D

Tables for Double Groups

In this appendix we provide tables useful for handling problems associated with double groups. Many of these tables can be found in two references, one by Koster et al. [48] and another by Miller and Love [54]. The first reference book "Properties of the Thirty-Two Point Groups," by G.F. Koster, J.O. Dimmock, R.G. Wheeler, and H. Statz gives many tables for each of the 32 point groups, while the second gives many character tables for the group of the wave vector for each of the high symmetry points for each of the 230 space groups and many other kinds of related space groups.

The tables in the first reference for the 32 point groups include:

1. A character table including the double group representations (see, for example Table D.1 for groups O and T_d).
2. A table giving the decomposition of the direct product of any two irreducible representations (an example of such a table is given in Table D.2).
3. Tables of coupling coefficients for the product of any two basis functions. Two examples of tables of coupling coefficients are given in Tables D.3 and D.4.[1]
4. Compatibility tables between point groups (e.g., Table D.7).
5. Compatibility tables with the Full Rotation Group (e.g., Table D.8).

We now illustrate some examples of these tables. Table D.1 shows the double group character table for the group O, which is tabulated together with T_d and includes classes, irreducible representations and basis functions for the double group. For example, the basis functions for $\Gamma_4(\Gamma_{15})$ are S_x, S_y, S_z which refer to the three Cartesian components of the angular momentum (integral values of angular momentum)[1] [47]. The basis functions for the Γ_6 and Γ_8 irreducible representations are written in the basic form $\phi(j, m_j)$ for the angular momentum and all the m_j partners are listed. Koster et al. use the notation $\overline{E}$ for $\mathcal{R}$ (rotation by 2π) and the notation $\overline{C}_3$ for class $\mathcal{R}C_3$. The meaning of the time

[1] Table 83 of [47] is continued over 10 pages of the book pages 90–99. We have reproduced some of the sections of this complete compilation.

Table D.1. Character table and basis functions for double groups O and T_d

O	E	$\overline{E}$	$8C_3$	$8\overline{C}_3$	$3C_2$ $3\overline{C}_2$	$6C_4$	$6\overline{C}_4$	$6C_2'$ $6\overline{C}_2'$			
T_d	E	$\overline{E}$	$8C_3$	$8\overline{C}_3$	$3C_2$ $3\overline{C}_2$	$6S_4$	$6\overline{S}_4$	$6\sigma_d$ $6\overline{\sigma}_d$	time inversion	bases for O	bases for T_d
Γ_1	1	1	1	1	1	1	1	1	a	R	R or xyz
Γ_2	1	1	1	1	1	−1	−1	−1	a	xyz	$S_xS_yS_z$
$\Gamma_3(\Gamma_{12})$	2	2	−1	−1	2	0	0	0	a	$(2z^2-x^2-y^2)$, $\sqrt{3}(x^2-y^2)$	$(2z^2-x^2-y^2)$, $\sqrt{3}(x^2-y^2)$
$\Gamma_4(\Gamma_{15})$	3	3	0	0	−1	1	1	−1	a	S_x, S_y, S_z	S_x, S_y, S_z
$\Gamma_5(\Gamma_{25})$	3	3	0	0	−1	−1	−1	1	a	yz, xz, xy	x, y, z
Γ_6	2	−2	1	−1	0	$\sqrt{2}$	$-\sqrt{2}$	0	c	$\phi(1/2, -1/2)$, $\phi(1/2, 1/2)$	$\phi(1/2, -1/2)$, $\phi(1/2, 1/2)$
Γ_7	2	−2	1	−1	0	$-\sqrt{2}$	$\sqrt{2}$	0	c	$\Gamma_6 \otimes \Gamma_2$	$\Gamma_6 \otimes \Gamma_2$
Γ_8	4	−4	−1	1	0	0	0	0	c	$\phi(3/2,-3/2)$, $\phi(3/2,-1/2)$, $\phi(3/2,1/2)$, $\phi(3/2,3/2)$	$\phi(3/2,-3/2)$, $\phi(3/2,-1/2)$, $\phi(3/2,1/2)$, $\phi(3/2,3/2)$

inversion (Time Inversion) entries a, b and c are explained in Chap. 16 where *time inversion symmetry* is discussed.

Table D.2 for groups O and T_d gives the decomposition of the direct product of any irreducible representation Γ_i labeling a column with another irreducible representation Γ_j labeling a row. The irreducible representations contained in the decomposition of the direct product are $\Gamma_i \otimes \Gamma_j$ entered in the matrix position of their intersection.

