Inelastic neutron scattering selection rules of αHgI2

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INELASTIC NEUTRON SCATTERING SELECTION RULES OF α HgI_2

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Résumé. — Les règles de sélection de diffusion neutronique inélastique ont été déduites de considérations de théorie des groupes pour α HgI_2, dans les directions Δ, Σ et Λ.

Abstract. — The inelastic neutron scattering selection rules of α HgI_2 in the directions Δ, Σ and Λ are derived by using group theoretical techniques.

Introduction. — Inelastic neutron scattering is a powerful technique for the determination of the phonon dispersion curves. Nevertheless, before applying this method to a given crystal, it is necessary to know the relative orientations of the crystal and the neutron beam which are the most favourable for the determination of the phonons belonging to various branches.

The coherent inelastic scattering cross section, where one phonon is created or destroyed, is given by Born's approximation [1]. The expression obtained contains a structure factor which depends on the geometry of the experiment and on the polarization vectors of the phonons which transform as a particular irreducible group representation.

The conditions under which the sums of the structure factors resulting from phonon branches of the same irreducible representation are zero, can be determined by group theory.

This method is applied in this paper to the case of α HgI_2, a member of the important layer structure family [2]. The C13 deficit structure [3] suggests that α HgI_2 is rather a transition compound from tridimensional to layered crystals. At the present time there is little information on the lattice dynamics of this compound out of the centrum of the Brillouin zone (B.Z.) [4]. Now, the understanding of the well-known optical [5], electrical [6], nuclear [7] etc... properties, which are perhaps in relation with the bidimensional character of α HgI_2, deserve fundamental investigations of the phonon branches in the B.Z. Neutron spectroscopy serves this purpose and requires a preliminary group theoretical examination. This is the aim of this paper.

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1. **Theory.** — All representations are based on the irreducible multiplier representations of the space-group [8]. To each operation $S = (R \mid \mathbf{t})$ of the space-group is associated an operator T which forms the so-called multiplier representation and is explicitly given by the matrix :

$$T_{\alpha\beta}(jj' \mid \mathbf{q}S) = R_{\alpha\beta}\, \delta_{((j)-(j'))}\, \mathrm{e}^{i\mathbf{q}\cdot(\mathbf{r}(j) - R\mathbf{r}(j'))} \qquad (1)$$

where :

j, j' refer respectively to the jth and j'th atom in the unit cell : α, β = 1, 2, 3 ;

$\mathbf{r}(j)$ is the equilibrium position of the jth atom in the unit cell ;

$\delta_{((j)-(j'))} = 1$ if atom j is transformed into atom j' under the symmetry operation S ;

$R_{\alpha\beta}$ is an element of the rotational matrix R associated with the operator S ;

$\mathbf{q}$ is the phonon wavevector.

$$\mathbf{t} = \mathbf{m} + \mathbf{v} \; ;$$

$\mathbf{m}$ = lattice translation,
$\mathbf{v}$ = fractional lattice translation.

The operations S are uniquely those of the little group $G(\mathbf{q})$ of $\mathbf{q}$. The T matrices provide a $3\,s$ dimensional unitary multiplier representation of the point group $G_0(\mathbf{q})$ of $\mathbf{q}$ (s being the number of atoms in the unit cell).

The T matrices are in general reducible. Let χ^λ be the character of the λth representation contained in T.

Devine and Peckham [1] have shown that a knowledge of the polarization vectors allows one to calculate the structure factors for inelastic neutron scattering experiments. The starting point is the discussion of the dynamical structure factor g_λ as given by Born's approximation :

$$g_\lambda = \sum_j (b_j/\sqrt{m_j}) \exp(-W_j)\, \mathbf{Q}.\mathbf{e}(j\mathbf{q}\lambda) \exp[i\mathbf{Q}.\mathbf{r}(j)]. \quad (2)$$

where b_j is the scattering length, W_j the Debye-Waller factor, and m_j the mass of the jth atom. $\mathbf{Q}$ is the scattering vector. The scattered structure factor is the sum of the individual atomic structure factors.

