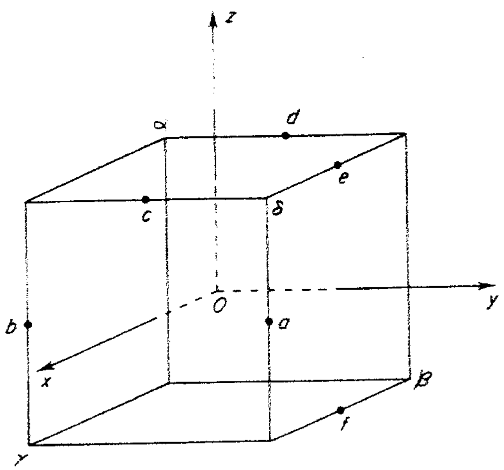
Character Tables of Point Groups

1 The single crystallographic point groups

The 32 crystallographic point groups will be listed in roughly decreasing order of complexity. For each group the following details are given:

(a) ***The group elements***. The notation for rotations is as in Chapter 1, Section 2(a), C_{nj} denoting a proper rotation through $2\pi/n$ in the right-hand screw sense about the axis Oj and I denoting the spatial inversion operator. All the axes involved are indicated in Figures D.1



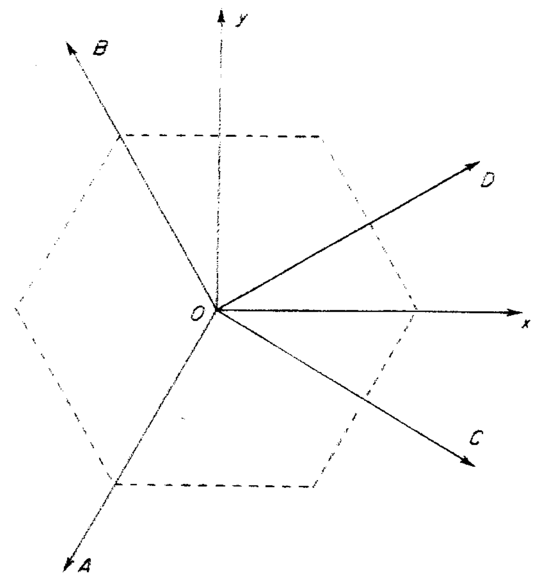


Figure D.2 The axes OA, OB, OC and OD. (All these axes lie in the plane Oxy.)

and D.2. The matrices **R**(T) for every relevant proper rotation are specified in Table D.1. The rotations are listed in classes.

(b) ***The character table***. Several alternative systems of labelling are given, the first column merely giving an arbitrary listing. In the labelling of the second column one-dimensional representations are

$$\mathbf{R}(E)=\begin{bmatrix}1&0&0\\0&1&0\\0&0&1\end{bmatrix},\quad \mathbf{R}(C_{3\alpha})=\begin{bmatrix}0&1&0\\0&0&-1\\-1&0&0\end{bmatrix},$$

$$\mathbf{R}(C_{3\beta})=\begin{bmatrix}0&-1&0\\0&0&-1\\1&0&0\end{bmatrix},\quad \mathbf{R}(C_{3\gamma})=\begin{bmatrix}0&-1&0\\0&0&1\\-1&0&0\end{bmatrix},$$

$$\mathbf{R}(C_{3\delta})=\begin{bmatrix}0&1&0\\0&0&1\\1&0&0\end{bmatrix},\quad \mathbf{R}(C_{3\alpha}^{-1})=\begin{bmatrix}0&0&-1\\1&0&0\\0&-1&0\end{bmatrix},$$

$$\mathbf{R}(C_{3\beta}^{-1})=\begin{bmatrix}0&0&1\\-1&0&0\\0&-1&0\end{bmatrix},\quad \mathbf{R}(C_{3\gamma}^{-1})=\begin{bmatrix}0&0&-1\\-1&0&0\\0&1&0\end{bmatrix},$$

Table D.1 The matrices **R**(T) for the proper rotations T appearing in various crystallographic point groups.

$$R(C_{3\delta}^{-1}) = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}, \quad R(C_{2x}) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix},$$

$$R(C_{2y}) = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}, \quad R(C_{2z}) = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix},$$

$$R(C_{4x}) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{bmatrix}, \quad R(C_{4y}) = \begin{bmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix},$$

$$R(C_{4z}) = \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad R(C_{4x}^{-1}) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix},$$

$$R(C_{4y}^{-1}) = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{bmatrix}, \quad R(C_{4z}^{-1}) = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix},$$

$$R(C_{2a}) = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}, \quad R(C_{2b}) = \begin{bmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix},$$

$$R(C_{2c}) = \begin{bmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \quad R(C_{2d}) = \begin{bmatrix} 0 & 0 & -1 \\ 0 & -1 & 0 \\ -1 & 0 & 0 \end{bmatrix},$$

$$R(C_{2e}) = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}, \quad R(C_{2f}) = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{bmatrix},$$

$$R(C_{3z}) = \begin{bmatrix} -\frac{1}{2} & \frac{1}{2}\sqrt{3} & 0 \\ -\frac{1}{2}\sqrt{3} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad R(C_{3z}^{-1}) = \begin{bmatrix} -\frac{1}{2} & -\frac{1}{2}\sqrt{3} & 0 \\ \frac{1}{2}\sqrt{3} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix},$$

$$R(C_{6z}) = \begin{bmatrix} \frac{1}{2} & \frac{1}{2}\sqrt{3} & 0 \\ -\frac{1}{2}\sqrt{3} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad R(C_{6z}^{-1}) = \begin{bmatrix} \frac{1}{2} & -\frac{1}{2}\sqrt{3} & 0 \\ \frac{1}{2}\sqrt{3} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix},$$

$$R(C_{2A}) = \begin{bmatrix} -\frac{1}{2} & \frac{1}{2}\sqrt{3} & 0 \\ \frac{1}{2}\sqrt{3} & \frac{1}{2} & 0 \\ 0 & 0 & -1 \end{bmatrix}, \quad R(C_{2B}) = \begin{bmatrix} -\frac{1}{2} & -\frac{1}{2}\sqrt{3} & 0 \\ -\frac{1}{2}\sqrt{3} & \frac{1}{2} & 0 \\ 0 & 0 & -1 \end{bmatrix},$$

$$R(C_{2C}) = \begin{bmatrix} \frac{1}{2} & -\frac{1}{2}\sqrt{3} & 0 \\ -\frac{1}{2}\sqrt{3} & -\frac{1}{2} & 0 \\ 0 & 0 & -1 \end{bmatrix}, \quad R(C_{2D}) = \begin{bmatrix} \frac{1}{2} & \frac{1}{2}\sqrt{3} & 0 \\ \frac{1}{2}\sqrt{3} & -\frac{1}{2} & 0 \\ 0 & 0 & -1 \end{bmatrix}.$$

Table D.1 *(continued)*

denoted by A or B, two-dimensional irreducible representations by E and three-dimensional irreducible representations by T, in all cases with subscripts and/or superscripts attached. (The subscripts g and u (standing for ***gerade*** and ***ungerade***) indicated representations that are even and odd under I respectively.) However, pairs of one-dimensional complex conjugate representations are bracketed together and labelled as a two-dimensional representation, as they correspond to degenerate eigenvalues (see Chapter 6, Section 5(*a*) and Chapter 7, Section 3(*f*)).

For a point group that is isomorphic to a group $\mathscr{G}_0(\mathbf{k})$ (see Chapter 9, Section 2(*a*)) for O_h^1, O_h^5 and O_h^9, the third column gives the labelling convention of Bouckaert *et al.* (1936). In such cases the corresponding **k**-vector is as defined in Tables 9.1, 9.2 or 9.3. As described in Chapter 9, Section 2(*b*), it is possible for two or more **k**-vectors in different stars to have point groups $\mathscr{G}_0(\mathbf{k})$ that are isomorphic. The group elements for each such $\mathscr{G}_0(\mathbf{k})$ belonging to O_h^1, O_h^5 and O_h^9 are specified when this occurs.

