} | \mathbf{t})_{ij} \boldsymbol{\varepsilon}(\mu, \mathbf{T} | \mathbf{q}, i)$$

$$\mathbf{k} = \mathbf{k}' + \mathbf{q} - \mathbf{H}$$



$$F_j^{\text{tr}}(\mathbf{Q}) = (1/N) \sum_{\mu} b_{\mu} [\mathbf{R} \boldsymbol{\varepsilon}(\mu, \mathbf{T} | \mathbf{q}, j) \cdot \mathbf{Q}] e^{i\mathbf{Q} \cdot (\mathbf{R} \mathbf{r}_{\mu} + \mathbf{T}) + \mathbf{t}}$$

$$F_j^{\text{tr}}(\mathbf{Q}) = (1/N) \sum_{\mu} b_{\mu} [\sum_i D^{q,\tau}(\mathbf{R} | \mathbf{t})_{ij} \boldsymbol{\varepsilon}(\mu, \mathbf{T} | \mathbf{q}, i) \cdot \mathbf{Q}] e^{i\mathbf{Q} \cdot (\mathbf{R} \mathbf{r}_{\mu} + \mathbf{T}) + \mathbf{t}}$$

$$F_j^{\text{tr}}(\mathbf{R}\mathbf{Q}) = e^{i\mathbf{R}\mathbf{Q} \cdot \mathbf{t}} F_j(\mathbf{Q})$$

$$F_j^{\text{tr}}(\mathbf{Q}) = \sum_i D^{q,\tau}(\mathbf{R} | \mathbf{t})_{ij} F_i(\mathbf{Q})$$

dynamic phonon structure factor transforms according to mode irrep  $D^{q,\tau}$

symmetry property of the phonon dynamic structure factor

$$F_i(\mathbf{R}\mathbf{Q}) = e^{i\mathbf{R}\mathbf{Q} \cdot \mathbf{t}} \sum_j D^{q,\tau}(\mathbf{R} | \mathbf{t})_{ij}^* F_j(\mathbf{Q})$$

point group  $\mathbf{P}^s_{\mathbf{Q}}$ , all operations  $\mathbf{R}$  such that  $\mathbf{R}\mathbf{Q} = \mathbf{Q}$

$$F_i(\mathbf{Q}) = e^{i\mathbf{Q} \cdot \mathbf{t}} \sum_j D^{q,\tau}(\mathbf{R} | \mathbf{t})_{ij}^* F_j(\mathbf{Q})$$

representation of  $\mathbf{P}^s_{\mathbf{Q}}$

**Extinction:** For  $F_i(\mathbf{Q}) \neq 0$  this representation should contain the identity irrep, otherwise  $F_i(\mathbf{Q}) = 0$

# NEUTRON: Phonon selection rules for neutron and X-ray inelastic scattering

## Input:

Bilbao Crystallographic Server → NEUTRON Help

### Inelastic Neutron Scattering Selection Rules

**Neutron scattering Selection Rules**

This program calculates systematic absences in inelastic neutron scattering spectra, due to the phonon symmetry.

**Input data :**

- Space group number as given in ITA.
- k-vector data :**
  - Reciprocal lattice basis type, which may be primitive (as in Cracknell-Davies-Miller-Love tables [1]), dual to the conventional (ITA), or dual to non-conventional (see 3.)
  - k-vector coordinates** relative to chosen basis as any three decimal numbers or fractions.
  - Label of the **k-vector** (up to three letters).