The extensive tables of coupling coefficients are perhaps the most useful tables in Koster et al. [48] These tables give the basis functions for the irreducible representations obtained by taking the direct product of two irreducible representations. We illustrate in Table D.3 the basis functions obtained by taking the direct product of each of the two partners of the Γ_{12} representation (denoted by Koster et al. as u_1^3 and u_2^3) with each of the three partners of the Γ_{15} representation (denoted by v_x^4, v_y^4, v_z^4) to yield three partners with Γ_{15} symmetry (denoted by $\psi_x^4, \psi_y^4, \psi_z^4$) and 3 partners with Γ_{25} symmetry (denoted by $\psi_{yz}^5, \psi_{zx}^5, \psi_{xy}^5$). This is Table 83 on p. 91 of Koster et al. [48]. From Table D.3 we see that the appropriate linear combinations for the ψ^4 and ψ^5 functions are (see Sect. 14.8)

Table D.2. Table of direct products of irreducible representations for the groups O and T_d

Γ_1	Γ_2	Γ_3	Γ_4	Γ_5	Γ_6	Γ_7	Γ_8	
Γ_1	Γ_2	Γ_3	Γ_4	Γ_5	Γ_6	Γ_7	Γ_8	Γ_1
	Γ_1	Γ_3	Γ_5	Γ_4	Γ_7	Γ_6	Γ_8	Γ_2
		$\Gamma_1+\Gamma_2+\Gamma_3$	$\Gamma_4+\Gamma_5$	$\Gamma_4+\Gamma_5$	Γ_8	Γ_8	$\Gamma_6+\Gamma_7+\Gamma_8$	Γ_3
			$\Gamma_1+\Gamma_3+\Gamma_4+\Gamma_5$	$\Gamma_2+\Gamma_3+\Gamma_4+\Gamma_5$	$\Gamma_6+\Gamma_8$	$\Gamma_7+\Gamma_8$	$\Gamma_6+\Gamma_7+2\Gamma_8$	Γ_4
				$\Gamma_1+\Gamma_3+\Gamma_4+\Gamma_5$	$\Gamma_7+\Gamma_8$	$\Gamma_6+\Gamma_8$	$\Gamma_6+\Gamma_7+2\Gamma_8$	Γ_5
					$\Gamma_1+\Gamma_4$	$\Gamma_2+\Gamma_5$	$\Gamma_3+\Gamma_4+\Gamma_5$	Γ_6
						$\Gamma_1+\Gamma_4$	$\Gamma_3+\Gamma_4+\Gamma_5$	Γ_7
							$\Gamma_1+\Gamma_2+\Gamma_3$ $+2\Gamma_4+2\Gamma_5$	Γ_8

Table D.3. Coupling coefficients for selected basis functions for single group O

	$u_1^3v_x^4$	$u_1^3v_y^4$	$u_1^3v_z^4$	$u_2^3v_x^4$	$u_2^3v_y^4$	$u_2^3v_z^4$
ψ_x^4	$-1/2$	0	0	$\sqrt{3}/2$	0	0
ψ_y^4	0	$-1/2$	0	0	$-\sqrt{3}/2$	0
ψ_z^4	0	0	1	0	0	0
ψ_{yz}^5	$-\sqrt{3}/2$	0	0	$-1/2$	0	0
ψ_{xz}^5	0	$\sqrt{3}/2$	0	0	$-1/2$	0
ψ_{xy}^5	0	0	0	0	0	1

Table D.4. Coupling coefficient tables for the indicated basis functions for double group O_h

	$u_x^4v_{-1/2}^6$	$u_x^4v_{1/2}^6$	$u_y^4v_{-1/2}^6$	$u_y^4v_{1/2}^6$	$u_z^4v_{-1/2}^6$	$u_z^4v_{1/2}^6$
$\psi_{-1/2}^6$	0	$-i/\sqrt{3}$	0	$-1/\sqrt{3}$	$i/\sqrt{3}$	0
$\psi_{1/2}^6$	$-i/\sqrt{3}$	0	$1/\sqrt{3}$	0	0	$-i/\sqrt{3}$
$\psi_{-3/2}^8$	$i/\sqrt{2}$	0	$1/\sqrt{2}$	0	0	0
$\psi_{-1/2}^8$	0	$i/\sqrt{6}$	0	$1/\sqrt{6}$	$i\sqrt{2}/\sqrt{3}$	0
$\psi_{1/2}^8$	$-i/\sqrt{6}$	0	$1/\sqrt{6}$	0	0	$i\sqrt{2}/\sqrt{3}$
$\psi_{3/2}^8$	0	$-i/\sqrt{2}$	0	$1/\sqrt{2}$	0	0