Group theory refers to the three dimensional vectors, with respect to $\mathbf{Q}$

$$\Phi(j, \alpha) = Q_\alpha \exp[i\mathbf{Q}.\mathbf{r}(j)] . \quad (3)$$

Using group theoretical arguments, inspection of this factor enables one to determine when the scattered structure factor is zero, or not zero.

The space of representations for the vectors $\mathbf{\Phi}$ is the direct product of the spaces of transformation of $\mathbf{Q}$ and the vectors (in respect to $\mathbf{Q}$) $\exp[i\mathbf{Q}.r(j)]$. Then, the character of $\mathbf{\Phi}$ is the product of the characters of the representations for these two types of vectors.

1.1 CHARACTERS ASSOCIATED WITH THE SPACE SPANNED BY $\mathbf{Q}$. — Three different cases can occur, according to the dimension of the space associated with $\mathbf{Q}$ and its transforms :

(i) $\mathbf{Q}$ unchanged, except for its sign :

$$\chi_{\mathbf{Q}} = \pm 1 . \quad (4)$$

(ii) $\mathbf{Q}$ spans a two-dimensional space :

$$\begin{aligned} &\chi_{\mathbf{Q}} = 2 \text{ for } E \\ &\chi_{\mathbf{Q}} = 2\cos\varphi \text{ for } C_\varphi \quad (\varphi = \text{rotation angle}) \\ &\chi_{\mathbf{Q}} = 0 \text{ for a mirror} . \end{aligned} \quad (5)$$

(iii) $\mathbf{Q}$ spans a three-dimensional space :

$$\chi_{\mathbf{Q}} = 3 \text{ for } E$$

$$\chi_{\mathbf{Q}} = \pm(1 + 2\cos\varphi) \begin{cases} + \text{ proper rotations} \\ - \text{ improper rotations} \end{cases} \quad (6)$$

$$\chi_{\mathbf{Q}} = 1 \text{ for a mirror} .$$

1.2 CHARACTERS ASSOCIATED WITH $\exp[i\mathbf{Q}.\mathbf{r}(j)]$. — The vectors $\exp[i\mathbf{Q}.\mathbf{r}(j)]$ are transformed to : $\exp[i\mathbf{Q}.\{R \mid \mathbf{m} + \mathbf{v}\}^{-1}\mathbf{r}(j)]$ by the action of the operators $\{R \mid \mathbf{m} + \mathbf{v}\}$. The theory requires one to consider the star $G_{0\mathbf{Q}}$ of $\mathbf{Q}$, which contains all the elements of $G_{0\mathbf{q}}$ leaving the vector $\exp[i\mathbf{Q}.\mathbf{r}(j)]$ unchanged except for a multiplication factor $\theta(R \mid \mathbf{t}, \mathbf{Q})$ defined by :

$$\theta(R \mid \mathbf{t}, \mathbf{Q}) = \exp[i\,\tau_R\, \mathbf{r}(j)] \exp[-i\boldsymbol{\tau}.\mathbf{t})] \quad (7)$$

with :

$$\begin{aligned} R\mathbf{Q} &= \mathbf{Q} + \\ \mathbf{Q} &= \mathbf{q} + \boldsymbol{\tau} = \mathbf{k}_1 - \mathbf{k}_0 \end{aligned} \quad (8)$$

$\boldsymbol{\tau}$ and $\boldsymbol{\tau}_R$ belong to the reciprocal lattice and $\mathbf{k}_0$, $\mathbf{k}_1$ are the wave vectors of the incident and scattered neutrons respectively.

Application of the decomposition to the product representation leads to :

$$C_\lambda = \frac{1}{h_{\mathbf{Q}}} \cdot \sum_{R \in G_{0\mathbf{q}}} \chi_{\mathbf{Q}}(R) \exp[i\tau_R.\mathbf{r}(j)] \times \times \exp(-i\boldsymbol{\tau}.\mathbf{t})\, \chi^*(R) \quad (9)$$

where :

$h_{\mathbf{Q}}$ = dimension of the group $G_{0\mathbf{Q}}$;

$\chi^\lambda(R)$ = character of the λth representation.

$$\boldsymbol{\tau} = p\mathbf{a}^* + q\mathbf{b}^* + r\mathbf{c}^* \quad (10)$$

where $\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$ are the basic reciprocal vectors.

