THE MATHEMATICAL THEORY OF SYMMETRY IN SOLIDS

Representation theory for point groups and space groups

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TABLE 6.5

The double-valued representations of the crystallographic point groups

($\omega = \exp(2\pi i/3)$; $\tilde{\omega} = \sqrt{2} + i$; $\theta = (1 + i)/\sqrt{2}$)

$1\ (C_1)$		E	$\bar{E}$
A	Γ_1	1	1
$\bar{A}$	Γ_2	1	-1

$\bar{1}\ (C_i)$		E	I	$\bar{E}$	$\bar{I}$
A_g	Γ_1^+	1	1	1	1
A_u	Γ_1^-	1	-1	1	-1
$\bar{A}_g$	Γ_2^+	1	1	-1	-1
$\bar{A}_u$	Γ_2^-	1	-1	-1	1

$2\ (C_2)$				E	C_{2z}	$\bar{E}$	$\bar{C}_{2z}$
		$m\ (C_{1h})$		E	σ_z	$\bar{E}$	$\bar{\sigma}_z$
A	Γ_1	A'	Γ_1	1	1	1	1
$^1\bar{E}$	Γ_3	$^1\bar{E}$	Γ_3	1	i	-1	$-i$
B	Γ_2	A''	Γ_2	1	-1	1	-1
$^2\bar{E}$	Γ_4	$^2\bar{E}$	Γ_4	1	$-i$	-1	i

$2/m = 2 \otimes \bar{1}$ $(C_{2h} = C_2 \otimes C_i)$.

$mm2\ (C_{2v})$				E	$\bar{E}$	$\sigma_x, \bar{\sigma}_x$	$\sigma_y, \bar{\sigma}_y$	$C_{2z}, \bar{C}_{2z}$
		$222\ (D_2)$		E	$\bar{E}$	$C_{2x}, \bar{C}_{2x}$	$C_{2y}, \bar{C}_{2y}$	$C_{2z}, \bar{C}_{2z}$
A_1	Γ_1	A	Γ_1	1	1	1	1	1
B_2	Γ_4	B_3	Γ_4	1	1	1	-1	-1
B_1	Γ_2	B_2	Γ_2	1	1	-1	1	-1
A_2	Γ_3	B_1	Γ_3	1	1	-1	-1	1
$\bar{E}$	Γ_5	$\bar{E}$	Γ_5	2	-2	0	0	0

$mm2\ (C_{2v})$				σ_x	σ_y
		$222\ (D_2)$		C_{2x}	C_{2y}
$\bar{E}$	Γ_5	$\bar{E}$	Γ_5	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}$

$mmm = 222 \otimes \bar{1}$ $(D_{2h} = D_2 \otimes C_i)$.

$4\ (C_4)$	$\bar{4}\ (S_4)$	E E	C_{4z}^- S_{4z}^+	C_{2z} C_{2z}	$\bar{C}_{4z}^+$ $\bar{S}_{4z}^-$	$\bar{E}$ $\bar{E}$	$\bar{C}_{4z}^-$ $\bar{S}_{4z}^+$	$\bar{C}_{2z}$ $\bar{C}_{2z}$	C_{4z}^+ S_{4z}^-
$A\ \Gamma_1$	$A\ \Gamma_1$	1	1	1	1	1	1	1	1
${}^2\bar{E}_1\ \Gamma_5$	${}^2\bar{E}_1\ \Gamma_5$	1	θ	i	$-\theta^*$	-1	$-\theta$	$-$i	θ^*
${}^1E\ \Gamma_4$	${}^1E\ \Gamma_4$	1	i	-1	$-$i	1	i	-1	$-$i
${}^1\bar{E}_2\ \Gamma_8$	${}^1\bar{E}_2\ \Gamma_8$	1	$-\theta^*$	$-$i	θ	-1	θ^*	i	$-\theta$
$B\ \Gamma_2$	$B\ \Gamma_2$	1	-1	1	-1	1	-1	1	-1
${}^2\bar{E}_2\ \Gamma_7$	${}^2\bar{E}_2\ \Gamma_7$	1	$-\theta$	i	θ^*	-1	θ	$-$i	$-\theta^*$
${}^2E\ \Gamma_3$	${}^2E\ \Gamma_3$	1	$-$i	-1	i	1	$-$i	-1	i
${}^1\bar{E}_1\ \Gamma_6$	${}^1\bar{E}_1\ \Gamma_6$	1	θ^*	$-$i	$-\theta$	-1	$-\theta^*$	i	θ

$4/m = 4 \otimes \bar{1}\ (C_{4h} = C_4 \otimes C_i)$.

