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SELECTION RULES FOR THE DOUBLE SPACE GROUP OF THE BETA-WOLFRAM STRUCTURE

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Résumé. — Les produits directs de représentations irréductibles du groupe double de la structure béta-tungstène sont réduits pour les quatre points de symétrie maximum de la zone de Brillouin.

Abstract. — The direct products of irreducible representations of the double space group of the beta-wolfram structure are reduced for the four points of highest symmetry of the Brillouin zone.

1. **Introduction.** — The binary intermetallic compounds having A_3B composition and the β-wolfram structure are of great theoretical interest and outstanding practical importance. They include materials with the highest transition temperatures to the superconducting state that have been observed, such as Nb_3Ge, Nb_3Sn, Nb_3Al, V_3Si, V_3Ga, etc.

We present the selection rules for the double space group of the β-wolfram or A-15 structure.

2. **The A-15 structure.** — The A-15 or β-wolfram structure for the compound formula A_3B is shown on figure 1. The A atom is a transition metal and B is usually but not always a nontransition metal. The B atoms occupy the body-centered cubic positions. The A atoms are situated on the faces of the simple cube, forming three orthogonal linear chains in the extended structure [1]. The point-group symmetry at the B atom site is $T_h(m3)$ and at the A atom site $D_{2h}(\overline{4}2m)$.

The space group of the A-15 structure is O_h^3 i.e. Pm3n which is a nonsymmorphic space group with a simple cubic Bravais lattice. The first Brillouin zone for the simple cubic Bravais lattice is shown in figure 2.

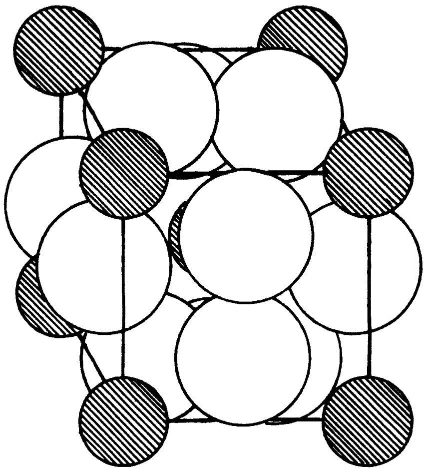

FIG. 1. — Atoms in the unit cell of the A_3B compounds having the β-wolfram structure. The A-atoms are represented by touching spheres centered on the faces of the simple cubic unit cell. The B-atom spheres occupy body-centered cubic positions, and are not drawn to their full radii.

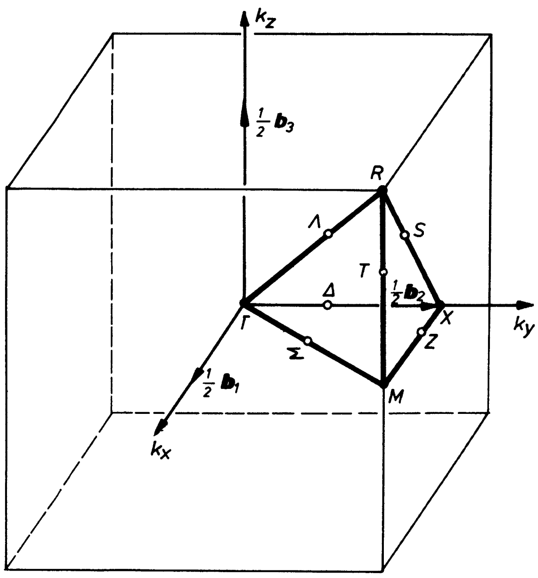

FIG. 2. — The first Brillouin zone and the representation domain indicated by heavy lines for the space group O_h^3. The basic vectors of the reciprocal lattice are b_1, b_2, b_3.