If $C_\lambda = 0$, $\mathbf{\Phi}$ does not contain components which transform according to the λth representation and the scattered structure factor is zero for the branches belonging to this representation.

2. **Structure of α HgI_2.** — The space group of α HgI_2 [2] is D_{4h}^{15} (P 4_2/nmc). There are two molecules (6 atoms) in the tetragonal unit cell, which is represented in figure 1. The primitive translations of the lattice are defined by :

$$\begin{aligned} \mathbf{m}_1 &= a\mathbf{i} \\ \mathbf{m}_2 &= a\mathbf{j} \\ \mathbf{m}_3 &= c\mathbf{k} \end{aligned}$$

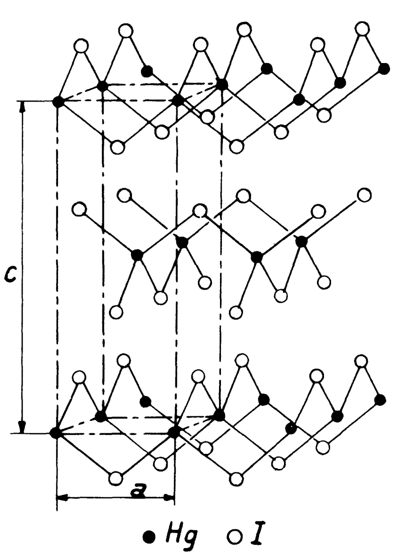

FIG. 1. — Structure of α HgI_2.

with :

$$\begin{aligned} a &= 4.369 \text{ Å} \\ c &= 12.439 \text{ Å} . \end{aligned}$$

The origin of the rectangular coordinate system is coincident with the inversion centre. The positions of

TABLE I

The positions of the atoms within the unit cell

$u = 0.14$

	Chemical nature of the ion	Origin at 0	Origin at centre of inversion
Atom 1	I	$0\ \frac{1}{2}\ u$	$\bar{\frac{1}{4}}\ \frac{3}{4}\ u - \frac{1}{4}$
Atom 2	I	$\bar{\frac{1}{2}}\ 0\ \bar{u}$	$\bar{\frac{3}{4}}\ \frac{1}{4}\ -u - \frac{1}{4}$
Atom 3	I	$0\ \frac{1}{2}\ \frac{1}{2} + u$	$\bar{\frac{1}{4}}\ \frac{3}{4}\ \frac{1}{4} + u$
Atom 4	I	$\bar{\frac{1}{2}}\ 0\ \frac{1}{2} - u$	$\bar{\frac{3}{4}}\ \frac{1}{4}\ \bar{\frac{1}{4}} - u$
Atom 5	Hg	$0\ 0\ 0$	$\bar{\frac{1}{4}}\ \frac{1}{4}\ \bar{\frac{1}{4}}$
Atom 6	Hg	$\frac{1}{2}\ \frac{1}{2}\ \frac{1}{2}$	$\frac{1}{4}\ \frac{3}{4}\ \frac{1}{4}$

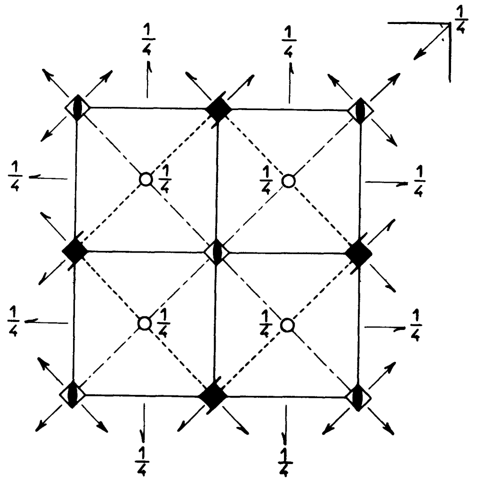

FIG. 2. — Symmetry operations of α HgI_2 (D_{4h}^{15}).