$3\ (C_3)$	E	C_3^+	$\bar{C}_3^-$	$\bar{E}$	$\bar{C}_3^+$	C_3^-
$A\ \Gamma_1$	1	1	1	1	1	1
${}^2\bar{E}\ \Gamma_5$	1	$-\omega^*$	ω	-1	ω^*	$-\omega$
${}^2E\ \Gamma_2$	1	ω	ω^*	1	ω	ω^*
$\bar{A}\ \Gamma_6$	1	-1	1	-1	1	-1
${}^1E\ \Gamma_3$	1	ω^*	ω	1	ω^*	ω
${}^1\bar{E}\ \Gamma_4$	1	$-\omega$	ω^*	-1	ω	$-\omega^*$

$\bar{3} = 3 \otimes \bar{1}\ (C_{3i} = C_3 \otimes C_i)$.

$32\ (D_3)$	$3m\ (C_{3v})$	E E	$\bar{E}$ $\bar{E}$	C_3^+, C_3^- C_3^+, C_3^-	$\bar{C}_3^-, \bar{C}_3^+$ $\bar{C}_3^-, \bar{C}_3^+$	$C'_{21}, C'_{22}, C'_{23}$ $\sigma_{d1}, \sigma_{d2}, \sigma_{d3}$	$\bar{C}'_{21}, \bar{C}'_{22}, \bar{C}'_{23}$ $\bar{\sigma}_{d1}, \bar{\sigma}_{d2}, \bar{\sigma}_{d3}$
$A_1\ \Gamma_1$	$A_1\ \Gamma_1$	1	1	1	1	1	1
$A_2\ \Gamma_2$	$A_2\ \Gamma_2$	1	1	1	1	-1	-1
${}^1\bar{E}\ \Gamma_5$	${}^1\bar{E}\ \Gamma_5$	1	-1	-1	1	i	$-$i
${}^2\bar{E}\ \Gamma_6$	${}^2\bar{E}\ \Gamma_6$	1	-1	-1	1	$-$i	i
$E\ \Gamma_3$	$E\ \Gamma_3$	2	2	-1	-1	0	0
$\bar{E}_1\ \Gamma_4$	$\bar{E}_1\ \Gamma_4$	2	-2	1	-1	0	0

$32\ (D_3)$	$3m\ (C_{3v})$	C_3^+ C_3^+	C'_{21} σ_{d1}
$\bar{E}_1\ \Gamma_4$	$\bar{E}_1\ \Gamma_4$	$\begin{pmatrix} \frac{1}{2} & -\frac{1}{2}\sqrt{3} \\ \frac{1}{2}\sqrt{3} & \frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} \mathrm{i} & 0 \\ 0 & -\mathrm{i} \end{pmatrix}$

$\bar{3}m = 32 \otimes \bar{1}\ (D_{3d} = D_3 \otimes C_i)$.