(*c*) ***Matrices for the irreducible representations of dimension greater than one.*** (Of course these are only unique up to a similarity transformation.) For one-dimensional representations the characters themselves are the matrix elements.

The notation employed for the point groups is that of Schönfliess (1923). More information on these groups may be found in the book of Koster *et al.* (1964), which is wholly devoted to this subject, and in the articles of Altmann (1962, 1963).

(1) O_h:

(*a*) Classes [for $\mathscr{G}_0(\mathbf{k})$ of Γ, H and R]:

$$\mathscr{C}_1 = E;\ \mathscr{C}_2 = C_{3\alpha}, C_{3\beta}, C_{3\gamma}, C_{3\delta}, C_{3\alpha}^{-1}, C_{3\beta}^{-1}, C_{3\gamma}^{-1}, C_{3\delta}^{-1};$$
$$\mathscr{C}_3 = C_{2x}, C_{2y}, C_{2z};\ \mathscr{C}_4 = C_{4x}, C_{4y}, C_{4z}, C_{4x}^{-1}, C_{4y}^{-1}, C_{4z}^{-1};$$
$$\mathscr{C}_5 = C_{2a}, C_{2b}, C_{2c}, C_{2d}, C_{2e}, C_{2f};\ \mathscr{C}_6 = I;$$
$$\mathscr{C}_7 = IC_{3\alpha}, IC_{3\beta}; IC_{3\gamma}, IC_{3\delta}, IC_{3\alpha}^{-1}, IC_{3\beta}^{-1}, IC_{3\gamma}^{-1}, IC_{3\delta}^{-1};$$
$$\mathscr{C}_8 = IC_{2x}, IC_{2y}, IC_{2z};\ \mathscr{C}_9 = IC_{4x}, IC_{4y}, IC_{4z}, IC_{4x}^{-1}, IC_{4y}^{-1}, IC_{4z}^{-1};$$
$$\mathscr{C}_{10} = IC_{2a}, IC_{2b}, IC_{2c}, IC_{2d}, IC_{2e}, IC_{2f}.$$

(*b*) The character table is given in Table D.2.

(*c*) Matrices for irreducible representations of dimension greater

			$\mathscr{C}_1$	$\mathscr{C}_2$	$\mathscr{C}_3$	$\mathscr{C}_4$	$\mathscr{C}_5$	$\mathscr{C}_6$	$\mathscr{C}_7$	$\mathscr{C}_8$	$\mathscr{C}_9$	$\mathscr{C}_{10}$
Γ^1	A_{1g}	$\Gamma_1 H_1 R_1$	1	1	1	1	1	1	1	1	1	1
Γ^2	A_{2g}	$\Gamma_2 H_2 R_2$	1	1	1	−1	−1	1	1	1	−1	−1
Γ^3	E_g	$\Gamma_{12} H_{12} R_{12}$	2	−1	2	0	0	2	−1	2	0	0
Γ^4	T_{1g}	$\Gamma_{15'} H_{15'} R_{15'}$	3	0	−1	1	−1	3	0	−1	1	−1
Γ^5	T_{2g}	$\Gamma_{25'} H_{25'} R_{25'}$	3	0	−1	−1	1	3	0	−1	−1	1
Γ^6	A_{1u}	$\Gamma_{1'} H_{1'} R_{1'}$	1	1	1	1	1	−1	−1	−1	−1	−1
Γ^7	A_{2u}	$\Gamma_{2'} H_{2'} R_{2'}$	1	1	1	−1	−1	−1	−1	−1	1	1
Γ^8	E_u	$\Gamma_{12'} H_{12'} R_{12'}$	2	−1	2	0	0	−2	1	−2	0	0
Γ^9	T_{1u}	$\Gamma_{15} H_{15} R_{15}$	3	0	−1	1	−1	−3	0	1	−1	1
Γ^{10}	T_{2u}	$\Gamma_{25} H_{25} R_{25}$	3	0	−1	−1	1	−3	0	1	1	−1

Table D.2 Character table for O_h.

than one, for any proper rotation C_{nj} of O_h:

$$\mathbf{\Gamma}^3(C_{nj}) = \mathbf{\Gamma}^8(C_{nj}) = \mathbf{\Gamma}''(C_{nj});\ \mathbf{\Gamma}^3(IC_{nj}) = -\mathbf{\Gamma}^8(IC_{nj}) = \mathbf{\Gamma}''(C_{nj});$$

$$\mathbf{\Gamma}^4(C_{nj}) = \mathbf{\Gamma}^9(C_{nj}) = \mathbf{R}(C_{nj});$$

$$\mathbf{\Gamma}^4(IC_{nj}) = -\mathbf{\Gamma}^9(IC_{nj}) = \mathbf{R}(C_{nj});\ \mathbf{\Gamma}^5(C_{nj}) = \mathbf{\Gamma}^{10}(C_{nj}) = \mathbf{\Gamma}'(C_{nj});$$

$$\mathbf{\Gamma}^5(IC_{nj}) = -\mathbf{\Gamma}^{10}(IC_{nj}) = \mathbf{\Gamma}'(C_{nj});$$

where the matrices $\mathbf{\Gamma}'(C_{nj})$, $\mathbf{\Gamma}''(C_{nj})$ and $\mathbf{R}(C_{nj})$ are given in Tables D.3, D.4 and D.1 respectively.

(2) D_{6h}:

(*a*) Classes:

$$\mathscr{C}_1 = E;\ \mathscr{C}_2 = C_{6z}, C_{6z}^{-1};\ \mathscr{C}_3 = C_{3z}, C_{3z}^{-1};\ \mathscr{C}_4 = C_{2z};\ \mathscr{C}_5 = C_{2x}, C_{2A}, C_{2B};$$

$$\mathscr{C}_6 = C_{2y}, C_{2C}, C_{2D};\ \mathscr{C}_7 = I;\ \mathscr{C}_8 = IC_{6z}, IC_{6z}^{-1};\ \mathscr{C}_9 = IC_{3z}, IC_{3z}^{-1};\ \mathscr{C}_{10} = IC_{2z};$$

$$\mathscr{C}_{11} = IC_{2x}, IC_{2A}, IC_{2B};\ \mathscr{C}_{12} = IC_{2y}, IC_{2C}, IC_{2D}.$$

(*b*) The character table is given in Table D.5.

(*c*) Matrices for irreducible representations of dimension greater than one, for any proper rotation C_{nj} of D_{6h}:

$$\mathbf{\Gamma}^5(C_{nj}) = \mathbf{\Gamma}^{11}(C_{nj}) = \mathbf{D}'(C_{nj});\ \mathbf{\Gamma}^5(IC_{nj}) = -\mathbf{\Gamma}^{11}(IC_{nj}) = \mathbf{D}'(C_{nj});$$

$$\mathbf{\Gamma}^6(C_{nj}) = \mathbf{\Gamma}^{12}(C_{nj}) = \mathbf{D}''(C_{nj});\ \mathbf{\Gamma}^6(IC_{nj}) = -\mathbf{\Gamma}^{12}(IC_{nj}) = \mathbf{D}''(C_{nj});$$

where the matrices $\mathbf{D}'(C_{nj})$ and $\mathbf{D}''(C_{nj})$ are given in Tables D.6 and D.7 respectively.