Table D.5. Coupling coefficient table for coupling the basis functions of $\Gamma_3 \otimes \Gamma_6^+$ to Γ_8 where $\Gamma_3 \otimes \Gamma_6^+ = \Gamma_8$ in the double group for O_h

	$u_1^3v_{-1/2}^6$	$u_1^3v_{+1/2}^6$	$u_2^3v_{-1/2}^6$	$u_2^3v_{+1/2}^6$
$\psi_{-3/2}^8$	0	0	0	1
$\psi_{-1/2}^8$	1	0	0	0
$\psi_{+1/2}^8$	0	-1	0	0
$\psi_{+3/2}^8$	0	0	-1	0

$$
\begin{aligned}
\psi_x^4 &= -(1/2)u_1^3v_x^4 + (\sqrt{3}/2)u_2^3v_x^4 \\
\psi_y^4 &= -(1/2)u_1^3v_y^4 - (\sqrt{3}/2)u_2^3v_y^4 \\
\psi_z^4 &= u_1^3v_z^4 \\
\psi_{yz}^5 &= -(\sqrt{3}/2)u_1^3v_x^4 - (1/2)u_2^3v_x^4 \\
\psi_{xz}^5 &= (\sqrt{3}/2)u_1^3v_y^4 - (1/2)u_2^3v_y^4 \\
\psi_{xy}^5 &= u_2^3v_z^4 \,.
\end{aligned}
$$

Note that the basis functions for the ψ^4 and ψ^5 functions depend on the choice of basis functions for u and v. Journal articles often use the notation

$$
\Gamma_{15} \otimes \Gamma_{12} = \Gamma_{15} + \Gamma_{25}\,, \tag{D.1}
$$

Table D.6. Coupling coefficient table for coupling the basis functions of $\Gamma_5 \otimes \Gamma_6^+$ to the basis functions Γ_7 and Γ_8 in the double group for O_h

	$u_x^5 v_{-1/2}^6$	$u_x^5 v_{+1/2}^6$	$u_y^5 v_{-1/2}^6$	$u_y^5 v_{+1/2}^6$	$u_z^5 v_{-1/2}^6$	$u_z^5 v_{+1/2}^6$
$\psi_{-1/2}^7$	0	$-i/\sqrt{3}$	0	$-1/\sqrt{3}$	$i/\sqrt{3}$	0
$\psi_{+1/2}^7$	$-i/\sqrt{3}$	0	$1/\sqrt{3}$	0	0	$-i/\sqrt{3}$
$\psi_{-3/2}^8$	$-i/\sqrt{6}$	0	$1/\sqrt{6}$	0	0	$i\sqrt{2}/\sqrt{3}$
$\psi_{-1/2}^8$	0	$i/\sqrt{2}$	0	$-1/\sqrt{2}$	0	0
$\psi_{+1/2}^8$	$-i/\sqrt{2}$	0	$-1/\sqrt{2}$	0	0	0
$\psi_{+3/2}^8$	0	$i/\sqrt{6}$	0	$1/\sqrt{6}$	$i\sqrt{2}/\sqrt{3}$	0

where $\Gamma_4 \leftrightarrow \Gamma_{15}$ and $\Gamma_3 \leftrightarrow \Gamma_{12}$. Thus taking the direct product between irreducible representations Γ_3 and Γ_4 in O or T_d symmetries yields:

$$\Gamma_4 \otimes \Gamma_3 = \Gamma_4 + \Gamma_5 \,, \tag{D.2}$$

where $\Gamma_5 \leftrightarrow \Gamma_{25}$.

We next illustrate the use of a typical coupling coefficient table relevant to the introduction of spin into the electronic energy level problem. In this case we need to take a direct product of Γ_6^+ with a single group representation, where Γ_6^+ is the representation for the spinor ($D_{1/2}$). For example, for a p-level $\Gamma_{15}^- \otimes \Gamma_6^+ = \Gamma_6^- + \Gamma_8^-$ and the appropriate coupling coefficient table is Table D.4 (in Koster et al. Table 83, p. 92).