6 (C_6)		$\bar{6}$ (C_{3h})		E	C_6^+	C_3^+	$\bar{C}_2$	$\bar{C}_3^-$	$\bar{C}_6^-$	$\bar{E}$	$\bar{C}_6^+$	$\bar{C}_3^+$	C_2	C_3^-	C_6^-
				E	S_3^-	C_3^+	$\bar{\sigma}_h$	$\bar{C}_3^-$	$\bar{S}_3^+$	$\bar{E}$	$\bar{S}_3^-$	$\bar{C}_3^+$	σ_h	C_3^-	S_3^+
A	Γ_1	A'	Γ_1	1	1	1	1	1	1	1	1	1	1	1	1
${}^2\bar{E}_3$	Γ_8	${}^2\bar{E}_3$	Γ_8	1	$-\mathrm{i}\omega$	$-\omega^*$	i	ω	$-\mathrm{i}\omega^*$	-1	$\mathrm{i}\omega$	ω^*	$-\mathrm{i}$	$-\omega$	$\mathrm{i}\omega^*$
${}^2E_2$	Γ_2	${}^2E''$	Γ_5	1	$-\omega^*$	ω	-1	ω^*	$-\omega$	1	$-\omega^*$	ω	-1	ω^*	$-\omega$
${}^1\bar{E}_1$	Γ_{11}	${}^1\bar{E}_1$	Γ_{11}	1	i	-1	$-\mathrm{i}$	1	i	-1	$-\mathrm{i}$	1	i	-1	$-\mathrm{i}$
${}^1E_1$	Γ_6	${}^1E'$	Γ_3	1	ω	ω^*	1	ω	ω^*	1	ω	ω^*	1	ω	ω^*
${}^2\bar{E}_2$	Γ_9	${}^2\bar{E}_2$	Γ_9	1	$-\mathrm{i}\omega^*$	$-\omega$	i	ω^*	$-\mathrm{i}\omega$	-1	$\mathrm{i}\omega^*$	ω	$-\mathrm{i}$	$-\omega^*$	$\mathrm{i}\omega$
B	Γ_4	A''	Γ_4	1	-1	1	-1	1	-1	1	-1	1	-1	1	-1
${}^1\bar{E}_2$	Γ_{10}	${}^1\bar{E}_2$	Γ_{10}	1	$\mathrm{i}\omega$	$-\omega^*$	$-\mathrm{i}$	ω	$\mathrm{i}\omega^*$	-1	$-\mathrm{i}\omega$	ω^*	i	$-\omega$	$-\mathrm{i}\omega^*$
${}^2E_1$	Γ_5	${}^2E'$	Γ_2	1	ω^*	ω	1	ω^*	ω	1	ω^*	ω	1	ω^*	ω
${}^2\bar{E}_1$	Γ_{12}	${}^2\bar{E}_1$	Γ_{12}	1	$-\mathrm{i}$	-1	i	1	$-\mathrm{i}$	-1	i	1	$-\mathrm{i}$	-1	i
${}^1E_2$	Γ_3	${}^1E''$	Γ_6	1	$-\omega$	ω^*	-1	ω	$-\omega^*$	1	$-\omega$	ω^*	-1	ω	$-\omega^*$
${}^1\bar{E}_3$	Γ_7	${}^1\bar{E}_3$	Γ_7	1	$\mathrm{i}\omega^*$	$-\omega$	$-\mathrm{i}$	ω^*	$\mathrm{i}\omega$	-1	$-\mathrm{i}\omega^*$	ω	i	$-\omega^*$	$-\mathrm{i}\omega$

$6/m = 6 \otimes \bar{1}$ ($C_{6h} = C_6 \otimes C_i$).

422 (D_4)						E	$\bar{E}$	$C_{2z}, \bar{C}_{2z}$	C_{4z}^-, C_{4z}^+	$\bar{C}_{4z}^+, \bar{C}_{4z}^-$	C_{2x}, C_{2y} $\bar{C}_{2x}, \bar{C}_{2y}$	C_{2a}, C_{2b} $\bar{C}_{2a}, \bar{C}_{2b}$
		4mm (C_{4v})				E	$\bar{E}$	$C_{2z}, \bar{C}_{2z}$	C_{4z}^-, C_{4z}^+	$\bar{C}_{4z}^+, \bar{C}_{4z}^-$	σ_x, σ_y $\bar{\sigma}_x, \bar{\sigma}_y$	σ_{da}, σ_{db} $\bar{\sigma}_{da}, \bar{\sigma}_{db}$
				$\bar{4}2m$ (D_{2d})		E	$\bar{E}$	$C_{2z}, \bar{C}_{2z}$	S_{4z}^+, S_{4z}^-	$\bar{S}_{4z}^-, \bar{S}_{4z}^+$	C_{2x}, C_{2y} $\bar{C}_{2x}, \bar{C}_{2y}$	σ_{da}, σ_{db} $\bar{\sigma}_{da}, \bar{\sigma}_{db}$
A_1	Γ_1	A_1	Γ_1	A_1	Γ_1	1	1	1	1	1	1	1
A_2	Γ_2	A_2	Γ_2	A_2	Γ_2	1	1	1	1	1	-1	-1
B_1	Γ_3	B_1	Γ_3	B_1	Γ_3	1	1	1	-1	-1	1	-1
B_2	Γ_4	B_2	Γ_4	B_2	Γ_4	1	1	1	-1	-1	-1	1
E	Γ_5	E	Γ_5	E	Γ_5	2	2	-2	0	0	0	0
$\bar{E}_1$	Γ_6	$\bar{E}_1$	Γ_6	$\bar{E}_1$	Γ_6	2	-2	0	$\sqrt{2}$	$-\sqrt{2}$	0	0
$\bar{E}_2$	Γ_7	$\bar{E}_2$	Γ_7	$\bar{E}_2$	Γ_7	2	-2	0	$-\sqrt{2}$	$\sqrt{2}$	0	0