$$\mathbf{\Gamma}'(E) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad \mathbf{\Gamma}'(C_{3\alpha}) = \begin{bmatrix} 0 & -1 & 0 \\ 0 & 0 & 1 \\ -1 & 0 & 0 \end{bmatrix},$$

$$\mathbf{\Gamma}'(C_{3\beta}) = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & -1 \\ -1 & 0 & 0 \end{bmatrix}, \quad \mathbf{\Gamma}'(C_{3\gamma}) = \begin{bmatrix} 0 & -1 & 0 \\ 0 & 0 & -1 \\ 1 & 0 & 0 \end{bmatrix},$$

$$\mathbf{\Gamma}'(C_{3\delta}) = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}, \quad \mathbf{\Gamma}'(C_{3\alpha}^{-1}) = \begin{bmatrix} 0 & 0 & -1 \\ -1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix},$$

$$\mathbf{\Gamma}'(C_{3\beta}^{-1}) = \begin{bmatrix} 0 & 0 & -1 \\ 1 & 0 & 0 \\ 0 & -1 & 0 \end{bmatrix}, \quad \mathbf{\Gamma}'(C_{3\gamma}^{-1}) = \begin{bmatrix} 0 & 0 & 1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \end{bmatrix},$$

$$\mathbf{\Gamma}'(C_{3\delta}^{-1}) = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}, \quad \mathbf{\Gamma}'(C_{2x}) = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix},$$

$$\mathbf{\Gamma}'(C_{2y}) = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad \mathbf{\Gamma}'(C_{2z}) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix},$$

$$\mathbf{\Gamma}'(C_{4x}) = \begin{bmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ -1 & 0 & 0 \end{bmatrix}, \quad \mathbf{\Gamma}'(C_{4y}) = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix},$$

$$\mathbf{\Gamma}'(C_{4z}) = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix}, \quad \mathbf{\Gamma}'(C_{4x}^{-1}) = \begin{bmatrix} 0 & 0 & -1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{bmatrix},$$

$$\mathbf{\Gamma}'(C_{4y}^{-1}) = \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}, \quad \mathbf{\Gamma}'(C_{4z}^{-1}) = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{bmatrix},$$

$$\mathbf{\Gamma}'(C_{2a}) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{bmatrix}, \quad \mathbf{\Gamma}'(C_{2b}) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix},$$

$$\mathbf{\Gamma}'(C_{2c}) = \begin{bmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad \mathbf{\Gamma}'(C_{2d}) = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix},$$

$$\mathbf{\Gamma}'(C_{2e}) = \begin{bmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{bmatrix}, \quad \mathbf{\Gamma}'(C_{2f}) = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix}.$$

Table D.3 The matrices $\mathbf{\Gamma}'$ for O_h, T_d, O, T_h and T.

$$\Gamma''(E) = \Gamma''(C_{2x}) = \Gamma''(C_{2y}) = \Gamma''(C_{2z}) = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix},$$

$$\Gamma''(C_{3\alpha}) = \Gamma''(C_{3\beta}) = \Gamma''(C_{3\gamma}) = \Gamma''(C_{3\delta}) = \begin{bmatrix} -\tfrac{1}{2} & -\tfrac{1}{2}\sqrt{3} \\ \tfrac{1}{2}\sqrt{3} & -\tfrac{1}{2} \end{bmatrix},$$

$$\Gamma''(C_{3\alpha}^{-1}) = \Gamma''(C_{3\beta}^{-1}) = \Gamma''(C_{3\gamma}^{-1}) = \Gamma''(C_{3\delta}^{-1}) = \begin{bmatrix} -\tfrac{1}{2} & \tfrac{1}{2}\sqrt{3} \\ -\tfrac{1}{2}\sqrt{3} & -\tfrac{1}{2} \end{bmatrix},$$

$$\Gamma''(C_{4x}) = \Gamma''(C_{4x}^{-1}) = \Gamma''(C_{2e}) = \Gamma''(C_{2f}) = \begin{bmatrix} \tfrac{1}{2} & -\tfrac{1}{2}\sqrt{3} \\ -\tfrac{1}{2}\sqrt{3} & -\tfrac{1}{2} \end{bmatrix},$$

$$\Gamma''(C_{4y}) = \Gamma''(C_{4y}^{-1}) = \Gamma''(C_{2c}) = \Gamma''(C_{2d}) = \begin{bmatrix} \tfrac{1}{2} & \tfrac{1}{2}\sqrt{3} \\ \tfrac{1}{2}\sqrt{3} & -\tfrac{1}{2} \end{bmatrix},$$

$$\Gamma''(C_{4z}) = \Gamma''(C_{4z}^{-1}) = \Gamma''(C_{2a}) = \Gamma''(C_{2b}) = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}.$$

Table D.4 The matrices $\mathbf{\Gamma}''$ for O_h, T_d, O, D_{3d} and C_{3v}.

		$\mathscr{C}_1$	$\mathscr{C}_2$	$\mathscr{C}_3$	$\mathscr{C}_4$	$\mathscr{C}_5$	$\mathscr{C}_6$	$\mathscr{C}_7$	$\mathscr{C}_8$	$\mathscr{C}_9$	$\mathscr{C}_{10}$	$\mathscr{C}_{11}$	$\mathscr{C}_{12}$
Γ^1	A_{1g}	1	1	1	1	1	1	1	1	1	1	1	1
Γ^2	A_{2g}	1	1	1	1	−1	−1	1	1	1	1	−1	−1
Γ^3	B_{1g}	1	−1	1	−1	1	−1	1	−1	1	−1	1	−1
Γ^4	B_{2g}	1	−1	1	−1	−1	1	1	−1	1	−1	−1	1
Γ^5	E_{2g}	2	−1	−1	2	0	0	2	−1	−1	2	0	0
Γ^6	E_{1g}	2	1	−1	−2	0	0	2	1	−1	−2	0	0
Γ^7	A_{1u}	1	1	1	1	1	1	−1	−1	−1	−1	−1	−1
Γ^8	A_{2u}	1	1	1	1	−1	−1	−1	−1	−1	−1	1	1
Γ^9	B_{1u}	1	−1	1	−1	1	−1	−1	1	−1	1	−1	1
Γ^{10}	B_{2u}	1	−1	1	−1	−1	1	−1	1	−1	1	1	−1
Γ^{11}	E_{2u}	2	−1	−1	2	0	0	−2	1	1	−2	0	0
Γ^{12}	E_{1u}	2	1	−1	−2	0	0	−2	−1	1	2	0	0

Table D.5 Character table for D_{6h}.

$$\mathbf{D}'(E) = \mathbf{D}'(C_{2z}) = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \qquad \mathbf{D}'(C_{6z}) = \mathbf{D}'(C_{3z}^{-1}) = \begin{bmatrix} -\tfrac{1}{2} & -\tfrac{1}{2}\sqrt{3} \\ \tfrac{1}{2}\sqrt{3} & -\tfrac{1}{2} \end{bmatrix},$$

$$\mathbf{D}'(C_{6z}^{-1}) = \mathbf{D}'(C_{3z}) = \begin{bmatrix} -\tfrac{1}{2} & \tfrac{1}{2}\sqrt{3} \\ -\tfrac{1}{2}\sqrt{3} & -\tfrac{1}{2} \end{bmatrix}, \qquad \mathbf{D}'(C_{2x}) = \mathbf{D}'(C_{2y}) = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix},$$

$$\mathbf{D}'(C_{2A}) = \mathbf{D}'(C_{2C}) = \begin{bmatrix} \tfrac{1}{2} & -\tfrac{1}{2}\sqrt{3} \\ -\tfrac{1}{2}\sqrt{3} & -\tfrac{1}{2} \end{bmatrix}, \qquad \mathbf{D}'(C_{2B}) = \mathbf{D}'(C_{2D}) = \begin{bmatrix} \tfrac{1}{2} & \tfrac{1}{2}\sqrt{3} \\ \tfrac{1}{2}\sqrt{3} & -\tfrac{1}{2} \end{bmatrix}.$$

Table D.6 The matrices $\mathbf{D}'$ for D_{6h}, D_{3h}, C_{6v} and D_6.