the atoms within the unit cell are indicated in table I. The symmetry operations are illustrated in figure 2. The tetragonal reciprocal lattice is defined by :

$$\mathbf{a}^* = \frac{2\pi}{a}\mathbf{i}\,,\qquad \mathbf{b}^* = \frac{2\pi}{a}\mathbf{j}\,,\qquad \mathbf{c}^* = \frac{2\pi}{c}\mathbf{k}\,.$$

The symmetry operators [9] are :

$$E\,;\ (I \mid 0\ 0\ 0)\,;\ \left(C_2 \middle| \frac{a}{2}\ \frac{a}{2}\ 0\right);\ \left(\sigma^x \middle| \frac{a}{2}\ 0\ 0\right);$$
$$\left(\sigma^y \mid 0\ \frac{a}{2}\ 0\right);\ \left(\sigma^{\bar{x}y} \mid 0\ 0\ \frac{c}{2}\right);\ \left(\sigma^{xy} \middle| \frac{a}{2}\ \frac{a}{2}\ \frac{c}{2}\right);$$
$$\left(C_4 \middle| \frac{a}{2}\ 0\ \frac{c}{2}\right);\ \left(C_4^3 \mid 0\ \frac{a}{2}\ \frac{c}{2}\right).$$
$$\left(C_2''^{\bar{x}y} \mid 0\ 0\ \frac{c}{2}\right);\ \left(C_2''^{xy} \middle| \frac{a}{2}\ \frac{a}{2}\ \frac{c}{2}\right);\ \left(\sigma^z \middle| \frac{a}{2}\ \frac{a}{2}\ 0\right);$$
$$\left(S_4 \middle| \frac{a}{2}\ 0\ \frac{c}{2}\right);\ \left(S_4^3 \mid 0\ \frac{a}{2}\ \frac{c}{2}\right);\ \left(C_2'^y \mid 0\ \frac{a}{2}\ 0\right);$$
$$\left(C_2'^x \middle| \frac{a}{2}\ 0\ 0\right)$$

where $C_2'^x$ and $C_2'^y$ indicate rotations by π around the coordinate axis x and y respectively, $C_2''^{\bar{x}y}$ and $C_2''^{xy}$ indicate rotations by π around the axis $\bar{x}y$ ($x + y = 0$, $z = 0$) and xy ($x = y$, $z = 0$) respectively.

3. **Selection rules for inelastic neutron scattering in α HgI_2.** — Table II gives the characters associated with the different spaces spanned by $\mathbf{Q}$ in the case of α HgI_2.

TABLE II

Characters $\chi_{\mathbf{Q}}(R)$

R	E	$(C_4 \mid \frac{1}{2}\ 0\ \frac{1}{2})$ $(C_4^3 \mid 0\ \frac{1}{2}\ \frac{1}{2})$	$(C_2 \mid \frac{1}{2}\ \frac{1}{2}\ 0)$	$(\sigma_v^x \mid \frac{1}{2}\ 0\ 0)$ $(\sigma_v^y \mid 0\ \frac{1}{2}\ 0)$	$(\sigma^{xy} \mid 0\ 0\ \frac{1}{2})$ $(\sigma^{\bar{x}y} \mid \frac{1}{2}\ \frac{1}{2}\ \frac{1}{2})$	I	$(C_2''^{\bar{x}y} \mid \frac{1}{2}\ \frac{1}{2}\ \frac{1}{2})$ $(C_2''^{xy} \mid 0\ 0\ \frac{1}{2})$	$(\sigma^z \mid \frac{1}{2}\ \frac{1}{2}\ 0)$	$(S_4^3 \mid 0\ \frac{1}{2}\ \frac{1}{2})$ $(S_4 \mid \frac{1}{2}\ 0\ \frac{1}{2})$	$(C_2'^x \mid 0\ \frac{1}{2}\ 0)$ $(C_2'^y \mid \frac{1}{2}\ 0\ 0)$
$\chi_{\mathbf{Q}}^{(3)}(R)$	3	1	− 1	1	1	− 3	− 1	1	− 1	− 1
$\chi_{\mathbf{Q}}^{(2)}(R)$	2	0	− 2	0	0	− 2	0	2	0	0
$\chi_{\mathbf{Q}}^{(1)}(R)$	1	± 1	± 1	± 1	± 1	± 1	± 1	± 1	± 1	± 1