422 (D_4)						C_{4z}^-	C_{2x}
		4mm (C_{4v})				C_{4z}^-	σ_x
				$\bar{4}2m$ (D_{2d})		S_{4z}^+	C_{2x}
$\bar{E}_1$	Γ_6	$\bar{E}_1$	Γ_6	$\bar{E}_1$	Γ_6	$\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & \mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}$
$\bar{E}_2$	Γ_7	$\bar{E}_2$	Γ_7	$\bar{E}_2$	Γ_7	$\frac{1}{\sqrt{2}}\begin{pmatrix} -1 & 1 \\ -1 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & \mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}$

$4/mmm = 422 \otimes \bar{1}$ ($D_{4h} = D_4 \otimes C_i$).

622 (D_6)	6mm (C_{6v})	$\bar{6}2m$ (D_{3h})									
622 (D_6)			E	$\bar{E}$	$\bar{C}_3^+, \bar{C}_3^-$	C_3^+, C_3^-	$\bar{C}_2, C_2$	C_6^+, C_6^-	$\bar{C}_6^-, \bar{C}_6^+$	$C'_{21}, \bar{C}'_{21}$ $C'_{22}, \bar{C}'_{22}$ $C'_{23}, \bar{C}'_{23}$	$C''_{21}, \bar{C}''_{21}$ $C''_{22}, \bar{C}''_{22}$ $C''_{23}, \bar{C}''_{23}$
	6mm (C_{6v})		E	$\bar{E}$	$\bar{C}_3^+, \bar{C}_3^-$	C_3^+, C_3^-	$\bar{C}_2, C_2$	C_6^+, C_6^-	$\bar{C}_6^-, \bar{C}_6^+$	$\sigma_{d1}, \bar{\sigma}_{d1}$ $\sigma_{d2}, \bar{\sigma}_{d2}$ $\sigma_{d3}, \bar{\sigma}_{d3}$	$\sigma_{v1}, \bar{\sigma}_{v1}$ $\sigma_{v2}, \bar{\sigma}_{v2}$ $\sigma_{v3}, \bar{\sigma}_{v3}$
		$\bar{6}2m$ (D_{3h})	E	$\bar{E}$	$\bar{C}_3^+, \bar{C}_3^-$	C_3^+, C_3^-	$\bar{\sigma}_h, \sigma_h$	S_3^-, S_3^+	$\bar{S}_3^+, \bar{S}_3^-$	$C'_{21}, \bar{C}'_{21}$ $C'_{22}, \bar{C}'_{22}$ $C'_{23}, \bar{C}'_{23}$	$\sigma_{v1}, \bar{\sigma}_{v1}$ $\sigma_{v2}, \bar{\sigma}_{v2}$ $\sigma_{v3}, \bar{\sigma}_{v3}$
A_1 Γ_1	A_1 Γ_1	A'_1 Γ_1	1	1	1	1	1	1	1	1	1
A_2 Γ_2	A_2 Γ_2	A'_2 Γ_2	1	1	1	1	1	1	1	−1	−1
B_1 Γ_3	B_2 Γ_3	A''_1 Γ_3	1	1	1	1	−1	−1	−1	1	−1
B_2 Γ_4	B_1 Γ_4	A''_2 Γ_4	1	1	1	1	−1	−1	−1	−1	1
E_1 Γ_5	E_1 Γ_5	E'' Γ_5	2	2	−1	−1	−2	1	1	0	0
E_2 Γ_6	E_2 Γ_6	E' Γ_6	2	2	−1	−1	2	−1	−1	0	0
$\bar{E}_1$ Γ_7	$\bar{E}_1$ Γ_7	$\bar{E}_1$ Γ_7	2	−2	−1	1	0	$\sqrt{3}$	$-\sqrt{3}$	0	0
$\bar{E}_2$ Γ_8	$\bar{E}_2$ Γ_8	$\bar{E}_2$ Γ_8	2	−2	−1	1	0	$-\sqrt{3}$	$\sqrt{3}$	0	0
$\bar{E}_3$ Γ_9	$\bar{E}_3$ Γ_9	$\bar{E}_3$ Γ_9	2	−2	2	−2	0	0	0	0	0