Table D.4 gives us the following relations between basis functions:

$$\begin{aligned}
\psi_{-1/2}^6 &= \left|\frac{1}{2}, -\frac{1}{2}\right\rangle = -(i/\sqrt{3})(u_x^4 - iu_y^4)\uparrow + (i/\sqrt{3})u_z^4 \downarrow \\
\psi_{1/2}^6 &= \left|\frac{1}{2}, \frac{1}{2}\right\rangle = -(i/\sqrt{3})(u_x^4 + iu_y^4)\downarrow - (i/\sqrt{3})u_z^4 \uparrow \\
\psi_{-3/2}^8 &= \left|\frac{3}{2}, -\frac{3}{2}\right\rangle = (i/\sqrt{2})(u_x^4 - iu_y^4)\downarrow \\
\psi_{-1/2}^8 &= \left|\frac{3}{2}, -\frac{1}{2}\right\rangle = (i/\sqrt{6})(u_x^4 - iu_y^4)\uparrow + (i\sqrt{2}/\sqrt{3})u_z^4 \downarrow \\
\psi_{1/2}^8 &= \left|\frac{3}{2}, \frac{1}{2}\right\rangle = -(i/\sqrt{6})(u_x^4 + iu_y^4)\downarrow + (i\sqrt{2}/\sqrt{3})u_z^4 \uparrow \\
\psi_{3/2}^8 &= \left|\frac{3}{2}, \frac{3}{2}\right\rangle = -(i/\sqrt{2})(u_x^4 + iu_y^4)\uparrow \,,
\end{aligned} \tag{D.3}$$

and $v_{-1/2}^6 = \downarrow$. The relations in (D.3) give the transformation of basis functions in the $|\ell s m_\ell m_s\rangle$ representation to the $|j \ell s m_j\rangle$ representation, appropriate to

Table D.7. Compatibility table for the decomposition of the irreducible representations of the double groups O and T_d into the irreducible representations of their subgroups

T_d	O	Γ_1	Γ_2	Γ_3	Γ_4
T	T	Γ_1	Γ_1	$\Gamma_2 + \Gamma_3$	Γ_4
D_{2d}	D_4	Γ_1	Γ_3	$\Gamma_1 + \Gamma_3$	$\Gamma_2 + \Gamma_5$
$C_{3v}; E(w)$	D_3	Γ_1	Γ_2	Γ_3	$\Gamma_2 + \Gamma_3$
$S_4 : H(z)$	$C_4 : H(z) : E(z)$	Γ_1	Γ_1	$\Gamma_2 + \Gamma_3$	$\Gamma_1 + \Gamma_2 + \Gamma_3$
$C_{2v} : E(z)$		Γ_1	Γ_3	$\Gamma_1 + \Gamma_3$	$\Gamma_2 + \Gamma_3 + \Gamma_4$
$C_s : E(v) : H(v)$	$C_2 : E(v) : H(v)$	Γ_1	Γ_2	$\Gamma_1 + \Gamma_2$	$\Gamma_1 + 2\Gamma_2$
T_d	O	Γ_5	Γ_6	Γ_7	Γ_8
T	T	Γ_4	Γ_5	Γ_5	$\Gamma_6 + \Gamma_7$
D_{2d}	D_4	$\Gamma_4 + \Gamma_5$	Γ_6	Γ_7	$\Gamma_6 + \Gamma_7$
$C_{3v}; E(w)$	D_3	$\Gamma_1 + \Gamma_3$	Γ_4	Γ_4	$\Gamma_4 + \Gamma_5 + \Gamma_6$
$S_4 : H(z)$	$C_4 : H(z) : E(z)$	$\Gamma_1 + \Gamma_2 + \Gamma_3$	$\Gamma_4 + \Gamma_5$	$\Gamma_4 + \Gamma_5$	$\Gamma_5 + \Gamma_6 + \Gamma_7 + \Gamma_8$
$C_{2v} : E(z)$		$\Gamma_1 + \Gamma_2 + \Gamma_4$	Γ_5	Γ_5	$2\Gamma_5$
$C_s : E(v) : H(v)$	$2\Gamma_1 + \Gamma_2$	$C_2 : E(v) : H(v)$	$\Gamma_3 + \Gamma_4$	$\Gamma_3 + \Gamma_4$	$2\Gamma_3 + 2\Gamma_4$