TABLE III

Wave vectors' point group and irreducible representations

Line	Wave vectors' point group	Elements of the wave vectors' point group	Irreducible representations (Zak notation)
Δ	$C_{2v}^{(y)}$	$\{ E, \sigma_v^x, \sigma_h, C_2'^y \}$	$6\,\Delta_1 \oplus 6\,\Delta_2 \oplus 3\,\Delta_3 \oplus 3\,\Delta_4$
Σ	$C_{2v}^{(xy)}$	$\{ E, \sigma^{\bar{x}y}, C_2''^{xy}, \sigma_h \}$	$4\,\Sigma_1 \oplus 5\,\Sigma_2 \oplus 4\,\Sigma_3 \oplus 5\,\Sigma_4$
Λ	C_{4v}	$\{ E, C_4, C_2, C_4^3, \sigma^x, \sigma^y, \sigma^{xy}, \sigma^{\bar{x}y} \}$	$3\,\Lambda_1 \oplus 3\,\Lambda_3 \oplus 6\,\Lambda_5$

Table III summarizes the elements of the wave-vectors' point groups for the Δ, Σ and Λ lines of the B.Z.

Table IV gives the characters of the phonons representations [10] corresponding to these points Δ, Σ and Λ.

Three cases are examined successively. In all the cases, $\boldsymbol{\tau}_R$ can be taken equal to zero.

3.1 SÉLECTION RULES FOR $\mathbf{q}$ ALONG U_y ($\Gamma\Delta$ DIRECTION) : $\mathbf{q} = (0, q, 0)$.

$$G_\Delta = \{ E, \sigma^x, \sigma^z, C_2'^y \} .$$

3.1.1 **Q** *general, or* **Q** *in the plane* σ^{xy}. — The star of **Q** spans three dimensions. For Hg and I, G_{0Q} contains only the identity. Substituting in equation (9) gives the following values for C_λ :

	Hg, I
Δ_1	3
Δ_2	3
Δ_3	3
Δ_4	3

3.1.2 **Q** *in the glide plane* σ^x, *or in the plane* σ^z. — The star of **Q** spans two dimensions, because the transformed vectors σ^x **Q** and σ^y **Q** are coplanar to **Q**. G_{0Q} now contains E and σ^x. Taking into account that $\chi_Q^{(2)}(\sigma^x) = 0$ (see table II) and $\chi_Q^{(2)}(E) = 2$, we found :

	Hg, I
Δ_1	1
Δ_2	1
Δ_3	1
Δ_4	1

3.1.3 **Q** *along* $C_2'^y$. — The star of **Q** is one dimensional. The group G_{0Q} contains all elements of $G_{0\mathbf{q}}$. The value C_λ is the same for Hg and I.

Recalling that :

$$\boldsymbol{\tau} = p\mathbf{a}^* + q\mathbf{b}^* + r\mathbf{c}^* \tag{10}$$

and taking into account the expressions of $\mathbf{t}(R)$ (see table I) :

$$e^{-i\boldsymbol{\tau}.\mathbf{t}(\sigma^x)} = e^{-i\pi p} ; \quad e^{-i\boldsymbol{\tau}.\mathbf{t}(\sigma^z)} = e^{-i\pi(p+q)} ;$$
$$e^{-i\boldsymbol{\tau}.\mathbf{t}(C_2'^y)} = e^{-i\pi q} .$$