$$\mathbf{D}''(E) = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \qquad \mathbf{D}''(C_{6z}) = \begin{bmatrix} \tfrac{1}{2} & \tfrac{1}{2}\sqrt{3} \\ -\tfrac{1}{2}\sqrt{3} & \tfrac{1}{2} \end{bmatrix},$$

$$\mathbf{D}''(C_{6z}^{-1}) = \begin{bmatrix} \tfrac{1}{2} & -\tfrac{1}{2}\sqrt{3} \\ \tfrac{1}{2}\sqrt{3} & \tfrac{1}{2} \end{bmatrix}, \qquad \mathbf{D}''(C_{3z}) = \begin{bmatrix} -\tfrac{1}{2} & \tfrac{1}{2}\sqrt{3} \\ -\tfrac{1}{2}\sqrt{3} & -\tfrac{1}{2} \end{bmatrix},$$

$$\mathbf{D}''(C_{3z}^{-1}) = \begin{bmatrix} -\tfrac{1}{2} & -\tfrac{1}{2}\sqrt{3} \\ \tfrac{1}{2}\sqrt{3} & -\tfrac{1}{2} \end{bmatrix}, \qquad \mathbf{D}''(C_{2z}) = \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix},$$

$$\mathbf{D}''(C_{2x}) = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \qquad \mathbf{D}''(C_{2A}) = \begin{bmatrix} -\tfrac{1}{2} & \tfrac{1}{2}\sqrt{3} \\ \tfrac{1}{2}\sqrt{3} & \tfrac{1}{2} \end{bmatrix},$$

$$\mathbf{D}''(C_{2B}) = \begin{bmatrix} -\tfrac{1}{2} & -\tfrac{1}{2}\sqrt{3} \\ -\tfrac{1}{2}\sqrt{3} & \tfrac{1}{2} \end{bmatrix}, \qquad \mathbf{D}''(C_{2y}) = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix},$$

$$\mathbf{D}''(C_{2C}) = \begin{bmatrix} \tfrac{1}{2} & -\tfrac{1}{2}\sqrt{3} \\ -\tfrac{1}{2}\sqrt{3} & -\tfrac{1}{2} \end{bmatrix}, \qquad \mathbf{D}''(C_{2D}) = \begin{bmatrix} \tfrac{1}{2} & \tfrac{1}{2}\sqrt{3} \\ \tfrac{1}{2}\sqrt{3} & -\tfrac{1}{2} \end{bmatrix}.$$

Table D.7 The matrices $\mathbf{D}''$ for D_{6h}, C_{6v}, D_6 and D_3.

(3) T_d:

(*a*) Classes [for $\mathscr{G}_0(\mathbf{k})$ of *P*]:

$$\mathscr{C}_1 = E,\ \mathscr{C}_2 = C_{3\alpha}, C_{3\beta}, C_{3\gamma}, C_{3\delta}, C_{3\alpha}^{-1}, C_{3\beta}^{-1}, C_{3\gamma}^{-1}, C_{3\delta}^{-1};$$

$$\mathscr{C}_3 = C_{2x}, C_{2y}, C_{2z};\ \mathscr{C}_4 = IC_{4x}, IC_{4y}, IC_{4z}, IC_{4x}^{-1}, IC_{4y}^{-1}, IC_{4z}^{-1};$$

$$\mathscr{C}_5 = IC_{2a}, IC_{2b}, IC_{2c}, IC_{2d}, IC_{2e}, IC_{2f}.$$

(*b*) The character table is given in Table D.8.

(*c*) Matrices for irreducible representations of dimension greater than one, for proper rotations C_{nj} of T_d:

$$\mathbf{\Gamma}^3(C_{nj}) = \mathbf{\Gamma}''(C_{nj});\ \mathbf{\Gamma}^4(C_{nj}) = \mathbf{R}(C_{nj});\ \mathbf{\Gamma}^5(C_{nj}) = \mathbf{\Gamma}'(C_{nj});$$

and for the improper rotations IC_{nj} of T_d:

$$\mathbf{\Gamma}^3(IC_{nj}) = -\mathbf{\Gamma}''(C_{nj});\ \mathbf{\Gamma}^4(IC_{nj}) = -\mathbf{R}(C_{nj});\ \mathbf{\Gamma}^5(IC_{nj}) = -\mathbf{\Gamma}'(C_{nj});$$

where the matrices $\mathbf{\Gamma}'(C_{nj})$, $\mathbf{\Gamma}''(C_{nj})$ and $\mathbf{R}(C_{nj})$ are given in Tables D.3, D.4 and D.1 respectively.

			$\mathscr{C}_1$	$\mathscr{C}_2$	$\mathscr{C}_3$	$\mathscr{C}_4$	$\mathscr{C}_5$
Γ^1	A_1	P_1	1	1	1	1	1
Γ^2	A_2	P_2	1	1	1	−1	−1
Γ^3	E	P_3	2	−1	2	0	0
Γ^4	T_2	P_4	3	0	−1	−1	1
Γ^5	T_1	P_5	3	0	−1	1	−1

Table D.8 Character table for T_d and O.

(4) O:

(*a*) Classes:

$$\mathscr{C}_1 = E;\ \mathscr{C}_2 = C_{3\alpha}, C_{3\beta}, C_{3\gamma}, C_{3\delta}, C_{3\alpha}^{-1}, C_{3\beta}^{-1}, C_{3\gamma}^{-1}, C_{3\delta}^{-1};$$

$$\mathscr{C}_3 = C_{2x}, C_{2y}, C_{2z};\ \mathscr{C}_4 = C_{4x}, C_{4y}, C_{4z}, C_{4x}^{-1}, C_{4y}^{-1}, C_{4z}^{-1};$$

$$\mathscr{C}_5 = C_{2a}, C_{2b}, C_{2c}, C_{2d}, C_{2e}, C_{2f}.$$

(*b*) The character table is given in Table D.8.
(*c*) Matrices for irreducible representations of dimension greater than one, for all rotations C_{nj} of O:

$$\mathbf{\Gamma}^3(C_{nj}) = \mathbf{\Gamma}''(C_{nj});\ \mathbf{\Gamma}^4(C_{nj}) = \mathbf{\Gamma}'(C_{nj});\ \mathbf{\Gamma}^5(C_{nj}) = \mathbf{R}(C_{nj});$$

where the matrices $\mathbf{\Gamma}'(C_{nj})$, $\mathbf{\Gamma}''(C_{nj})$ and $\mathbf{R}(C_{nj})$ are given in Tables D.3, D.4 and D.1 respectively.

(5) T_h:

(*a*) Classes:

$$\mathscr{C}_1 = E;\ \mathscr{C}_2 = C_{3\alpha}, C_{3\beta}, C_{3\gamma}, C_{3\delta};\ \mathscr{C}_3 = C_{3\alpha}^{-1}, C_{3\beta}^{-1}, C_{3\gamma}^{-1}, C_{3\delta}^{-1};$$

$$\mathscr{C}_4 = C_{2x}, C_{2y}, C_{2z};\ \mathscr{C}_5 = I;\ \mathscr{C}_6 = IC_{3\alpha}, IC_{3\beta}, IC_{3\gamma}, IC_{3\delta};$$

$$\mathscr{C}_7 = IC_{3\alpha}^{-1}, IC_{3\beta}^{-1}, IC_{3\gamma}^{-1}, IC_{3\delta}^{-1},\ \mathscr{C}_8 = IC_{2x}, IC_{2y}, IC_{2z}.$$

(*b*) The character table is given in Table D.9.
(*c*) Matrices for irreducible representations of dimension greater than one, for any proper rotation C_{nj} of T_h:

$$\mathbf{\Gamma}^4(C_{nj}) = \mathbf{\Gamma}^8(C_{nj}) = \mathbf{\Gamma}'(C_{nj});\ \mathbf{\Gamma}^4(IC_{nj}) = -\mathbf{\Gamma}^8(IC_{nj}) = \mathbf{\Gamma}'(C_{nj});$$

where the matrices $\mathbf{\Gamma}'(C_{nj})$ are given in Table D.3.

		$\mathscr{C}_1$	$\mathscr{C}_2$	$\mathscr{C}_3$	$\mathscr{C}_4$	$\mathscr{C}_5$	$\mathscr{C}_6$	$\mathscr{C}_7$	$\mathscr{C}_8$
Γ^1	A_g	1	1	1	1	1	1	1	1
Γ^2	E_g	1	ϕ	ϕ^2	1	1	ϕ	ϕ^2	1
Γ^3	E_g	1	ϕ^2	ϕ	1	1	ϕ^2	ϕ	1
Γ^4	T_g	3	0	0	−1	3	0	0	−1
Γ^5	A_u	1	1	1	1	−1	−1	−1	−1
Γ^6	E_u	1	ϕ	ϕ^2	1	−1	$-\phi$	$-\phi^2$	−1
Γ^7	E_u	1	ϕ^2	ϕ	1	−1	$-\phi^2$	$-\phi$	−1
Γ^8	T_u	3	0	0	−1	−3	0	0	1

Table D.9 Character table for T_h ($\phi = \exp(\frac{2}{3}\pi i)$).