It is known that the A-15 structure is liable to lattice instabilites, defects, etc. and that the effects of disorder along the chains in the A-15 structure dominate its superconducting properties [2-5]. Matthias,

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Geballe and Compton [6] have tabulated the forty-odd compounds with this structure. Some of the interesting electronic properties which these compounds possess, in addition to their high-superconducting transition temperature, have been summarized previously by Clogston and Jaccarino [7], and more recently, by others [8, 9, 10]. The symmetry properties for the space group O_h^3 have been investigated by Gorzkowski [11, 12] and Mattheiss [13]. The energy bands in the free-electron approximation for V_3X compounds have been calculated by Mattheiss [8] and the APW-LCAO band model for A-15 compounds has been presented [14]. The results of this APW-LCAO model was applied to evaluate the accuracy of the Labbé-Friedel [1] linear-chain and the Weger-Goldberg [20] coupled-chain band models for the A-15 compounds.

A simplified theory of symmetry changes in second-order phase transitions, lattice instabilities, etc. applied to V_3Si was proposed by Birman [15, 16] and discussed in [17]. Experimental results relating structural instability and superconductivity have been compiled in several papers [5, 18, 19]. A more detailed discussion and extensive references can be found in the recent review articles on these materials by Weger and Goldberg [20], Testardi [21, 22], Dew-Hughes [9] and others [23-27].

3. **Selection rules.** — Selection rules are useful in the investigation of the electron band symmetries, optical transitions, infrared lattice absorption, electron scattering and tunnelling, neutron scattering, magnon sidebands, etc. [17]. Analysis of scattering processes involving photons, phonons or magnons in crystalline solids generally requires knowledge of the appropriate selection rules.

Recently much attention has been directed to the Clebsch-Gordan coefficients of the space group representations [28-35].

In particular, Birman and coworkers [33-35] have shown that the elements of the first order, one excitation, scattering tensor are precisely certain Clebsch-Gordan coefficients or prescribed linear combinations. The elements of the second-order, two-excitation, process are a particular sum of products of Clebsch-Gordan coefficients. The factorization of a matrix element or a scattering tensor element into a Clebsch-Gordan coefficient and a reduced matrix element can provide significant simplifications related to the symmetry of a problem. For a calculation of the Clebsch-Gordan coefficients or scattering tensor an elaboration of the selection rules is a first necessary step. In fact, a reduction of products of the irreducible representations of the relevant crystal group gives the frequency of occurrence of each irreducible representations in a product and thus a survey of the matrix elements which vanish by symmetry alone and of those which remain for which the calculation of the Clebsch-Gordan coefficients is required.

4. **Decomposition formula.** — The transition amplitude of an electron from the state $\psi_q^{\mathbf{m}}$ to the state $\psi_r^{\mathbf{h}}$ due to an interaction described by the operator $\psi_p^{\mathbf{k}}$ is proportional to the integral [36-39]

$$\int \psi_r^{*\mathbf{h}}(x)\, \psi_p^{\mathbf{k}}(x)\, \psi_q^{\mathbf{m}}(x)\, \mathrm{d}_3 x\,. \tag{1}$$

The integral vanishes unless the representation $D_r^{\mathbf{h}}$ is contained in the product $D_p^{\mathbf{k}} \times D_q^{\mathbf{m}}$. Thus the selection rules are obtained from decomposition of the Kronecker product of two irreducible representations into irreducible ones. The irreducible representations are labelled by the wave vectors **k**, **m**, **h** and indices p, q, r respectively. $C_{pq,r}^{\mathbf{km},\mathbf{h}}$ are coefficients expressing the frequency of occurrence of the representation $D_r^{\mathbf{h}}$ in $D_p^{\mathbf{k}} \times D_q^{\mathbf{m}}$

$$D_p^{\mathbf{k}} \times D_q^{\mathbf{m}} = \sum_{\mathbf{h},r} C_{pq,r}^{\mathbf{km},\mathbf{h}}\, D_r^{\mathbf{h}}\,. \tag{2}$$

For the space group G with the elements $\{\alpha \mid \mathbf{V}\}$ and with the characters $\chi_p^{\mathbf{k}}$, $\chi_q^{\mathbf{m}}$, $\chi_r^{\mathbf{h}}$ of the irreducible representations $D_p^{\mathbf{k}}$, $D_q^{\mathbf{m}}$, $D_r^{\mathbf{h}}$ respectively, the frequencies of occurrence are given by

$$C_{pq,r}^{\mathbf{km},\mathbf{h}} = \frac{1}{|G|} \times \\ \times \sum_{\{\alpha|\mathbf{V}\}\in G} \chi_p^{\mathbf{k}}(\{\alpha \mid \mathbf{V}\})\, \chi_q^{\mathbf{m}}(\{\alpha \mid \mathbf{V}\})\, \chi_r^{*\mathbf{h}}(\{\alpha \mid \mathbf{V}\})\,. \tag{3}$$