Space Group number: Please, enter the sequential number of group as given in <i>International Tables for Crystallography</i> , Vol. A or choose it:		<input type="text" value="34"/>
<b>k vector data</b>	Reciprocal basis	primitive (CDML) <input type="button" value="v"/>
	Coordinates	$k_x$ <input type="text" value="0"/> $k_y$ <input type="text" value="0"/> $k_z$ <input type="text" value="0"/>
	Label	<input type="text" value="GM"/>

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

Rotational part			Origin shift		
<input type="text" value="1"/>	<input type="text" value="0"/>	<input type="text" value="0"/>	<input type="text" value="0"/>	<input type="text" value="0"/>	<input type="text" value="0"/>
<input type="text" value="0"/>	<input type="text" value="1"/>	<input type="text" value="0"/>	<input type="text" value="0"/>	<input type="text" value="0"/>	<input type="text" value="0"/>
<input type="text" value="0"/>	<input type="text" value="0"/>	<input type="text" value="1"/>	<input type="text" value="0"/>	<input type="text" value="0"/>	<input type="text" value="0"/>

OR

# NEUTRON: Phonon selection rules for neutron and X-ray inelastic scattering

## Output:

### Inelastic Neutron Scattering Selection Rules for group 34 (*Pnn2*)

“small” irreps of the little group are constructed and labelled:

\*\*\*\*\* Space-group data \*\*\*\*\*

Space group G34 , number 34  
Lattice type : oP

Number of generators : 3

1	0	0	0	-1	0	0	0	1	0	0	1/2
0	1	0	0	0	-1	0	0	0	-1	0	1/2
0	0	1	0	0	0	1	0	0	0	1	1/2

Translation coset representatives : 4

1	0	0	0	-1	0	0	0	1	0	0	1/2	-1	0	0	1/2
0	1	0	0	0	-1	0	0	0	-1	0	1/2	0	1	0	1/2
0	0	1	0	0	0	1	0	0	0	1	1/2	0	0	1	1/2

\*\*\*\*\* q-vector data \*\*\*\*\*

q-vector GM :  
in primitive basis : 0.000 0.000 0.000  
in standard dual basis : 0.000 0.000 0.000

The little group of the q-vector has the following 4 translation coset representatives :

1	0	0	0	-1	0	0	0	1	0	0	1/2	-1	0	0	1/2
0	1	0	0	0	-1	0	0	0	-1	0	1/2	0	1	0	1/2
0	0	1	0	0	0	1	0	0	0	1	1/2	0	0	1	1/2

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

Irrep (GM)(1) , dimension 1

1	2	3	4
(1.000, 0.0)	(1.000, 0.0)	(1.000, 0.0)	(1.000, 0.0)

Irrep (GM)(2) , dimension 1

1	2	3	4
(1.000, 0.0)	(1.000, 0.0)	(1.000,180.0)	(1.000,180.0)

Irrep (GM)(3) , dimension 1

1	2	3	4
(1.000, 0.0)	(1.000,180.0)	(1.000, 0.0)	(1.000,180.0)

Irrep (GM)(4) , dimension 1

1	2	3	4
(1.000, 0.0)	(1.000,180.0)	(1.000,180.0)	(1.000, 0.0)

# NEUTRON: Phonon selection rules for neutron and X-ray inelastic scattering

## Output:

\*\*\*\*\* Q-vector types and extinction rules \*\*\*\*\*

General form of Q-vectors:  $Q = (h, k, l)$

There are 3 types of special Q-vectors.

Brillouin zones with selection rules for the q chosen

$H[1] = (0, 0, 1)$ ,  $Q[1] = (0, 0, 1)$   
with parameters:  $l=any$

$H=(001)$

The elements of the little co-group, which leaves Q invariant (strict point group) are:  
1 2 3 4