Table D.8. Full rotation group compatibility table for the group O

S	D_0^+	Γ_1
P	D_1^-	Γ_4
D	D_2^+	$\Gamma_3 + \Gamma_5$
F	D_3^-	$\Gamma_2 + \Gamma_4 + \Gamma_5$
G	D_4^+	$\Gamma_1 + \Gamma_3 + \Gamma_4 + \Gamma_5$
H	D_5^-	$\Gamma_3 + 2\Gamma_4 + \Gamma_5$
I	D_6^+	$\Gamma_1 + \Gamma_2 + \Gamma_3 + \Gamma_4 + 2\Gamma_5$
	$D_{1/2}^\pm$	Γ_6
	$D_{3/2}^\pm$	Γ_8
	$D_{5/2}^\pm$	$\Gamma_7 + \Gamma_8$
	$D_{7/2}^\pm$	$\Gamma_6 + \Gamma_7 + \Gamma_8$
	$D_{9/2}^\pm$	$\Gamma_6 + 2\Gamma_8$
	$D_{11/2}^\pm$	$\Gamma_6 + \Gamma_7 + 2\Gamma_8$
	$D_{13/2}^\pm$	$\Gamma_6 + 2\Gamma_7 + 2\Gamma_8$
	$D_{15/2}^\pm$	$\Gamma_6 + \Gamma_7 + 3\Gamma_8$

energy bands for which the spin–orbit interaction is included. These linear combinations are basically the *Clebsch–Gordan coefficients* in quantum mechanics [18]. We make use of (D.3) when we introduce spin and spin–orbit interaction into the plane wave relations of the energy eigenvalues and eigenfunctions of the empty lattice.

Tables similar to Table D.4, but allowing us to find the basis functions for the direct products $\Gamma_{12}^\pm \otimes \Gamma_6^+$ and $\Gamma_{25}^\pm \otimes \Gamma_6^+$, are given in Tables D.5 and D.6, respectively, where $\Gamma_{12}^\pm$ and $\Gamma_{25}^\pm$ are denoted by $\Gamma_3^\pm$ and $\Gamma_5^\pm$, respectively, in the Koster tables [47].

Table D.7 gives the point groups that are subgroups of groups T_d and O, and gives the decomposition of the irreducible representations of T_d and O into the irreducible representations of the lower symmetry group. Note in Table D.7 that E refers to the electric field and H to the magnetic field. The table can be used for many applications such as finding the resulting symmetries under crystal field splittings as for example $O_h \to D_3$.

The notation for each of the irreducible representations is consistent with that given in the character tables of Koster's book [47,48]. The decompositions of the irreducible representations of the full rotation group into irreducible representations of groups O and T_d are given, respectively, in Tables D.8 and D.9. Note that all the irreducible representations of the full rotation group are listed, with the $\pm$ sign denoting the parity (even or odd under inversion) and the subscript giving the angular momentum quantum number (j), so that the dimensionality of the irreducible representation $D_j^\pm$ is $(2j + 1)$. In

Table D.9. Full rotation group compatibility table for the group T_d

D_0^+	Γ_1	D_0^-	Γ_2
D_1^+	Γ_4	D_1^-	Γ_5
D_2^+	$\Gamma_3 + \Gamma_5$	D_2^-	$\Gamma_3 + \Gamma_4$
D_3^+	$\Gamma_2 + \Gamma_4 + \Gamma_5$	D_3^-	$\Gamma_1 + \Gamma_4 + \Gamma_5$
D_4^+	$\Gamma_1 + \Gamma_3 + \Gamma_4 + \Gamma_5$	D_4^-	$\Gamma_2 + \Gamma_3 + \Gamma_4 + \Gamma_5$
D_5^+	$\Gamma_3 + 2\Gamma_4 + \Gamma_5$	D_5^-	$\Gamma_3 + \Gamma_4 + 2\Gamma_5$
D_6^+	$\Gamma_1 + \Gamma_2 + \Gamma_3 + \Gamma_4 + 2\Gamma_5$	D_6^-	$\Gamma_1 + \Gamma_2 + \Gamma_3 + 2\Gamma_4 + \Gamma_5$
$D_{1/2}^+$	Γ_6	$D_{1/2}^-$	Γ_7
$D_{3/2}^+$	Γ_8	$D_{3/2}^-$	Γ_8
$D_{5/2}^+$	$\Gamma_7 + \Gamma_8$	$D_{5/2}^-$	$\Gamma_6 + \Gamma_8$
$D_{7/2}^+$	$\Gamma_6 + \Gamma_7 + \Gamma_8$	$D_{7/2}^-$	$\Gamma_6 + \Gamma_7 + \Gamma_8$
$D_{9/2}^+$	$\Gamma_6 + 2\Gamma_8$	$D_{9/2}^-$	$\Gamma_7 + 2\Gamma_8$
$D_{11/2}^+$	$\Gamma_6 + \Gamma_7 + 2\Gamma_8$	$D_{11/2}^-$	$\Gamma_6 + \Gamma_7 + 2\Gamma_8$
$D_{13/2}^+$	$\Gamma_6 + 2\Gamma_7 + 2\Gamma_8$	$D_{13/2}^-$	$2\Gamma_6 + \Gamma_7 + 2\Gamma_8$

summary, we note that the double group character table shown in Table D.1 is applicable to a symmorphic space group, like the O_h point group ($O_h = O \otimes i$) which applies to the group of the wave vector at $k = 0$ for cubic space groups #221, #225, and #229. A double group character table like Table D.1 is also useful for specifying the group of the wave vector for high symmetry points of a nonsymmorphic space group where the double group has to be modified to take into account symmetry operations involving translations. For illustrative purposes we consider the nonsymmorphic space group #194 that applies to 3D graphite ($P6_3/mmc$) or D_{6h}^4 with $ABAB$ layer stacking (see Fig. C.1).