			$\mathscr{C}_1$	$\mathscr{C}_2$	$\mathscr{C}_3$	$\mathscr{C}_4$	$\mathscr{C}_5$	$\mathscr{C}_6$	$\mathscr{C}_7$	$\mathscr{C}_8$	$\mathscr{C}_9$	$\mathscr{C}_{10}$
Γ^1	A_{1g}	X_1, M_1	1	1	1	1	1	1	1	1	1	1
Γ^2	B_{1g}	X_2, M_2	1	1	1	−1	−1	1	1	1	−1	−1
Γ^3	B_{2g}	X_3, M_3	1	−1	1	−1	1	1	−1	1	−1	1
Γ^4	A_{2g}	X_4, M_4	1	−1	1	1	−1	1	−1	1	1	−1
Γ^5	E_g	X_5, M_5	2	0	−2	0	0	2	0	−2	0	0
Γ^6	A_{1u}	$X_{1'}, M_{1'}$	1	1	1	1	1	−1	−1	−1	−1	−1
Γ^7	B_{1u}	$X_{2'}, M_{2'}$	1	1	1	−1	−1	−1	−1	−1	1	1
Γ^8	B_{2u}	$X_{3'}, M_{3'}$	1	−1	1	−1	1	−1	1	−1	1	−1
Γ^9	A_{2u}	$X_{4'}, M_{4'}$	1	−1	1	1	−1	−1	1	−1	−1	1
Γ^{10}	E_u	$X_{5'}, M_{5'}$	2	0	−2	0	0	−2	0	2	0	0

Table D.10 Character table for D_{4h}.

(6) D_{4h}:

(*a*) Classes [for $\mathscr{G}_0(\mathbf{k})$ of *X*]:

$$\mathscr{C}_1 = E;\ \mathscr{C}_2 = C_{2x}, C_{2y};\ \mathscr{C}_3 = C_{2z};\ \mathscr{C}_4 = C_{4z}, C_{4z}^{-1};$$

$$\mathscr{C}_5 = C_{2a}, C_{2b};\ \mathscr{C}_6 = I;\ \mathscr{C}_7 = IC_{2x}, IC_{2y};\ \mathscr{C}_8 = IC_{2z};\ \mathscr{C}_9 = IC_{4z}, IC_{4z}^{-1};$$

$$\mathscr{C}_{10} = IC_{2a}, IC_{2b}.$$

Classes [for $\mathscr{G}_0(\mathbf{k})$ of *M*]:

$$\mathscr{C}_1 = E,\ \mathscr{C}_2 = C_{2y}, C_{2z};\ \mathscr{C}_3 = C_{2x};\ \mathscr{C}_4 = C_{4x}, C_{4x}^{-1};\ \mathscr{C}_5 = C_{2e}, C_{2f};\ \mathscr{C}_6 = I;$$

$$\mathscr{C}_7 = IC_{2y}, IC_{2z};\ \mathscr{C}_8 = IC_{2x};\ \mathscr{C}_9 = IC_{4x}, IC_{4x}^{-1};\ \mathscr{C}_{10} = IC_{2e}, IC_{2f}.$$

(*b*) The character table is given in Table D.10.
(*c*) Matrices for irreducible representations of dimension greater than one, for any proper rotation C_{nj} of D_{4h}:

$$\mathbf{\Gamma}^5(C_{nj}) = \mathbf{\Gamma}^{10}(C_{nj}) = \mathbf{D}(C_{nj});\ \mathbf{\Gamma}^5(IC_{nj}) = -\mathbf{\Gamma}^{10}(IC_{nj}) = \mathbf{D}(C_{nj});$$

where for $\mathscr{G}_0(\mathbf{k})$ of *M* the matrices $\mathbf{D}(C_{nj})$ are given in Table D.11, while for $\mathscr{G}_0(\mathbf{k})$ of *X* they are given in Table D.12.

$$\mathbf{D}(E) = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix},\quad \mathbf{D}(C_{2x}) = \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix},\quad \mathbf{D}(C_{2y}) = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix},$$

$$\mathbf{D}(C_{2z}) = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix},\quad \mathbf{D}(C_{4x}) = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix},\quad \mathbf{D}(C_{4x}^{-1}) = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix},$$

$$\mathbf{D}(C_{2e}) = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix},\quad \mathbf{D}(C_{2f}) = \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix}.$$

Table D.11 The matrices **D** for D_{4h} for $\mathscr{G}_0(\mathbf{k})$ of *M*.

$$\mathbf{D}(E)=\begin{bmatrix}1&0\\0&1\end{bmatrix},\quad \mathbf{D}(C_{2x})=\begin{bmatrix}1&0\\0&-1\end{bmatrix},\quad \mathbf{D}(C_{2y})=\begin{bmatrix}-1&0\\0&1\end{bmatrix},$$

$$\mathbf{D}(C_{2z})=\begin{bmatrix}-1&0\\0&-1\end{bmatrix},\quad \mathbf{D}(C_{4z})=\begin{bmatrix}0&1\\-1&0\end{bmatrix},\quad \mathbf{D}(C_{4z}^{-1})=\begin{bmatrix}0&-1\\1&0\end{bmatrix},$$

$$\mathbf{D}(C_{2a})=\begin{bmatrix}0&1\\1&0\end{bmatrix},\quad \mathbf{D}(C_{2b})=\begin{bmatrix}0&-1\\-1&0\end{bmatrix}.$$

Table D.12 The matrices $\mathbf{D}$ for D_{4h} for $\mathscr{G}_0(\mathbf{k})$ of X.

(7) D_{3h}:

(*a*) Classes

$$\mathscr{C}_1=E;\ \mathscr{C}_2=C_{3z}, C_{3z}^{-1};\ \mathscr{C}_3=C_{2x}, C_{2A}, C_{2B};\ \mathscr{C}_4=IC_{2z};\ \mathscr{C}_5=IC_{6z}, IC_{6z}^{-1};$$
$$\mathscr{C}_6=IC_{2y}, IC_{2C}, IC_{2D}.$$

(*b*) The character table is given in Table D.13.

(*c*) Matrices for irreducible representations of dimension greater than one, for any proper rotation C_{nj} of D_{3h}:

$$\Gamma^3(C_{nj})=\Gamma^6(C_{nj})=\mathbf{D}'(C_{nj});$$

and for any improper rotation IC_{nj} of D_{3h}:

$$\Gamma^3(IC_{nj})=-\Gamma^6(IC_{nj})=\mathbf{D}'(C_{nj});$$

where the matrices $\mathbf{D}'(C_{nj})$ are given in Table D.6.

(8) D_{3d}:

(*a*) Classes [for $\mathscr{G}_0(\mathbf{k})$ of L]:

$$\mathscr{C}_1=E;\ \mathscr{C}_2=C_{3\delta}, C_{3\delta}^{-1};\ \mathscr{C}_3=C_{2b}, C_{2d}, C_{2f};\ \mathscr{C}_4=I;\ \mathscr{C}_5=IC_{3\delta}, IC_{3\delta}^{-1};$$
$$\mathscr{C}_6=IC_{2b}, IC_{2d}, IC_{2f}.$$

(*b*) The character table is given in Table D.13.

	D_{3h}	D_{3d}	C_{6v}	D_6		$\mathscr{C}_1$	$\mathscr{C}_2$	$\mathscr{C}_3$	$\mathscr{C}_4$	$\mathscr{C}_5$	$\mathscr{C}_6$
Γ^1	A_1'	A_{1g}	A_1	A_1	L_1	1	1	1	1	1	1
Γ^2	A_2'	A_{2g}	A_2	A_2	L_2	1	1	−1	1	1	−1
Γ^3	E'	E_g	E_2	E_2	L_3	2	−1	0	2	−1	0
Γ^4	A_1''	A_{1u}	B_1	B_1	L_1'	1	1	1	−1	−1	−1
Γ^5	A_2''	A_{2u}	B_2	B_2	L_2'	1	1	−1	−1	−1	1
Γ^6	E''	E_u	E_1	E_1	L_3'	2	−1	0	−2	1	0

Table D.13 Character table for D_{3h}, D_{3d}, C_{6v} and D_6.