Here the vectors **k**, **m**, **h** belong to the suitably chosen $1/|\overline{G}|$ part of the Brillouin zone, the so-called representation domain Φ, containing one arm from each star. The integer $|\overline{G}|$ is the order of the single point group $\overline{G}$ of the group G. An example of the representation domain of the space group O_h^3 is shown in figure 2 by heavy lines. Eq. (3) can be expressed in terms of the characters $\psi_p^{\mathbf{k}}$ of the small representations $d_p^{\mathbf{k}}$ which induce the representations $D_p^{\mathbf{k}}$ of G [37, 38]

$$C_{pq,r}^{\mathbf{km},\mathbf{h}} = \sum_{\alpha}{}' \frac{1}{|\overline{L}_\alpha|} \times \\ \times \sum_{S\in L_\alpha} \psi_{\alpha p}^{\mathbf{k}}(S \mid \tau_s)\, \psi_{\beta(\alpha)q}^{\mathbf{m}}(S \mid \tau_s)\, \psi_r^{*\mathbf{h}}(S \mid \tau_s)\,. \tag{4}$$

Here the sum indexed by α is taken over the relevant leading wave vector selection rules (LWVSRs), see Lewis [38], i.e. over the elements determined by the expansion of the point group $\overline{G}$ into double cosets ([37], p. 208),

$$\overline{G} = \sum_{\alpha} \overline{G}^{\mathbf{h}}\, \alpha \overline{G}^{\mathbf{k}}\,,$$

where $\overline{G}^{\mathbf{h}}$ is the point group of the wave vector group $G^{\mathbf{h}}$ of **h** and $\overline{G}^{\mathbf{k}}$ is the point group of $G^{\mathbf{k}}$. The index $\beta(\alpha)$ means that β is dependent on α, it is an arbitrary element of $\overline{G}$ satisfying

$$\alpha\mathbf{k} + \beta\mathbf{m} \equiv \mathbf{h} \tag{5}$$

where $\equiv$ means equality modulo a vector of the reciprocal lattice of the group G. The symbol $\sum'$ reminds us that, if for given $\mathbf{k}$, $\mathbf{m}$, $\mathbf{h}$ and α no element β of $\overline{\mathrm{G}}$ satisfying eq. (5) exists, then we have zero instead of the sum over S. $\overline{\mathrm{L}}_\alpha$ is the point group of

$$\mathrm{L}_\alpha = \mathrm{G}^{\alpha\mathbf{k}} \wedge \mathrm{G}^{\mathbf{h}},$$

the intersection of the group $\mathrm{G}^{\alpha\mathbf{k}}$ of the vector $\alpha\mathbf{k}$ and the group $\mathrm{G}^{\mathbf{h}}$ of $\mathbf{h}$. The $\boldsymbol{\tau}_s$, $\boldsymbol{\tau}_\alpha$ and $\boldsymbol{\tau}_\beta$ are fixed, e.g. the simplest ones, fractional translations associated with S, α and β, respectively, in the group G. $\psi^{\mathbf{k}}_{\alpha p}$ and $\psi^{\mathbf{m}}_{\beta q}$ are given by the relations of the type

$$\psi^{\mathbf{k}}_{\alpha p}(\mathrm{S} \mid \boldsymbol{\tau}_s) = \psi^{\mathbf{k}}_p(\{ \alpha \mid \boldsymbol{\tau}_\alpha \}^{-1} \{ \mathrm{S} \mid \boldsymbol{\tau}_s \} \{ \alpha \mid \boldsymbol{\tau}_\alpha \}) . \qquad (6)$$