The simplest case to consider is the group of the wave vector for $k = 0$ (the Γ point) where the phase factor is unity. Then the character table for this nonsymmorphic space group looks quite similar to that for a symmorphic space group, the only difference being the labeling of the classes, some of which include translations. This is illustrated in Table D.10 where eight of the classes require translations. Those classes with translations $\tau = (c/2)(0, 0, 1)$ correspond to symmetry operations occuring in group D_{6h} but not in D_{3d}, and are indicated in Table D.10 by a τ symbol underneath the class listing (see also Table C.24 for the corresponding ordinary irreducible representations for which spin is not considered).

As we move away from the Γ point in the k_z direction, the symmetry is lowered from D_{6h} to C_{6v} and the appropriate group of the wave vector is that for a Δ point, as shown in Table D.11. The corresponding point group is C_{6v} which has nine classes, as listed in the character table, showing a compatibility between the classes in C_{6v} and D_{6h} regarding which classes contain

Table D.10. Character table for the double group D_{6h} [48] appropriately modified to pertain to the group of the wave vector at the Γ point($k = 0$) for space group #194 $D_{6h}^4(P6_3/mmc)$[a]

D_{6h}	E	$\overline{E}$	C_2 / $\overline{C}_2$ (τ)	$2C_3$	$2\overline{C}_3$	$2C_6$ (τ)	$2\overline{C}_6$ (τ)	$3C'_2$ / $3\overline{C}'_2$	$3C''_2$ / $3\overline{C}''_2$ (τ)	I	$\overline{I}$	σ_h / $\overline{\sigma}_h$ (τ)	$2S_6$	$2\overline{S}_6$	$2S_3$ (τ)	$2\overline{S}_3$ (τ)	$3\sigma_d$ / $3\overline{\sigma}_d$	$3\sigma_v$ / $3\overline{\sigma}_v$ (τ)	time
Γ_1^+	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	a
Γ_2^+	1	1	1	1	1	1	1	−1	−1	1	1	1	1	1	1	1	−1	−1	a
Γ_3^+	1	1	−1	1	1	−1	−1	1	−1	1	1	−1	1	1	−1	−1	1	−1	a
Γ_4^+	1	1	−1	1	1	−1	−1	−1	1	1	1	−1	1	1	−1	−1	−1	1	a
Γ_5^+	2	2	−2	−1	−1	1	1	0	0	2	2	−2	−1	−1	1	1	0	0	a
Γ_6^+	2	2	2	−1	−1	−1	−1	0	0	2	2	2	−1	−1	−1	−1	0	0	a
Γ_1^-	1	1	1	1	1	1	1	1	1	−1	−1	−1	−1	−1	−1	−1	−1	−1	a
Γ_2^-	1	1	1	1	1	1	1	−1	−1	−1	−1	−1	−1	−1	−1	−1	1	1	a
Γ_3^-	1	1	−1	1	1	−1	−1	1	−1	−1	−1	1	−1	−1	1	1	−1	1	a
Γ_4^-	1	1	−1	1	1	−1	−1	−1	1	−1	−1	1	−1	−1	1	1	1	−1	a
Γ_5^-	2	2	−2	−1	−1	1	1	0	0	−2	−2	2	1	1	−1	−1	0	0	a
Γ_6^-	2	2	2	−1	−1	−1	−1	0	0	−2	−2	−2	1	1	1	1	0	0	a
Γ_7^+	2	−2	0	1	−1	$\sqrt{3}$	$-\sqrt{3}$	0	0	2	−2	0	1	−1	$\sqrt{3}$	$-\sqrt{3}$	0	0	c
Γ_8^+	2	−2	0	1	−1	$-\sqrt{3}$	$\sqrt{3}$	0	0	2	−2	0	1	−1	$-\sqrt{3}$	$\sqrt{3}$	0	0	c
Γ_9^+	2	−2	0	−2	2	0	0	0	0	2	−2	0	−2	2	0	0	0	0	c
Γ_7^-	2	−2	0	1	−1	$\sqrt{3}$	$-\sqrt{3}$	0	0	−2	2	0	−1	1	$-\sqrt{3}$	$\sqrt{3}$	0	0	c
Γ_8^-	2	−2	0	1	−1	$-\sqrt{3}$	$\sqrt{3}$	0	0	−2	2	0	−1	1	$\sqrt{3}$	$-\sqrt{3}$	0	0	c
Γ_9^-	2	−2	0	−2	2	0	0	0	0	−2	2	0	2	−2	0	0	0	0	c