(*c*) Matrices for irreducible representations of dimension greater than one, for any proper rotation C_{nj} of D_{3d}:

$$\Gamma^3(C_{nj})=\Gamma^6(C_{nj})=\Gamma''(C_{nj});\ \Gamma^3(IC_{nj})=-\Gamma^6(IC_{nj})=\Gamma''(C_{nj});$$

where the matrices $\Gamma''(C_{nj})$ are given in Table D.4.

(9) C_{6v}:

(*a*) Classes:

$$\mathscr{C}_1=E;\ \mathscr{C}_2=C_{3z}, C_{3z}^{-1};\ \mathscr{C}_3=IC_{2x}, IC_{2A}, IC_{2B};\ \mathscr{C}_4=C_{2z};$$
$$\mathscr{C}_5=C_{6z}, C_{6z}^{-1};\ \mathscr{C}_6=IC_{2y}, IC_{2C}, IC_{2D}.$$

(*b*) The character table is given in Table D.13.

(*c*) Matrices for irreducible representations of dimension greater than one, for any proper rotation C_{nj} of C_{6v}:

$$\Gamma^6(C_{nj})=\mathbf{D}''(C_{nj});\ \Gamma^3(C_{nj})=\mathbf{D}'(C_{nj});$$

and for any improper rotation IC_{nj} of C_{6v}:

$$\Gamma^6(IC_{nj})=\mathbf{D}''(C_{nj});\ \Gamma^3(IC_{nj})=\mathbf{D}'(C_{nj});$$

where the matrices $\mathbf{D}'(C_{nj})$ and $\mathbf{D}''(C_{nj})$ are given in Tables D.6 and D.7 respectively.

(10) C_{6h}:

(*a*) Classes:

$$\mathscr{C}_1=E;\ \mathscr{C}_2=C_{6z};\ \mathscr{C}_3=C_{3z};\ \mathscr{C}_4=C_{2z};\ \mathscr{C}_5=C_{3z}^{-1};\ \mathscr{C}_6=C_{6z}^{-1};\ \mathscr{C}_7=I;$$
$$\mathscr{C}_8=IC_{6z};\ \mathscr{C}_9=IC_{3z};\ \mathscr{C}_{10}=IC_{2z};\ \mathscr{C}_{11}=IC_{3z}^{-1};\ \mathscr{C}_{12}=IC_{6z}^{-1}.$$

(*b*) The character table is given in Table D.14.

(11) D_6:

(*a*) Classes:

$$\mathscr{C}_1=E;\ \mathscr{C}_2=C_{3z}, C_{3z}^{-1};\ \mathscr{C}_3=C_{2x}, C_{2A}, C_{2B};\ \mathscr{C}_4=C_{2z};\ \mathscr{C}_5=C_{6z}, C_{6z}^{-1};$$
$$\mathscr{C}_6=C_{2y}, C_{2C}, C_{2D}.$$

(*b*) The character table is given in Table D.13.

(*c*) Matrices for irreducible representations of dimension greater than one, for any rotation C_{nj} of D_6:

$$\Gamma^6(C_{nj})=\mathbf{D}''(C_{nj});\ \Gamma^3(C_{nj})=\mathbf{D}'(C_{nj});$$

where the matrices $\mathbf{D}'(C_{nj})$ and $\mathbf{D}''(C_{nj})$ are given in Tables D.6 and D.7 respectively.

		$\mathscr{C}_1$	$\mathscr{C}_2$	$\mathscr{C}_3$	$\mathscr{C}_4$	$\mathscr{C}_5$	$\mathscr{C}_6$	$\mathscr{C}_7$	$\mathscr{C}_8$	$\mathscr{C}_9$	$\mathscr{C}_{10}$	$\mathscr{C}_{11}$	$\mathscr{C}_{12}$
Γ^1	A_g	1	1	1	1	1	1	1	1	1	1	1	1
Γ^2	B_g	1	−1	1	−1	1	−1	1	−1	1	−1	1	−1
Γ^3	E'_g {	1	ω	ω^2	−1	$-\omega$	$-\omega^2$	1	ω	ω^2	−1	$-\omega$	$-\omega^2$
Γ^4		1	$-\omega^2$	$-\omega$	−1	ω^2	ω	1	$-\omega^2$	$-\omega$	−1	ω^2	ω
Γ^5	E''_g {	1	ω^2	$-\omega$	1	ω^2	$-\omega$	1	ω^2	$-\omega$	1	ω^2	$-\omega$
Γ^6		1	$-\omega$	ω^2	1	$-\omega$	ω^2	1	$-\omega$	ω^2	1	$-\omega$	ω^2
Γ^7	A_u	1	1	1	1	1	1	−1	−1	−1	−1	−1	−1
Γ^8	B_u	1	−1	1	−1	1	−1	−1	1	−1	1	−1	1
Γ^9	E'_u {	1	ω	ω^2	−1	$-\omega$	$-\omega^2$	−1	$-\omega$	$-\omega^2$	1	ω	ω^2
Γ^{10}		1	$-\omega^2$	$-\omega$	−1	ω^2	ω	−1	ω^2	ω	1	$-\omega^2$	$-\omega$
Γ^{11}	E''_u {	1	ω^2	$-\omega$	1	ω^2	$-\omega$	−1	$-\omega^2$	ω	−1	$-\omega^2$	ω
Γ^{12}		1	$-\omega$	ω^2	1	$-\omega$	ω^2	−1	ω	$-\omega^2$	−1	ω	$-\omega^2$

Table D.14 Character table for C_{6h} ($\omega = \exp(\frac{1}{3}\pi i)$).

(12) T:

(*a*) Classes:

$$\mathscr{C}_1 = E;\ \mathscr{C}_2 = C_{3\alpha}, C_{3\beta}, C_{3\gamma}, C_{3\delta};\ \mathscr{C}_3 = C_{3\alpha}^{-1}, C_{3\beta}^{-1}, C_{3\gamma}^{-1}, C_{3\delta}^{-1};$$
$$\mathscr{C}_4 = C_{2x}, C_{2y}, C_{2z}.$$

(*b*) The character table is given in Table D.15.

(*c*) Matrices for irreducible representation of dimension greater than one, for any rotation C_{nj} of T:

$$\Gamma^4(C_{nj}) = \Gamma'(C_{nj});$$

where the matrices $\Gamma'(C_{nj})$ are given in Table D.3.

(13) D_{2h} or V_h:

(*a*) Classes [for $\mathscr{G}_0(\mathbf{k})$ of *N*]:

$$\mathscr{C}_1 = E;\ \mathscr{C}_2 = C_{2x};\ \mathscr{C}_3 = C_{2e};\ \mathscr{C}_4 = C_{2f};\ \mathscr{C}_5 = I;\ \mathscr{C}_6 = IC_{2x};$$
$$\mathscr{C}_7 = IC_{2e};\ \mathscr{C}_8 = IC_{2f}.$$

(*b*) The character table is given in Table D.16.

		$\mathscr{C}_1$	$\mathscr{C}_2$	$\mathscr{C}_3$	$\mathscr{C}_4$
Γ^1	A	1	1	1	1
Γ^2	E {	1	ϕ	ϕ^2	1
Γ^3		1	ϕ^2	ϕ	1
Γ^4	T	3	0	0	−1

Table D.15 Character table for T ($\phi = \exp(\frac{2}{3}\pi i)$).