For the small representation $\mathrm{d}^{\mathbf{k}}_p$ of the unbarred primitive translation $\{ \mathrm{E} \mid \mathbf{t} \}$ we assume the convention

$$\mathrm{d}^{\mathbf{k}}_p(\{ \mathrm{E} \mid \mathbf{t} \}) = \hat{1} \exp(+ i\mathbf{kt})$$

i.e. we choose the + sign in the exponent on the right-hand side. $\hat{1}$ is the unit matrix having the dimension of the representation $\mathrm{d}^{\mathbf{k}}_p$. In the above considerations G can be a single or double space group. Correspondingly all the groups considered are single groups or double groups, respectively. If G is a double space group, we use the same symbols for the point operations of a double group as for corresponding operations of the single group. For given $\mathbf{k}$, $\mathbf{m}$ from the representation domain Φ all the vectors $\mathbf{h}$ for which the coefficient (4) may be different from zero can be found as follows [36, 46] : we consider the vectors $\mathbf{k}_i$ from the star of $\mathbf{k}$ and $\mathbf{m}_j$ from the star of $\mathbf{m}$. We construct the vectors $\mathbf{k}_i + \mathbf{m}_j$ with one of the vectors $\mathbf{k}_i$, $\mathbf{m}_j$ fixed and the second varied. In this way, on account of eq. (5), we obtain representants $\mathbf{h}_l = \mathbf{k}_i + \mathbf{m}_j$ of the star of the vector $\mathbf{h}$ for which the coefficient (4) may be nonvanishing.

5. **The effect of time reversal symmetry on selection rules.** — The existence of time reversal symmetry requires that the symmetrized or antisymmetrized Kronecker squares of representations have to be considered [39]. The symmetrized (antisymmetrized) Kronecker squares $[\mathrm{D}^2]_\pm$ of a representation D of an arbitrary group G with elements g has the characters

$$[\chi]^2_\pm(g) = \tfrac{1}{2}[\chi^2(g) \pm \chi(g^2)]$$

where $[\chi]^2_+$ and $[\chi]^2_-$ are respectively the characters of the symmetrized and the antisymmetrized Kronecker square of D and χ is the character of D. The formula for the coefficient $\mathrm{C}^{\mathbf{kh}}_{pr}(\pm)$ expressing how many times the symmetrized (antisymmetrized) square $[\mathrm{D}^{\mathbf{k}}_p]^2_\pm$ of a representation $\mathrm{D}^{\mathbf{k}}_p$ of a single or double group G with the character $\chi^{\mathbf{k}}_p$ contains a representation $\mathrm{D}^{\mathbf{h}}_r$ of G with the character $\chi^{\mathbf{h}}_r$ [37-39] is quoted here according to the results of Lewis [38], following his notation on the right-hand side of the equation :

$$\mathrm{C}^{\mathbf{kh}}_{pr}(\pm) = \frac{1}{2}\Bigg\{ \sum_{\alpha(\beta)}{}' \frac{|\mathrm{T}|}{|\mathrm{L}_\alpha|} \sum_{\mathrm{S}\in\overline{\mathrm{L}}_\alpha} \psi^{\mathbf{k}}_{\alpha p}(\{ \mathrm{S} \mid \boldsymbol{\tau}_s \}) \times$$
$$\times\ \psi^{\mathbf{k}}_{\beta q}(\{ \mathrm{S} \mid \boldsymbol{\tau}_s \})\, \psi^{*\mathbf{h}}_r(\{ \mathrm{S} \mid \boldsymbol{\tau}_s \})$$
$$\pm \sum_{\alpha}{}'' \frac{|\mathrm{T}|}{|\mathrm{L}_\alpha|} \sum_{\mathrm{S}\in\mathrm{Q}_\alpha} \psi^{\mathbf{k}}_{\alpha p}(\{ \mathrm{S} \mid \boldsymbol{\tau}_s \}^2)\, \psi^{*\mathbf{h}}_r(\{ \mathrm{S} \mid \boldsymbol{\tau}_s \}) \Bigg\} . \qquad (7)$$

The first term in (7) has been described before [36, 37]. The sum $\sum_\alpha''$ is taken over the LWVSRs capable of being expressed in the form $\alpha\mathbf{k} + \mathrm{S}\alpha\mathbf{k} \equiv \mathbf{h}$. The double prime reminds us that for given $\mathbf{k}$, $\mathbf{h}$, α the LWVSRs not capable of being expressed in the form $\alpha\mathbf{k} + \mathrm{S}\alpha\mathbf{k} \equiv \mathbf{h}$ will not contribute to the $\mathrm{C}^{\mathbf{kh}}_{pr}(\pm)$. The element $\mathrm{S} \in \mathrm{Q}_\alpha$ is defined by (i) $\mathrm{S} \in \overline{\mathrm{G}}^{\mathbf{h}}$ and (ii) $\alpha\mathbf{k} + \mathrm{S}\alpha\mathbf{k} \equiv \mathbf{h}$.