It is convenient to discuss several cases for p and q, even or odd. For example, if both p and q are even, then :

$$e^{-ip\pi} = e^{-iq\pi} = e^{-i(p+q)\pi} = 1$$

and from table IV :

$$C_{\Delta_1} = 1 ; \quad C_{\Delta_i} = 0 \qquad i = 2, 3, 4 .$$

TABLE IV

Characters [9] *of the phonons* [10] *irreducible representations for* Λ, Δ *and* Σ *points.*

C_{4v}	E	(C_4, C_4^3)	C_2	(σ^x, σ^y)	$(\sigma^{xy}, \sigma^{\bar{x}y})$
χ^{Λ_1}	1	1	1	1	1
χ^{Λ_3}	1	− 1	1	1	− 1
χ^{Λ_5}	2	0	− 2	0	0

$C_{2v}^{(y)}$	E	σ^z	σ^x	$C_2'^y$
χ^{Δ_1}	1	1	1	1
χ^{Δ_2}	1	1	− 1	− 1
χ^{Δ_3}	1	− 1	− 1	1
χ^{Δ_4}	1	− 1	1	− 1

$C_{2v}^{(xy)}$	E	$C_2''^{xy}$	$\sigma^{\bar{x}y}$	σ^z
χ^{Σ_1}	1	1	1	1
χ^{Σ_2}	1	− 1	1	− 1
χ^{Σ_3}	1	1	− 1	− 1
χ^{Σ_4}	1	− 1	− 1	1

Hg, I

$$\Delta_1, \quad \begin{cases} 1 & \text{if } p \text{ and } q \text{ even} \\ 0 & \text{otherwise} \end{cases}$$

$$\Delta_2 \quad \begin{cases} 1 & \text{if } p \text{ even and } q \text{ odd} \\ 0 & \text{otherwise} \end{cases}$$

$$\Delta_3 \quad \begin{cases} 1 & \text{if } p \text{ odd and } q \text{ even} \\ 0 & \text{otherwise} \end{cases}$$

$$\Delta_4 \quad \begin{cases} 1 & \text{if } p \text{ and } q \text{ odd} \\ 0 & \text{otherwise} \end{cases}$$

3.1.4 **Q** *along* C_4. — The star of **Q** is one dimensional. The group G_{0Q} contains E and σ^x.

Now :

$$\mathbf{t}(\sigma^x) = \left(\frac{a}{2}, 0, 0\right) \quad \text{and} \quad e^{-i\boldsymbol{\tau}.\mathbf{t}(\sigma^x)} = e^{-i\pi p} .$$

It is sufficient to discuss p, even or odd :

$$e^{-i\boldsymbol{\tau}.\mathbf{t}(\sigma^x)} = \begin{cases} 1 & \text{if } p \text{ even} \\ -1 & \text{if } p \text{ odd} \end{cases}$$

The values for C_λ are :

Hg, I	(e)	(o)
Δ_1	1	0
Δ_2	1	0
Δ_3	0	1
Δ_4	0	1

Columns (e) and (o) give the values for even and odd reciprocal lattice vectors τ respectively.

3.1.5 **Q** *along* $C_2''^{xy}$ *and* $C_2''^{\bar{x}y}$. — The star of **Q** is two dimensional. For Hg and I, G_{0Q} contains E and σ^z. Taking account of :

$$\mathbf{v}(\sigma^z) = (\tfrac{1}{2}, \tfrac{1}{2}, 0)$$

$$\tau = p\mathbf{a}^* + q\mathbf{b}^* + r\mathbf{c}^* \qquad (10)$$

and

$$e^{-i\tau.\mathbf{v}(\sigma^z)} = e^{-i\pi(p+q)}.$$

One finds, for p even and q odd for example, that : $e^{-i\pi(p+q)} = -1$ and from tables II and IV :

$$C_{\Delta_{1\text{ or }2}} = 0 ; \quad C_{\Delta_{3\text{ or }4}} = 2 ; \quad \text{etc}.$$

Hg, I	p and q both even or odd	p even and q odd (and rec.)
Δ_1	2	0
Δ_2	2	0
Δ_3	0	2
Δ_4	0	2