			$\mathscr{C}_1$	$\mathscr{C}_2$	$\mathscr{C}_3$	$\mathscr{C}_4$	$\mathscr{C}_5$	$\mathscr{C}_6$	$\mathscr{C}_7$	$\mathscr{C}_8$
Γ^1	A_{1g}	N_1	1	1	1	1	1	1	1	1
Γ^2	B_{1g}	N_2	1	−1	1	−1	1	−1	1	−1
Γ^3	B_{2g}	N_3	1	−1	−1	1	1	−1	−1	1
Γ^4	B_{3g}	N_4	1	1	−1	−1	1	1	−1	−1
Γ^5	A_{1u}	$N_{2'}$	1	1	1	1	−1	−1	−1	−1
Γ^6	B_{1u}	$N_{1'}$	1	−1	1	−1	−1	1	−1	1
Γ^7	B_{2u}	$N_{4'}$	1	−1	−1	1	−1	1	1	−1
Γ^8	B_{3u}	$N_{3'}$	1	1	−1	−1	−1	−1	1	1

Table D.16 Character table for D_{2h}.

(14) C_{4v}:

(*a*) Classes [for $\mathscr{G}_0(\mathbf{k})$ of Δ]:

$$\mathscr{C}_1 = E;\ \mathscr{C}_2 = C_{2z};\ \mathscr{C}_3 = C_{4z}, C_{4z}^{-1};\ \mathscr{C}_4 = IC_{2x}, IC_{2y};\ \mathscr{C}_5 = IC_{2a}, IC_{2b}.$$

Classes [for $\mathscr{G}_0(\mathbf{k})$ of *T*]:

$$\mathscr{C}_1 = E;\ \mathscr{C}_2 = C_{2x};\ \mathscr{C}_3 = C_{4x}, C_{4x}^{-1};\ \mathscr{C}_4 = IC_{2y}, IC_{2z};\ \mathscr{C}_5 = IC_{2e}, IC_{2f}.$$

(*b*) The character table is given in Table D.17.

(*c*) Matrices for irreducible representation of dimension greater than one, for any proper rotation C_{nj} of C_{4v}:

$$\Gamma^5(C_{nj}) = \mathbf{D}(C_{nj});$$

and for any improper rotation IC_{nj} of C_{4v}:

$$\Gamma^5(IC_{nj}) = -\mathbf{D}(C_{nj});$$

where for $\mathscr{G}_0(\mathbf{k})$ of Δ the matrices $\mathbf{D}(C_{nj})$ are given in Table D.12, while for $\mathscr{G}_0(\mathbf{k})$ of *T* they are given in Table D.11.

				$\mathscr{C}_1$	$\mathscr{C}_2$	$\mathscr{C}_3$	$\mathscr{C}_4$	$\mathscr{C}_5$
Γ^1	A_1	$\Delta_1, T_1,$	W_1	1	1	1	1	1
Γ^2	B_1	$\Delta_2, T_2,$	$W_{2'}$	1	1	−1	1	−1
Γ^3	A_2	$\Delta_{1'}, T_{1'},$	W_2	1	1	1	−1	−1
Γ^4	B_2	$\Delta_{2'}, T_{2'},$	$W_{1'}$	1	1	−1	−1	1
Γ^5	E	$\Delta_5, T_5,$	W_3	2	−2	0	0	0

Table D.17 Character table for C_{4v}, D_4 and D_{2d}.

(15) D_4:

(*a*) Classes:

$$\mathscr{C}_1 = E;\ \mathscr{C}_2 = C_{2y};\ \mathscr{C}_3 = C_{4y}, C_{4y}^{-1},\ \mathscr{C}_4 = C_{2x}, C_{2z};\ \mathscr{C}_5 = C_{2c}, C_{2d}.$$

(*b*) The character table is given in Table D.17.

(*c*) Matrices for irreducible representation of dimension greater than one, for any rotation C_{nj} of D_4:

$$\Gamma^5(C_{nj}) = \mathbf{S}(C_{nj});$$

where the matrices $\mathbf{S}(C_{nj})$ are given in Table D.18.

(16) D_{2d} or V_d:

(*a*) Classes [for $\mathscr{G}_0(\mathbf{k})$ of W]:

$$\mathscr{C}_1 = E;\ \mathscr{C}_2 = C_{2y};\ \mathscr{C}_3 = IC_{4y}, IC_{4y}^{-1};\ \mathscr{C}_4 = IC_{2x}, IC_{2z};\ \mathscr{C}_5 = C_{2c}, C_{2d}.$$

(*b*) The character table is given in Table D.17.

(*c*) Matrices for irreducible representation of dimension greater than one, for any proper rotation C_{nj} of D_{2d}:

$$\Gamma^5(C_{nj}) = \mathbf{S}(C_{nj});$$

and for any improper rotation IC_{nj} of D_{2d}:

$$\Gamma^5(IC_{nj}) = -\mathbf{S}(C_{nj});$$

where the matrices $\mathbf{S}(C_{nj})$ are given in Table D.18.

(17) C_{4h}:

(*a*) Classes:

$$\mathscr{C}_1 = E;\ \mathscr{C}_2 = C_{4z};\ \mathscr{C}_3 = C_{2z};\ \mathscr{C}_4 = C_{4z}^{-1};\ \mathscr{C}_5 = I;\ \mathscr{C}_6 = IC_{4z};$$
$$\mathscr{C}_7 = IC_{2z};\ \mathscr{C}_8 = IC_{4z}^{-1}.$$

(*b*) The character table is given in Table D.19.

$$\mathbf{S}(E) = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix},\quad \mathbf{S}(C_{2y}) = \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix},\quad \mathbf{S}(C_{2c}) = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix},$$

$$\mathbf{S}(C_{2d}) = \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix},\quad \mathbf{S}(C_{4y}) = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix},\quad \mathbf{S}(C_{4y}^{-1}) = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix},$$

$$\mathbf{S}(C_{2x}) = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix},\quad \mathbf{S}(C_{2z}) = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}.$$

Table D.18 The matrices **S** for D_4 and D_{2d}.

		$\mathscr{C}_1$	$\mathscr{C}_2$	$\mathscr{C}_3$	$\mathscr{C}_4$	$\mathscr{C}_5$	$\mathscr{C}_6$	$\mathscr{C}_7$	$\mathscr{C}_8$
Γ^1	A_g	1	1	1	1	1	1	1	1
Γ^2	B_g	1	−1	1	−1	1	−1	1	−1
Γ^3	E_g	1	i	−1	$-i$	1	i	−1	$-i$
Γ^4		1	$-i$	−1	i	1	$-i$	−1	i
Γ^5	A_u	1	1	1	1	−1	−1	−1	−1
Γ^6	B_u	1	−1	1	−1	−1	1	−1	1
Γ^7	E_u	1	i	−1	$-i$	−1	$-i$	1	i
Γ^8		1	$-i$	−1	i	−1	i	1	$-i$

Table D.19 Character table for C_{4h}.

(18) C_{3h}:

(*a*) Classes:

$$\mathscr{C}_1 = E;\ \mathscr{C}_2 = IC_{6z};\ \mathscr{C}_3 = C_{3z};\ \mathscr{C}_4 = IC_{2z};\ \mathscr{C}_5 = C_{3z};\ \mathscr{C}_6 = IC_{6z}^{-1}.$$

(*b*) The character table is given in Table D.20.

	C_{3h}	C_{3i}	C_6	$\mathscr{C}_1$	$\mathscr{C}_2$	$\mathscr{C}_3$	$\mathscr{C}_4$	$\mathscr{C}_5$	$\mathscr{C}_6$
Γ^1	A′	A_g	A	1	1	1	1	1	1
Γ^2	A″	A_u	B	1	−1	1	−1	1	−1
Γ^3	E″	E_u	E′	1	ω	ω^2	−1	$-\omega$	$-\omega^2$
Γ^4				1	$-\omega^2$	$-\omega$	−1	ω^2	ω
Γ^5	E′	E_g	E″	1	ω^2	$-\omega$	1	ω^2	$-\omega$
Γ^6				1	$-\omega$	ω^2	1	$-\omega$	ω^2

Table D.20 Character table for C_{3h}, C_{3i} and C_6 ($\omega = \exp(\frac{1}{3}\pi i)$).