A particularly interesting application of the decomposition of the direct product of the irreducible representations into the sum of the irreducible representations arises in the construction of the symmetry adapted electron pair states and cell states in a given crystal lattice. The cell states have been constructed in the Wannier representation for the d-electrons in the beta-wolfram lattice, in the approximation of a contact interaction and a nearest-neighbour interaction [40]. Much remains to be done to derive further results by this method and the general selection rules may be of help in this approach.

6. **Description of tables.** — Table I lists coordinates of the symmetry points of the representation domain Φ for A-15 structure. Tables II-XI present the decomposition of the Kronecker products of the irreducible representations of the space group O^3_h into irreducible representations, eq. (2), where $\mathbf{k}$, $\mathbf{m}$ run over the four symmetry points of the Brillouin zone. We present

TABLE I

The symmetry points

Point	k	Point	k
Γ	(0, 0, 0)	R	$(\pi/a, \pi/a, \pi/a)$
X	$(0, \pi/a, 0)$	M	$(\pi/a, \pi/a, 0)$

TABLE II

$$\Gamma \times \Gamma = \Gamma_- \times \Gamma_- = \sum c_i \Gamma_i \qquad \Gamma_- \times \Gamma = \sum c_i \Gamma_{i-}$$

	Γ_1	Γ_2	Γ_3	Γ_4	Γ_5	Γ_6	Γ_7	Γ_8
Γ_1	[1]	2	3	4	5	6	7	8
Γ_2		[1]	3	5	4	7	6	8
Γ_3			[13] 2	45	45	8	8	678
Γ_4				[135] 4	2345	68	78	678^2
Γ_5					[135] 4	78	68	678^2
Γ_6						[4] 1	25	345
Γ_7							[4] 1	345
Γ_8								$[24^25]$ 135

TABLE III

$$\Gamma \times \mathrm{R} = \sum c_i \, \mathrm{R}_i$$

	$\Gamma_{1\pm,2\pm}$	Γ_{3+}	$\Gamma_{4\pm,5\pm}$	Γ_{3-}	$\Gamma_{6+,7+}$	Γ_{8+}	$\Gamma_{6-,7-}$	Γ_{8-}
R_1	1	23	4	23	5	67	5	67
R_2	2	13	4	12	7	56	6	57
R_3	3	12	4	13	6	57	7	56
R_4	4	4^2	1234^2	4^2	567	$5^26^27^2$	567	$5^26^27^2$
R_5	5	67	567	67	14	234^2	14	234^2
R_6	6	57	567	56	34	124^2	24	134^2
R_7	7	56	567	57	24	134^2	34	124^2

TABLE IV

$$\Gamma_{i+} \times \mathrm{M}_{j+} = \Gamma_{i-} \times \mathrm{M}_{j-} = \sum c_k \, \mathrm{M}_{k+}$$
$$\Gamma_{i-} \times \mathrm{M}_{j+} = \Gamma_{i+} \times \mathrm{M}_{j-} = \sum c_k \, \mathrm{M}_{k-}$$

	Γ_1	Γ_2	Γ_3	Γ_4	Γ_5	Γ_6	Γ_7	Γ_8
M_1	1	2	12	35	45	6	7	67
M_2	2	1	12	45	35	7	6	67
M_3	3	4	34	15	25	6	7	67
M_4	4	3	34	25	15	7	6	67
M_5	5	5	5^2	12345	12345	67	67	6^27^2
M_6	6	7	67	6^27	67^2	135	245	12345^2
M_7	7	6	67	67^2	6^27	245	135	12345^2