[a] For the group of the wave vector for $k = 0$ for the space group #194, the eight classes in the double group D_{6h} that are not in group D_{3d} [namely $(C_2, \overline{C}_2)$, $2C_6$, $2\overline{C}_6$, $(3C''_2, 3\overline{C}''_2)$, $(\sigma_h, \overline{\sigma}_h)$, $2S_3$, $2\overline{S}_3$, and $(3\sigma_v, 3\overline{\sigma}_v)$] have, in addition to the point group operations $\{R|0\}$ or $\{\overline{R}|0\}$, additional operations $\{R|\tau\}$ or $\{\overline{R}|\tau\}$ involving the translation $\tau = (0, 0, c/2)$. A phase factor $T = \exp(\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{\tau})$, which is equal to unity at $k = 0$, accompanies the characters for the classes corresponding to $\{R|\tau\}$ or $\{\overline{R}|\tau\}$. In listing the classes, the symbol τ is placed below the class symbol, such as $2C_6$, to distinguish the classes that involve translations $\{R|\tau\}$. For the special classes containing both the $\{R|0\}$ and $\{\overline{R}|0\}$ symmetry operations, the symbols are stacked above one another, as in $3\sigma_d$ and $3\overline{\sigma}_d$

translations τ and which do not. All characters corresponding to symmetry operations containing τ must be multiplied by a phase factor $T_\Delta = \exp[\mathrm{i}\pi\Delta]$ which is indicated in Table D.11 by T_Δ, where Δ is a dimensionless variable $0 \leq \Delta \leq 1$.

From Tables D.10 and D.11 we can write down compatibility relations between the Γ point and the Δ point representations (see Table D.12), and we note that in the limit $k \to 0$ all the phase factors $T_\Delta = \exp[\mathrm{i}\pi\Delta]$ in Table D.11 go to unity as Δ goes to zero.

Table D.11. Character table and basis functions for the double group C_{6v} [48] as modified to pertain to the group of the wave vector along the Δ direction for space group #194[a,b]

C_{6v} (6mm)			E	$\overline{E}$	$\overset{C_2}{\overline{C}_2}$ τ	$2C_3$	$2\overline{C}_3$	$2C_6$ τ	$2\overline{C}_6$ τ	$\overset{3\sigma_d}{3\overline{\sigma}_d}$	$\overset{3\sigma_v}{3\overline{\sigma}_v}$ τ	time inversion
x^2+y^2, z^2	z	Δ_1	1	1	$1\cdot T_\Delta$	1	1	$1\cdot T_\Delta$	$1\cdot T_\Delta$	1	$1\cdot T_\Delta$	a
	R_z	Δ_2	1	1	$1\cdot T_\Delta$	1	1	$1\cdot T_\Delta$	$1\cdot T_\Delta$	-1	$-1\cdot T_\Delta$	a
	x^3-3xy^2	Δ_3	1	1	$-1\cdot T_\Delta$	1	1	$-1\cdot T_\Delta$	$-1\cdot T_\Delta$	1	$-1\cdot T_\Delta$	a
	x^3-3yx^2	Δ_4	1	1	$-1\cdot T_\Delta$	1	1	$-1\cdot T_\Delta$	$-1\cdot T_\Delta$	-1	$1\cdot T_\Delta$	a
(xz, yz)	$\left.\begin{matrix}(x,y)\\(R_x,R_y)\end{matrix}\right\}$	Δ_5	2	2	$-2\cdot T_\Delta$	-1	-1	$1\cdot T_\Delta$	$1\cdot T_\Delta$	0	0	a
(x^2-y^2, xy)	$\Delta_3\otimes\Delta_5$	Δ_6	2	2	$2\cdot T_\Delta$	-1	-1	$-1\cdot T_\Delta$	$-1\cdot T_\Delta$	0	0	a
	$\left.\begin{matrix}\phi(1/2,1/2)\\\phi(1/2,-1/2)\end{matrix}\right\}$	Δ_7	2	-2	0	1	-1	$\sqrt{3}\cdot T_\Delta$	$-\sqrt{3}\cdot T_\Delta$	0	0	c
	$\Delta_3\otimes\Delta_7$	Δ_8	2	-2	0	1	-1	$-\sqrt{3}\cdot T_\Delta$	$\sqrt{3}\cdot T_\Delta$	0	0	c
	$\left.\begin{matrix}\phi(3/2,3/2)\\\phi(3/2,-3/2)\end{matrix}\right\}$	Δ_9	2	-2	0	-2	2	0	0	0	0	c