(19) C_{3v}:

(*a*) Classes [for $\mathscr{G}_0(\mathbf{k})$ of Λ]:

$$\mathscr{C}_1 = E;\ \mathscr{C}_2 = C_{3\delta}, C_{3\delta}^{-1};\ \mathscr{C}_3 = IC_{2b}, IC_{2d}, IC_{2f}.$$

Classes [for $\mathscr{G}_0(\mathbf{k})$ of F]:

$$\mathscr{C}_1 = E;\ \mathscr{C}_2 = C_{3\alpha}, C_{3\alpha}^{-1};\ \mathscr{C}_3 = IC_{2b}, IC_{2c}, IC_{2e}.$$

(*b*) The character table is given in Table D.21.

			$\mathscr{C}_1$	$\mathscr{C}_2$	$\mathscr{C}_3$
Γ^1	A_1	F_1, Λ_1	1	1	1
Γ^2	A_2	F_2, Λ_2	1	1	−1
Γ^3	E	F_3, Λ_3	2	−1	0

Table D.21 Character table for C_{3v} and D_3.

(*c*) Matrices for irreducible representation of dimension greater than one, for any proper rotation C_{nj} of C_{3v}:

$$\Gamma^3(C_{nj}) = \Gamma''(C_{nj});$$

and for any improper rotation IC_{nj} of C_{3v}:

$$\Gamma^3(IC_{nj}) = \Gamma''(C_{nj});$$

where the matrices $\Gamma''(C_{nj})$ are given in Table D.4.

(20) D_3:

(*a*) Classes:

$$\mathscr{C}_1 = E;\ \mathscr{C}_2 = C_{3z}, C_{3z}^{-1};\ \mathscr{C}_3 = C_{2x}, C_{2A}, C_{2B}.$$

(*b*) The character table is given in Table D.21.

(*c*) Matrices for irreducible representation of dimension greater than one, for any rotation C_{nj} of D_3:

$$\Gamma^3(C_{nj}) = \mathbf{D}'(C_{nj});$$

where the matrices $\mathbf{D}'(C_{nj})$ are given in Table D.6.

(21) C_{3i} or S_6:

(*a*) Classes:

$$\mathscr{C}_1 = E;\ \mathscr{C}_2 = IC_{3z}^{-1};\ \mathscr{C}_3 = C_{3z};\ \mathscr{C}_4 = I;\ \mathscr{C}_5 = C_{3z}^{-1};\ \mathscr{C}_6 = IC_{3z}.$$

(*b*) The character table is given in Table D.20.

(22) C_6:

(*a*) Classes:

$$\mathscr{C}_1 = E;\ \mathscr{C}_2 = C_{6z};\ \mathscr{C}_3 = C_{3z};\ \mathscr{C}_4 = C_{2z};\ \mathscr{C}_5 = C_{3z}^{-1},\ \mathscr{C}_6 = C_{6z}^{-1}.$$

(*b*) The character table is given in Table D.20.

(23) C_{2v}:

(*a*) Classes [for $\mathscr{G}_0(\mathbf{k})$ for Σ]:

$$\mathscr{C}_1 = E;\ \mathscr{C}_2 = C_{2e};\ \mathscr{C}_3 = IC_{2x};\ \mathscr{C}_4 = IC_{2f}.$$

Classes [for $\mathscr{G}_0(\mathbf{k})$ for D]:

$$\mathscr{C}_1 = E;\ \mathscr{C}_2 = C_{2x};\ \mathscr{C}_3 = IC_{2e};\ \mathscr{C}_4 = IC_{2f}.$$

Classes [for $\mathscr{G}_0(\mathbf{k})$ for S]:

$$\mathscr{C}_1 = E;\ \mathscr{C}_2 = C_{2a};\ \mathscr{C}_3 = IC_{2z};\ \mathscr{C}_4 = IC_{2b}.$$

	C_{2v}	C_{2h}	D_2						$\mathscr{C}_1$	$\mathscr{C}_2$	$\mathscr{C}_3$	$\mathscr{C}_4$
Γ^1	A_1	A_g	A_1	Σ_1	S_1	Z_1	G_1	D_1	1	1	1	1
Γ^2	A_2	A_u	B_1	Σ_2	S_2	Z_2	G_2	D_2	1	1	−1	−1
Γ^3	B_1	B_u	B_2	Σ_3	S_3	Z_3	G_3	D_3	1	−1	−1	1
Γ^4	B_2	B_g	B_3	Σ_4	S_4	Z_4	G_4	D_4	1	−1	1	−1

Table D.22 Character table for C_{2v}, C_{2h} and D_2.

Classes [for $\mathscr{G}_0(\mathbf{k})$ for Z]:

$$\mathscr{C}_1 = E;\ \mathscr{C}_2 = C_{2y};\ \mathscr{C}_3 = IC_{2z};\ \mathscr{C}_4 = IC_{2x}.$$

Classes [for $\mathscr{G}_0(\mathbf{k})$ for G]:

$$\mathscr{C}_1 = E;\ \mathscr{C}_2 = C_{2f};\ \mathscr{C}_3 = IC_{2x};\ \mathscr{C}_4 = IC_{2e}.$$

(*b*) The character table is given in Table D.22.

(24) C_{2h}:

(*a*) Classes:

$$\mathscr{C}_1 = E;\ \mathscr{C}_2 = C_{2z};\ \mathscr{C}_3 = I;\ \mathscr{C}_4 = IC_{2z}.$$

(*b*) The character table is given in Table D.22.

(25) D_2 or V:

(*a*) Classes:

$$\mathscr{C}_1 = E;\ \mathscr{C}_2 = C_{2x};\ \mathscr{C}_3 = C_{2y};\ \mathscr{C}_4 = C_{2z}.$$

(*b*) The character table is given in Table D.22.

(26) C_4:

(*a*) Classes:

$$\mathscr{C}_1 = E;\ \mathscr{C}_2 = C_{4z};\ \mathscr{C}_3 = C_{2z};\ \mathscr{C}_4 = C_{4z}^{-1}.$$

(*b*) The character table is given in Table D.23.

(27) S_4:

(*a*) Classes:

$$\mathscr{C}_1 = E;\ \mathscr{C}_2 = IC_{4y};\ \mathscr{C}_3 = C_{2y};\ \mathscr{C}_4 = IC_{4y}^{-1}.$$

(*b*) The character table is given in Table D.23.

		$\mathscr{C}_1$	$\mathscr{C}_2$	$\mathscr{C}_3$	$\mathscr{C}_4$
Γ^1	A	1	1	1	1
Γ^2	B	1	−1	1	−1
Γ^3	E	1	i	−1	$-i$
Γ^4	E	1	$-i$	−1	i

Table D.23 Character table for C_4 and S_4.

(28) C_3:

(*a*) Classes:

$$\mathscr{C}_1 = E;\ \mathscr{C}_2 = C_{3z};\ \mathscr{C}_3 = C_{3z}^{-1}.$$

(*b*) The character table is given in Table D.24.

		$\mathscr{C}_1$	$\mathscr{C}_2$	$\mathscr{C}_3$
Γ^1	A	1	1	1
Γ^2	E	1	ϕ	ϕ^2
Γ^3	E	1	ϕ^2	ϕ

Table D.24 Character table for C_3 ($\phi = \exp(\frac{2}{3}\pi i)$).

(29) C_s or C_{1h}:

(*a*) Classes:

$$\mathscr{C}_1 = E;\ \mathscr{C}_2 = IC_{2z}.$$

(*b*) The character table is given in Table D.25.

	C_s	C_2	C_i		$\mathscr{C}_1$	$\mathscr{C}_2$
Γ^1	A′	A	A_g	Q_1	1	1
Γ^2	A″	B	A_u	Q_2	1	−1

Table D.25 Character table for C_s, C_2 and C_i.

(30) C_2:

(*a*) Classes [for $\mathscr{G}_0(\mathbf{k})$ of Q]:

$$\mathscr{C}_1 = E;\ \mathscr{C}_2 = C_{2d}.$$

(*b*) The character table is given in Table D.25.

(31) C_i or S_2:

(*a*) Classes:

$$\mathscr{C}_1 = E;\ \mathscr{C}_2 = I.$$

(*b*) The character table is given in Table D.25

(32) C_1:

(*a*) This group consists of E alone.
(*b*) $\chi(E) = 1$.