also in tables II, IX, X and XI the decompositions of the Kronecker squares $\mathrm{D}_p^{\mathbf{k}} \times \mathrm{D}_p^{\mathbf{k}}$ of the irreducible representations of the group into symmetrized and antisymmetrized squares, $[\mathrm{D}_p^{\mathbf{k}}]_+^2$, $[\mathrm{D}_p^{\mathbf{k}}]_-^2$, respectively. We do this by writing the decomposition of $[\mathrm{D}_p^{\mathbf{k}}]_+^2$ in square brackets. To label the irreducible representations of the group O_h^3 we use the Miller and Love [41] labels of the corresponding small representations, numbers with the minus sign above correspond to the odd representations, numbered with $-$ sign, those with no sign correspond to even representations, numbered with $+$ sign. Powers correspond to the frequency of occurrence c_i of the given irreducible representation. In tables XII and XIII we summarize in the upper part, the notations of the single-valued representations and in the lower part, those of the spinor representations for the symmetry points Γ, R, M and X, according to various authors [47-52].

TABLE V

$$\Gamma \times \mathrm{X} = \sum c_i \, \mathrm{X}_i$$

	$\Gamma_{1+,2+}$	Γ_{3+}	$\Gamma_{4+,5+}$	$\Gamma_{1-,2-}$	Γ_{3-}	$\Gamma_{4-,5-}$	$\Gamma_{6\pm,7\pm}$	$\Gamma_{8\pm}$
X_1	1	1^2	234	2	2^2	134	5	5^2
X_2	2	2^2	134	1	1^2	234	5	5^2
X_3	3	3^2	124	3	3^2	124	5	5^2
X_4	4	4^2	123	4	4^2	123	5	5^2
X_5	5	5^2	5^3	5	5^2	5^3	1234	$1^22^23^24^2$

TABLE VI

$$\mathrm{R} \times \mathrm{M} = \sum c_i \, \mathrm{X}_i$$

	$\mathrm{R}_{1,2,3}$	R_4	$\mathrm{R}_{5,6,7}$
$\mathrm{M}_{1\pm,2\pm}$	3	124	5
$\mathrm{M}_{3\pm,4\pm}$	4	123	5
$\mathrm{M}_{5\pm}$	12	123^24^2	5^2
$\mathrm{M}_{6\pm,7\pm}$	5	5^3	1234

TABLE VII

$$\mathrm{R} \times \mathrm{X} = \sum c_i \, \mathrm{M}_i$$

	$\mathrm{R}_{1,2,3}$	R_4	$\mathrm{R}_{5,6,7}$
$\mathrm{X}_{1,2}$	$5\bar{5}$	$12345\bar{1}\bar{2}\bar{3}\bar{4}\bar{5}$	$67\bar{6}\bar{7}$
X_3	$12\bar{1}\bar{2}$	$345^2\bar{3}\bar{4}\bar{5}^2$	$67\bar{6}\bar{7}$
X_4	$34\bar{3}\bar{4}$	$125^2\bar{1}\bar{2}\bar{5}^2$	$67\bar{6}\bar{7}$
X_5	$67\bar{6}\bar{7}$	$6^37^3\bar{6}^3\bar{7}^3$	$12345^2\bar{1}\bar{2}\bar{3}\bar{4}\bar{5}^2$

Table VIII

$$M \times X = \sum c_i R_i + \sum c_j X_j$$

	$M_{1+,2+}$		$M_{3+,4+}$		M_{5+}		$M_{1-,2-}$		$M_{3-,4-}$		M_{5-}		$M_{6\pm,7\pm}$	
	R	X	R	X	R	X	R	X	R	X	R	X	R	X
X_1	4	24	4	23	1234	1^234	4	14	4	13	1234	2^234	567	5^2
X_2	4	14	4	13	1234	2^234	4	24	4	23	1234	1^234	567	5^2
X_3	123	3^2	4	12	4^2	124^2	123	3^2	4	12	4^2	124^2	567	5^2
X_4	4	12	123	4^2	4^2	123^2	4	12	123	4^2	4^2	123^2	567	5^2
X_5	567	5^2	567	5^2	$5^26^27^2$	5^4	567	5^2	567	5^2	$5^26^27^2$	5^4	1234^3	$1^22^23^24^2$