622 (D_6)	6mm (C_{6v})	$\bar{6}2m$ (D_{3h})	C_6^+ C_6^+ S_3^-	C'_{21} σ_{d1} C'_{21}
$\bar{E}_1$ Γ_7	$\bar{E}_1$ Γ_7	$\bar{E}_1$ Γ_7	$\begin{pmatrix} -i\omega & 0 \\ 0 & i\omega^* \end{pmatrix}$	$\begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}$
$\bar{E}_2$ Γ_8	$\bar{E}_2$ Γ_8	$\bar{E}_2$ Γ_8	$\begin{pmatrix} -i\omega^* & 0 \\ 0 & i\omega \end{pmatrix}$	$\begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}$
$\bar{E}_3$ Γ_9	$\bar{E}_3$ Γ_9	$\bar{E}_3$ Γ_9	$\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}$	$\begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}$

$6/mmm = 622 \otimes \bar{1}$ $(D_{6h} = D_6 \otimes C_i)$.

23 (T)	E	$\bar{E}$	C_{2x}, C_{2y}, C_{2z} $\bar{C}_{2x}, \bar{C}_{2y}, \bar{C}_{2z}$	C_{31}^-, C_{32}^- C_{33}^-, C_{34}^-	$\bar{C}_{31}^-, \bar{C}_{32}^-$ $\bar{C}_{33}^-, \bar{C}_{34}^-$	$\bar{C}_{31}^+, \bar{C}_{32}^+$ $\bar{C}_{33}^+, \bar{C}_{34}^+$	C_{31}^+, C_{32}^+ C_{33}^+, C_{34}^+
A Γ_1	1	1	1	1	1	1	1
^2E Γ_3	1	1	1	ω	ω	ω^*	ω^*
^1E Γ_2	1	1	1	ω^*	ω^*	ω	ω
$\bar{E}$ Γ_5	2	−2	0	1	−1	−1	1
$^1\bar{F}$ Γ_6	2	−2	0	ω	$-\omega$	$-\omega^*$	ω^*
$^2\bar{F}$ Γ_7	2	−2	0	ω^*	$-\omega^*$	$-\omega$	ω
T Γ_4	3	3	−1	0	0	0	0

23 (T)		C_{31}^-	C_{2x}	$\bar{C}_{2y}$
$\bar{E}$	Γ_5	$\frac{1}{2}\begin{pmatrix} 1-i & -1+i \\ 1+i & 1+i \end{pmatrix}$	$\begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$
${}^1\bar{F}$	Γ_6	$\frac{\omega}{2}\begin{pmatrix} 1-i & -1+i \\ 1+i & 1+i \end{pmatrix}$	$\begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$
${}^2\bar{F}$	Γ_7	$\frac{\omega^*}{2}\begin{pmatrix} 1-i & -1+i \\ 1+i & 1+i \end{pmatrix}$	$\begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$

$m3 = 23 \otimes \bar{1}$ $(T_h = T \otimes C_i)$.

432 (O)		$\bar{4}3m$ (T_d)		C_1	C_2	C_3	C_4	C_5	C_6	C_7	C_8
A_1	Γ_1	A_1	Γ_1	1	1	1	1	1	1	1	1
A_2	Γ_2	A_2	Γ_2	1	1	1	1	1	-1	-1	-1
E	Γ_3	E	Γ_3	2	2	2	-1	-1	0	0	0
T_1	Γ_4	T_1	Γ_4	3	3	-1	0	0	1	1	-1
T_2	Γ_5	T_2	Γ_5	3	3	-1	0	0	-1	-1	1
$\bar{E}_1$	Γ_6	$\bar{E}_1$	Γ_6	2	-2	0	1	-1	$\sqrt{2}$	$-\sqrt{2}$	0
$\bar{E}_2$	Γ_7	$\bar{E}_2$	Γ_7	2	-2	0	1	-1	$-\sqrt{2}$	$\sqrt{2}$	0
$\bar{F}$	Γ_8	$\bar{F}$	Γ_8	4	-4	0	-1	1	0	0	0

432 (O)