3.1.6 **Q** *perpendicular to* σ^x *or* σ^{xy}. — The star of **Q** is one dimensional and G_{0Q} contains E and σ^z. The same considerations as in 5 for **t**, τ and $e^{-i\tau.\mathbf{t}}$ give the following values for C_λ :

Hg, I	p and q both even or odd	p even and q odd (or rec.)
Δ_1	1	0
Δ_2	1	0
Δ_3	0	1
Δ_4	0	1

3.2 SELECTION RULES FOR **q** ALONG $C_2''^{xy}$ ($\Gamma\Sigma$ DIRECTION) : $\mathbf{q} = (q, q, 0)$.

$$G_\Sigma = \{ E, C_2''^{xy}, \sigma^{\bar{x}y}, \sigma^z \}.$$

3.2.1 **Q** *general or* **Q** *in the plane* σ^x. — The star of **Q** spans three dimensions. G_{0Q} contains only the identity E. Therefore :

Hg, I	
Σ_1	3
Σ_2	3
Σ_3	3
Σ_4	3

3.2.2 **Q** *in the plane* σ^z, *or along* C_2', *or along* C_2'', *or perpendicular to* σ_v *and* σ^{xy}. — The star of **Q** spans two dimensions. G_{0Q} contains E and σ^z. The factor

$$e^{-i\tau.\mathbf{t}(\sigma^z)} = e^{-i(p+q)\pi}$$

and table IV lead to the following results, similarly to A.5 :

Hg, I	p and q both even or odd	p even and q odd (or rec.)
Σ_1	2	0
Σ_2	2	0
Σ_3	0	2
Σ_4	0	2

3.2.3 **Q** *in the plane* σ^{xy}. — The star of **Q** is two dimensional. The group of G_{0Q} contains E and $\sigma^{\bar{x}y}$ and $\chi_{\mathbf{Q}}^{(2)}(\sigma^{\bar{x}y}) = 0$. Consequently :

$$C_{\Sigma_1,\Sigma_2,\Sigma_3,\Sigma_4} = 1 \quad \text{for Hg and I}.$$

3.2.4 **Q** *along* C_4. — The star of **Q** is one dimensional. The group of G_{0Q} contains E and $\sigma^{\bar{x}y}$. Columns (e) and (o) give the values of C_λ for even and odd reciprocal lattice τ respectively.

Hg, I	(e)	(o)
Σ_1	1	0
Σ_2	0	1
Σ_3	0	1
Σ_4	1	0

3.3 SELECTION RULES FOR **q** ALONG C_4 ($\Gamma\Lambda$ DIRECTION) : $\mathbf{q} = (0, 0, q)$.

$$G_\Lambda = \{ E, C_4, C_4^3, C_2, \sigma^x, \sigma^y, \sigma^{xy}, \sigma^{\bar{x}y} \}.$$

3.3.1 **Q** *general.* — The star of **Q** spans three dimensions. The group of G_{0Q} for Hg contains E and σ^{xy} and G_{0Q} for I contains only E. For Hg, the factor :

$$e^{-i\tau.\mathbf{t}(\sigma^{xy})} = e^{-i(p+q+r)\pi}$$

is equal to 1 if $p + q + r$ is even, and -1 if $p + q + r$ is odd. Consequently, taking account on tables II and IV, we find :

	Hg		I
	$p+q+r$ even	$p+q+r$ odd	
Λ_1	2	1	3
Λ_3	1	2	3
Λ_5	3	3	6

3.3.2 **Q** *in the plane σ^z and perpendicular to σ^{xy}.* — The star of **Q** is two dimensional. The group $G_{0\mathbf{Q}}$ contains E and σ^{xy} for Hg, and E for I. The character $\chi_{\mathbf{Q}}^{(2)}(\sigma^{xy}) = 0$ leads to :

	Hg, I
Λ_1	1
Λ_3	1
Λ_5	2

3.3.3 **Q** *along C_2'.* — The star of **Q** is two dimensional. The group $G_{0\mathbf{Q}}$ contains E, σ^{xy}, σ^x, C_4^3. All the characters $\chi_{\mathbf{Q}}^{(2)}(R)$ are zero, except for E.