Table IX

$$R \times R = \sum c_i \Gamma_i$$

	R_1	R_2	R_3	R_4	R_5	R_6	R_7
R_1	$[12\bar1]\,\bar2$	$3\bar3$	$3\bar3$	$45\bar4\bar5$	$67\bar6\bar7$	$8\bar8$	$8\bar8$
R_2		$[\bar13]\,\bar2$	$12\bar3$	$45\bar4\bar5$	$8\bar8$	$67\bar8$	$\bar6\bar78$
R_3			$[\bar13]\,\bar2$	$45\bar4\bar5$	$8\bar8$	$\bar6\bar78$	$67\bar8$
R_4				$[123^245\bar1\bar3\bar5^2]\,45\bar2\bar3\bar4^2$	$678^2\bar6\bar7\bar8^2$	$678^2\bar6\bar7\bar8^2$	$678^2\bar6\bar7\bar8^2$
R_5					$[45\bar2\bar4]\,12\bar1\bar5$	$345\bar3\bar4\bar5$	$345\bar3\bar4\bar5$
R_6						$[45\bar2\bar4]\,3\bar1\bar5$	$1245\bar3\bar4\bar5$
R_7							$[45\bar2\bar4]\,3\bar1\bar5$

Table X

$$M \times M = M_- \times M_- = \sum c_i \Gamma_i + \sum c_j M_j \qquad M_- \times M = \sum c_i \Gamma_{i-} + \sum c_j M_{j-}$$

	M_1		M_2		M_3		M_4		M_5		M_6		M_7	
	Γ	M	Γ	M	Γ	M	Γ	M	Γ	M	Γ	M	Γ	M
M_1	[13]	[1] 2	23	12	4	5	5	5	45	345	68	67	78	67
M_2			[13]	[1] 2	5	5	4	5	45	345	78	67	68	67
M_3					[13]	[4] 3	23	34	45	125	68	67	78	67
M_4							[13]	[4] 3	45	125	78	67	68	67
M_5									$[123^25]$ 4	[145] 235	678^2	6^27^2	678^2	6^27^2
M_6											$[4^25]$ 13	[235] 145	2345^2	12345^2
M_7													$[4^25]$ 13	[235] 145

Table XI

$$X \times X = \sum c_i \Gamma_i + \sum c_j M_j$$

	X_1		X_2		X_3		X_4		X_5	
	Γ	M	Γ	M	Γ	M	Γ	M	Γ	M
X_1	$[123^2\bar5]\bar4$	$[\bar1\bar45]\bar2\bar35$	$45\bar1\bar2\bar3^2$	$1234\bar5^2$	$45\bar4\bar5$	$345\bar3\bar4\bar5$	$45\bar4\bar5$	$125\bar1\bar2\bar5$	$67\bar6\bar7$	$6^27^2\bar6^2\bar7^2$
X_2			$[123^2\bar5]\bar4$	$[\bar1\bar45]\bar2\bar35$	$45\bar4\bar5$	$345\bar3\bar4\bar5$	$45\bar4\bar5$	$125\bar1\bar2\bar5$	$67\bar6\bar7$	$6^27^2\bar6^2\bar7^2$
X_3					$[123^2\bar1\bar3]\bar2\bar3$	$[12\bar1^2]12\bar2^2$	$45\bar4\bar5$	$5^2\bar5^2$	$67\bar6\bar7$	$6^27^2\bar6^2\bar7^2$
X_4							$[123^2\bar1\bar3]\bar2\bar3$	$[34\bar4^2]34\bar3^2$	$67\bar6\bar7$	$6^27^2\bar6^2\bar7^2$
X_5									$[4^35^3\bar2\bar3\bar4^2\bar5]123^2\bar1\bar3\bar4\bar5^2$	$[12345^2\bar2^2\bar3^2\bar5^2]12345^2\bar1^2\bar4^2\bar5^2$