Condition  $l=any$

For  $l = 1$

Irrep	Allowed
GM_1	NO
GM_2	YES
GM_3	NO
GM_4	NO

←  $l=odd$

For  $l = 2$

Irrep	Allowed
GM_1	YES
GM_2	NO
GM_3	NO
GM_4	NO

←  $l=even$

$H=(h0l)$

$H[2] = (h, 0, l)$ ,  $Q[2] = (h, 0, l)$   
with parameters:  $h=any, l=any$

The elements of the little co-group, which leaves Q invariant are:  
1 3

Condition  $h=any, l=any$

For  $h = 1, l = 1$

Irrep	Allowed
GM_1	YES
GM_2	NO
GM_3	YES
GM_4	NO

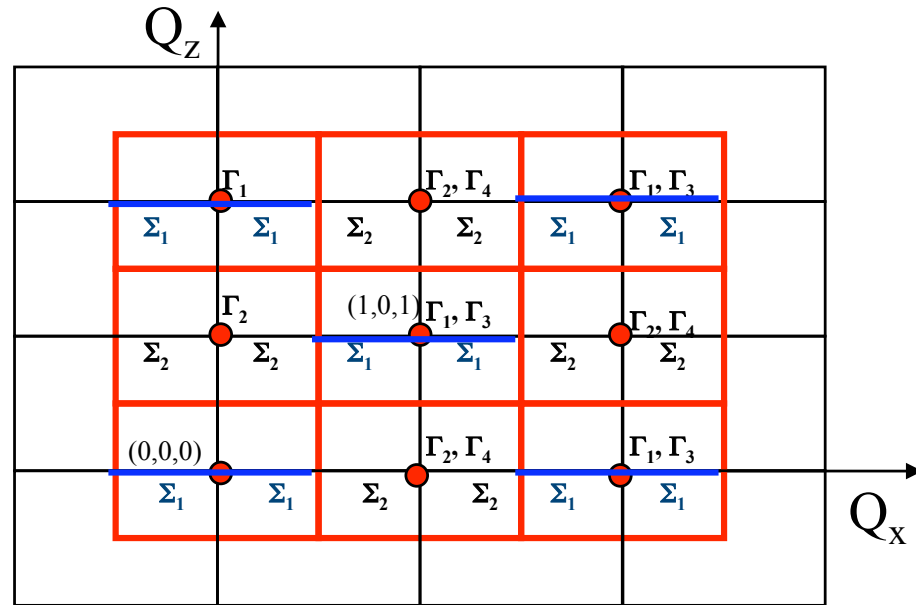
←  $h+l=even$

For  $h = 1, l = 2$

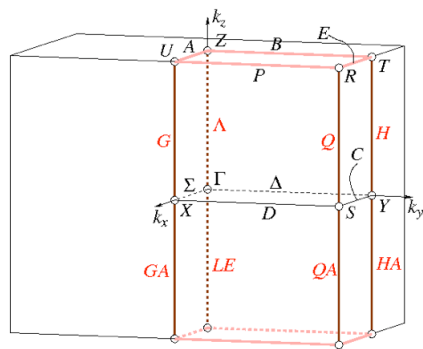
Irrep	Allowed
GM_1	NO
GM_2	YES
GM_3	NO
GM_4	YES

←  $h+l=odd$

# Example: Phonon selection rules for the line $\Sigma(\alpha,0,0)$ in Pnn2



		$q=(0\ 0\ 0)$	$q=(\alpha\ 0\ 0)$
<b>H</b>	condition	allowed	Allow.
$(0\ 0\ 1)$	l - even	$\Gamma_1$	$\Sigma_1$
	l - odd	$\Gamma_2$	$\Sigma_2$
$(h\ 0\ 1)$	h+l - even	$\Gamma_1, \Gamma_3$	$\Sigma_1$
	h+l - odd	$\Gamma_2, \Gamma_4$	$\Sigma_2$
$(0\ k\ 1)$	k+l - even	$\Gamma_1, \Gamma_4$	No restric.
	k+l - odd	$\Gamma_2, \Gamma_3$	



Brillouin zone Pnn2  
(KVEC)

irreps:

$q=(0\ 0\ 0)$

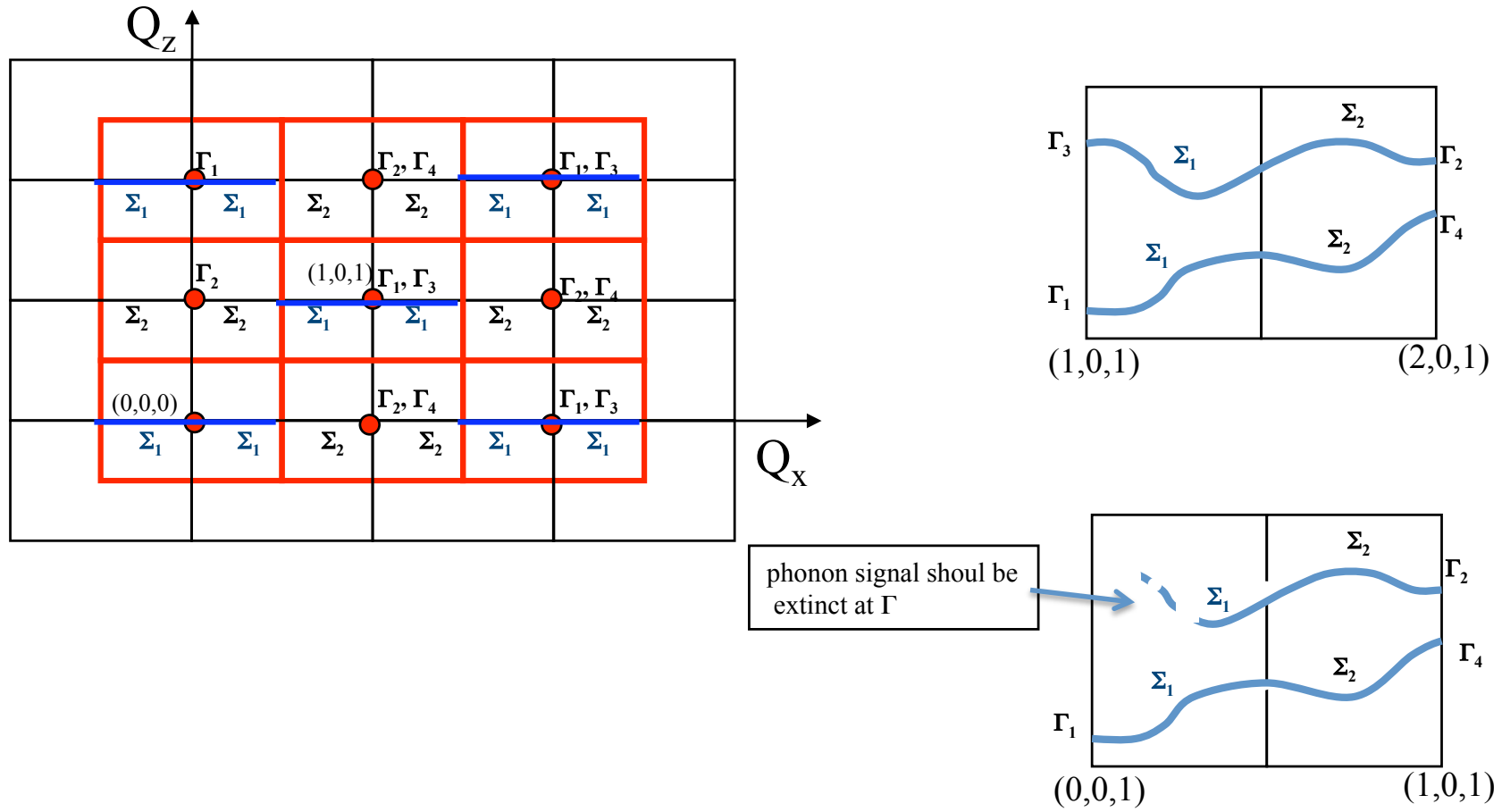
	E	$m_x$	$m_y$	$2_z$
$\Gamma_1$	1	1	1	1
$\Gamma_2$	1	-1	-1	1
$\Gamma_3$	1	-1	1	-1
$\Gamma_4$	1	1	-1	-1