[a] The notation for the symmetry elements and classes is the same as in Table D.10

[b] For the group of the wave vector for a k point along the Δ axis for group #194, the four classes in group C_{6v} that are not in group C_{3v} [namely $(C_2, \overline{C}_2)$, $2C_6$, $2\overline{C}_6$), and $(3\sigma_v, 3\overline{\sigma}_v)$] have, in addition to the point group operation R (or $\overline{R}$), a translation $\tau = (0,0,c/2)$ to form the operation $\{R|\tau\}$, and the irreducible representations have a phase factor $T_\Delta = \exp(\mathrm{i}\pi\Delta)$ for these classes. The remaining classes have symmetry operations of the form $\{R|0\}$ and have no phase factors.

Table D.12. Compatibility relations between the irreducible representations of the group of the wave vector at Γ ($k = 0$) and Δ [$k = (2\pi/a)(0, 0, \Delta)$] for space group #194

Γ point representation		Δ point representation	Γ point representation		Δ point representation
Γ_1^+	$\rightarrow$	Δ_1	Γ_1^-	$\rightarrow$	Δ_2
Γ_2^+	$\rightarrow$	Δ_2	Γ_2^-	$\rightarrow$	Δ_1
Γ_3^+	$\rightarrow$	Δ_3	Γ_3^-	$\rightarrow$	Δ_3
Γ_4^+	$\rightarrow$	Δ_4	Γ_4^-	$\rightarrow$	Δ_4
Γ_5^+	$\rightarrow$	Δ_5	Γ_5^-	$\rightarrow$	Δ_5
Γ_6^+	$\rightarrow$	Δ_6	Γ_6^-	$\rightarrow$	Δ_6
Γ_7^+	$\rightarrow$	Δ_7	Γ_7^-	$\rightarrow$	Δ_7
Γ_8^+	$\rightarrow$	Δ_8	Γ_8^-	$\rightarrow$	Δ_8
Γ_9^+	$\rightarrow$	Δ_9	Γ_9^-	$\rightarrow$	Δ_9

Table D.13. Character table for the group of the wave vector at the point A for space group #194 from Koster [48]

	E	$\overline{E}$	$2C_3$	$2\overline{C}_3$	$3C_2'$ $3\overline{C'}_2$	$3\sigma_d$ $3\overline{\sigma}_d$	time inversion
A_1	2	2	2	2	0	2	a
A_2	2	2	2	2	0	−2	a
A_3	4	4	−2	−2	0	0	a
A_4	2	−2	−2	2	$2i$	0	c
A_5	2	−2	−2	2	$-2i$	0	c
A_6	4	−4	2	−2	0	0	c

All classes have symmetry operations of the form $\{R|0\}$ or $\{\overline{R}|0\}$ and do not involve τ translations.

Table D.14. Compatibility relations between the irreducible representations of the group of the wave vector at A [$k = (2\pi/c)(001)$] and Δ [$k = (2\pi/c)(00\Delta)$] for space group #194

A point representation		Δ point representation
A_1	$\rightarrow$	$\Delta_1 + \Delta_3$
A_2	$\rightarrow$	$\Delta_2 + \Delta_4$
A_3	$\rightarrow$	$\Delta_5 + \Delta_6$
$A_4 + A_5$	$\rightarrow$	$2\Delta_9$
A_6	$\rightarrow$	$\Delta_7 + \Delta_8$

At the A point (D_{6h} symmetry) we have six irreducible representations, three of which are ordinary irreducible representations Γ_1^A, Γ_2^A, Γ_3^A and three of which are double group representations (Γ_4^A, Γ_5^A, Γ_6^A). There are only six classes with nonvanishing characters (see Table D.13) for the A point. We note that all the characters in the group of the wave vector are multiples of 2, consistent with bands sticking together. For example, the compatibility relations given in Table D.14 show Δ point bands sticking together in pairs at the A point. In the plane defined by $\Delta = 1$, containing the A point and the H point among others (see Fig. C.7), the structure factor vanishes and Bragg reflections do not occur.