TABLE XII

Labels of the irreducible representations for the point Γ

Miller, Love [41] p. 397	Zak, Casher, Glück, Gur [45] p. 36, 265	Kovalev [44] p. 58, 60	Bradley, Cracknell [37] p. 383, 252, 396 274, 557	Elliott [42] p. 340	Bouckaert, Smoluchowski, Wigner [43]	Gorzkowski [11, 12], Mattheiss [13]
GM1+	1	T 205 τ_1	A_{1g}	Γ_{1+}	Γ_1	Γ_{1+}
GM2+	2	T 205 τ_2	A_{2g}	Γ_{2+}	Γ_2	Γ_{2+}
GM3+	3	T 205 τ_3	E_g	Γ_{12+}	Γ_{12}	Γ_{3+}
GM4+	5	T 205 τ_5	T_{1g}	Γ_{15+}	$\Gamma_{15'}$	Γ_{4+}
GM5+	4	T 205 τ_4	T_{2g}	Γ_{25+}	$\Gamma_{25'}$	Γ_{5+}
GM1−	6	T 205 τ_6	A_{1u}	Γ_{1-}	$\Gamma_{1'}$	Γ_{1-}
GM2−	7	T 205 τ_7	A_{2u}	Γ_{2-}	$\Gamma_{2'}$	Γ_{2-}
GM3−	8	T 205 τ_8	E_u	Γ_{12-}	$\Gamma_{12'}$	Γ_{3-}
GM4−	10	T 205 τ_{10}	T_{1u}	Γ_{15-}	Γ_{15}	Γ_{4-}
GM5−	9	T 205 τ_9	T_{2u}	Γ_{25-}	Γ_{25}	Γ_{5-}
GM6+	$\bar{1}$	P 205 π_2	$\bar{E}_{1g}$	Γ_{6+}		Γ_{7+}
GM7+	$\bar{2}$	P 205 π_1	$\bar{E}_{2g}$	Γ_{7+}		Γ_{6+}
GM8+	$\bar{3}$	P 205 π_3	$\bar{F}_g$	Γ_{8+}		Γ_{8+}
GM6−	$\bar{4}$	P 205 π_5	$\bar{E}_{1u}$	Γ_{6-}		Γ_{7-}
GM7−	$\bar{5}$	P 205 π_4	$\bar{E}_{2u}$	Γ_{7-}		Γ_{6-}
GM8−	$\bar{6}$	P 205 π_6	$\bar{F}_u$	Γ_{8-}		Γ_{8-}

TABLE XIII

Labels of the irreducible representations for the points R, M *and* X

Miller, Love [41] p. 397, 398			Zak, Casher, Glück, Gur [45] p. 264, 263			Kovalev [44] p. 58, 60, 83, 94, 97			Bradley, Cracknell [37] p. 269, 383, 234, 228, 240, 556			Gorzkowski [11, 12] p. 915, 916, 917		
						T 209	T 208	T 157						
R	M	X	R	M	X	R	M	X	R	M	X	R	M	X
1	1_+	1	2	2	1	τ_1	τ_1	τ_3	E	A_{1g}	E′	3	4	1
2	2_+	2	3	4	3	τ_3	τ_5	τ_4	${}^2F$	B_{1g}	E″	1	8	2
3	3_+	3	4	3	2	τ_2	τ_3	τ_1	${}^1F$	A_{2g}	E_1	2	7	3
4	4_+	4	1	5	4	τ_4	τ_7	τ_2	H	B_{2g}	E_2	4	3	4
	5_+			1			τ_9			E_g			9	
	1_-			9			τ_2			A_{1u}			5	
	2_-			7			τ_6			B_{1u}			1	
	3_-			10			τ_4			A_{2u}			2	
	4_-			8			τ_8			B_{2u}			6	
	5_-			6			τ_{10}			E_u			10	
						p. 135 P 209	p. 135 P 208	p. 124 P 157	p. 568	p. 565	p. 567			
5	6_+	5	$\bar{1}$	$\bar{2}$	$\bar{1}$	π_1	π_3	π_1	$\bar{F}$	$\bar{E}_{2g}$	$\bar{F}$	7	14	5
6	7_+		$\bar{3}$	$\bar{1}$		π_2	π_1		${}^1\bar{M}$	$\bar{E}_{1g}$		5	13	
7	6_-		$\bar{2}$	$\bar{3}$		π_3	π_4		${}^2\bar{M}$	$\bar{E}_{2u}$		6	11	
	7_-			$\bar{4}$			π_2			$\bar{E}_{1u}$			12	

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