$q=(\alpha\ 0\ 0)$

	E	$m_y$
$\Sigma_1$	1	1
$\Sigma_2$	1	-1

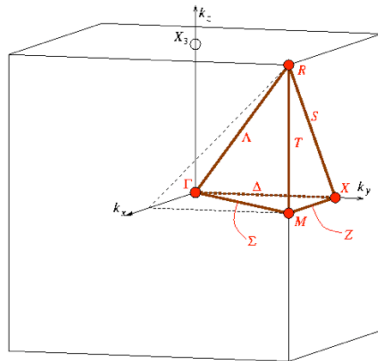


# Example: Phonon selection rules for the line $\Sigma(\alpha,0,0)$ in Pnn2



# Example: Phonon selection rules for Pn-3m

## line $\Gamma(0,0,0)$ - example



H[2] = ( h, h, h ) , Q[2] = ( h, h, h )  
with parameters: h=any

The elements of the little co-group, which leaves Q invariant (strict point group) are:  
1 5 9 38 44 47

Condition h=any

For h = 1

Irrep	Allowed
GM_1	YES
GM_2	NO
GM_3	NO
GM_4	YES
GM_5	NO
GM_6	NO
GM_7	NO
GM_8	YES
GM_9	YES
GM_10	NO

## line $\Delta(\alpha,0,0)$ - example

H[3] = ( h, k, k ) , Q[3] = ( h - 0.21, k, k )  
with parameters: h=any, k=any

The elements of the little co-group, which leaves Q invariant (strict point group) are:  
1 7

Condition h=any, k=any

For h = 1 , k = 1

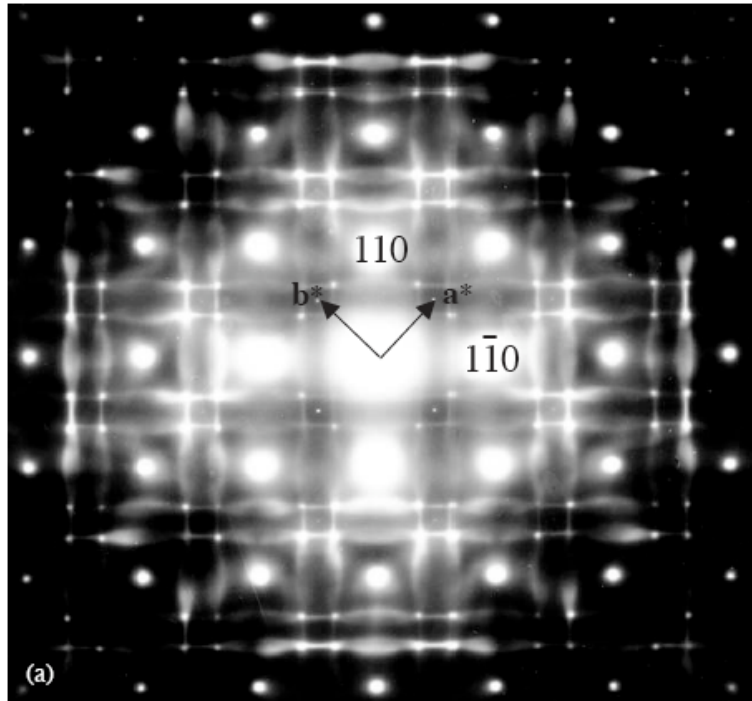
Irrep	Allowed
DT_1	YES
DT_2	NO
DT_3	NO
DT_4	YES
DT_5	YES

\*\*\*\*\* END \*\*\*\*\*

# Phonon/modes selection rules also present in diffuse scattering

NEUTRON can also be used to interpret patterns of diffuse scattering

ThAsSe (Withers et al., JSSC (2004))



P4/nmm

Diffuse streaks:  $(h,k,0) + \mathbf{q}$ ,  $\mathbf{q} = (\alpha,\beta,0)$

$$h+k = \text{odd}$$

program NEUTRON:

$\mathbf{q} = (\alpha,\beta,0)$  - 2 irreps:  $D_1, D_2$

$h+k = \text{even}$  ----  $D_1$  allowed

$h+k = \text{odd}$  ----  $D_2$  allowed