	Hg, I
Λ_1	1
Λ_3	1
Λ_5	2

3.3.4 **Q** *in the plane σ^{xy}.* — The star of **Q** spans two dimensions. The group $G_{0\mathbf{Q}}$ for Hg contains E, $\sigma^{\bar{x}y}$, σ^{xy}, C_2 and the characters $\chi_{\mathbf{Q}}^{(2)}(R)$ are zero, except for $\chi_{\mathbf{Q}}^{(2)}(E) = 2$ and $\chi_{\mathbf{Q}}^{(2)}(C_2) = -2$. The group $G_{0\mathbf{Q}}$ for I contains only E and $\sigma^{\bar{x}y}$, and $\chi_{\mathbf{Q}}^{(2)}(\sigma^{\bar{x}y}) = 0$. For Hg, taking account on the factor

$$e^{-i\tau.\mathbf{t}(C_2)} = e^{-i(p+q)\pi}$$

and table IV, one finds by analogy with 3.1.5

	Hg		I
	$p+q$ even	$p+q$ odd	
Λ_1	0	1	1
Λ_3	0	1	1
Λ_5	2	0	2

3.3.5 **Q** *along C_2''.* — The star of **Q** is two dimensional. For Hg, the group $G_{0\mathbf{Q}}$ contains E, $\sigma^{\bar{x}y}$, σ^{xy}, C_2, with

$$\chi_{\mathbf{Q}}^{(2)}(C_2) = -2 \quad \text{and} \quad \chi_{\mathbf{Q}}^{(2)}(E) = 2 .$$

The group $G_{0\mathbf{Q}}$ for I is E, $\sigma^{\bar{x}y}$.

	Hg		I
	$p+q$ even	$p+q$ odd	
Λ_1	0	1	1
Λ_3	0	1	1
Λ_5	2	0	2

3.3.6 **Q** *along C_4.* — The star of **Q** spans one dimension. For Hg and I, $G_{0\mathbf{Q}}$ contains all elements of $G_{0\mathbf{Q}}$.

Table II shows that except for $\chi_{\mathbf{Q}}^{(1)}(E) = 1$, all the χ's are equal to ± 1.

On the other hand, taking table I into account, the following expressions arise :

$$\begin{aligned}
e^{-i\tau.\mathbf{t}(C_2''^{xy})} &= e^{-ir\pi} \\
e^{-i\tau.\mathbf{t}(C_2''^{\bar{x}y})} &= e^{-i(p+q+r)\pi} \\
e^{-i\tau.\mathbf{t}(C_2)} &= e^{-i(p+q)\pi} \\
e^{-i\tau.\mathbf{t}(C_4)} &= e^{-i(p+r)\pi} \\
e^{-i\tau.\mathbf{t}(C_2'^y)} &= e^{-ip\pi} \\
e^{-i\tau.\mathbf{t}(C_2'^x)} &= e^{-iq\pi} \\
e^{-i\tau.\mathbf{t}(C_4^3)} &= e^{-i(q+r)\pi}
\end{aligned}$$

As an example :

$$C_{\Lambda_3} = \tfrac{1}{8}[1 - e^{-i(p+r)\pi} + e^{-i(p+q)\pi} - e^{-i(q+r)\pi} + e^{-ip\pi} - e^{-ir\pi} + e^{-iq\pi} - e^{-i(p+q+r)\pi}] .$$

Considering all the possibilities for p, q, r, it is easy to demonstrate that C_{Λ_3} is equal to zero, except for p, q even and r odd, in which case $C_{\Lambda_3} = 1$.

	Hg, I
Λ_1	$\begin{cases} 1 \text{ if } p, q, r \text{ all even} \\ 0 \text{ otherwise} \end{cases}$
Λ_3	$\begin{cases} 1 \text{ if } p \text{ and } q \text{ even and } r \text{ odd} \\ 0 \text{ otherwise} \end{cases}$
Λ_5	0

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