C_1 E
C_2 $\bar{E}$
C_3 $C_{2x}, C_{2y}, C_{2z}, \bar{C}_{2x}, \bar{C}_{2y}, \bar{C}_{2z}$
C_4 $C_{31}^-, C_{32}^-, C_{33}^-, C_{34}^-, C_{31}^+, C_{32}^+, C_{33}^+, C_{34}^+$
C_5 $\bar{C}_{31}^-, \bar{C}_{32}^-, \bar{C}_{33}^-, \bar{C}_{34}^-, \bar{C}_{31}^+, \bar{C}_{32}^+, \bar{C}_{33}^+, \bar{C}_{34}^+$
C_6 $C_{4x}^+, C_{4y}^+, C_{4z}^+, C_{4x}^-, C_{4y}^-, C_{4z}^-$
C_7 $\bar{C}_{4x}^+, \bar{C}_{4y}^+, \bar{C}_{4z}^+, \bar{C}_{4x}^-, \bar{C}_{4y}^-, \bar{C}_{4z}^-$
C_8 $C_{2a}, C_{2b}, C_{2c}, C_{2d}, C_{2e}, C_{2f}, \bar{C}_{2a}, \bar{C}_{2b}, \bar{C}_{2c}, \bar{C}_{2d}, \bar{C}_{2e}, \bar{C}_{2f}$

$\bar{4}3m$ (T_d)

C_1 E
C_2 $\bar{E}$
C_3 $C_{2x}, C_{2y}, C_{2z}, \bar{C}_{2x}, \bar{C}_{2y}, \bar{C}_{2z}$
C_4 $C_{31}^-, C_{32}^-, C_{33}^-, C_{34}^-, C_{31}^+, C_{32}^+, C_{33}^+, C_{34}^+$
C_5 $\bar{C}_{31}^-, \bar{C}_{32}^-, \bar{C}_{33}^-, \bar{C}_{34}^-, \bar{C}_{31}^+, \bar{C}_{32}^+, \bar{C}_{33}^+, \bar{C}_{34}^+$
C_6 $S_{4x}^-, S_{4y}^-, S_{4z}^-, S_{4x}^+, S_{4y}^+, S_{4z}^+$
C_7 $\bar{S}_{4x}^-, \bar{S}_{4y}^-, \bar{S}_{4z}^-, \bar{S}_{4x}^+, \bar{S}_{4y}^+, \bar{S}_{4z}^+$
C_8 $\sigma_{da}, \sigma_{db}, \sigma_{dc}, \sigma_{dd}, \sigma_{de}, \sigma_{df}, \bar{\sigma}_{da}, \bar{\sigma}_{db}, \bar{\sigma}_{dc}, \bar{\sigma}_{dd}, \bar{\sigma}_{de}, \bar{\sigma}_{df}$

432 (O)	$\bar{4}3m$ (T_d)	C_{4x}^+ S_{4x}^-	$\bar{C}_{31}^-$ $\bar{C}_{31}^-$	C_{2b} σ_{db}
$\bar{E}_1$ Γ_6	$\bar{E}_1$ Γ_6	$\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -i \\ -i & 1 \end{pmatrix}$	$\frac{1}{2}\begin{pmatrix} -1+i & 1-i \\ -1-i & -1-i \end{pmatrix}$	$\frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -1-i \\ 1-i & 0 \end{pmatrix}$
$\bar{E}_2$ Γ_7	$\bar{E}_2$ Γ_7	$\frac{1}{\sqrt{2}}\begin{pmatrix} -1 & i \\ i & -1 \end{pmatrix}$	$\frac{1}{2}\begin{pmatrix} -1+i & 1-i \\ -1-i & -1-i \end{pmatrix}$	$\frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1+i \\ -1+i & 0 \end{pmatrix}$
$\bar{F}$ Γ_8	$\bar{F}$ Γ_8	$\frac{1}{\sqrt{2}}\begin{pmatrix} \mu & -i\mu \\ -i\mu & \mu \end{pmatrix}$	$\frac{1}{2}\begin{pmatrix} (-1+i)\beta & (1-i)\beta \\ (-1-i)\beta & (-1-i)\beta \end{pmatrix}$	$\frac{1}{\sqrt{2}}\begin{pmatrix} 0 & (-1-i)\lambda \\ (1-i)\lambda & 0 \end{pmatrix}$

$$\beta = \begin{pmatrix} -\frac{1}{2} & \frac{1}{2}\sqrt{3} \\ -\frac{1}{2}\sqrt{3} & -\frac{1}{2} \end{pmatrix}; \quad \lambda = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}; \quad \mu = \begin{pmatrix} -\frac{1}{2} & -\frac{1}{2}\sqrt{3} \\ -\frac{1}{2}\sqrt{3} & \frac{1}{2} \end{pmatrix}.$$

$m3m = 432 \otimes \bar{1}$ $\quad (O_h = O \otimes C_i)$.

Notes to Table 6.5

(i) The names of the point groups are given in the top left-hand blocks of the tables and, where appropriate, several point groups are tabulated together.

(ii) The characters of the single-valued reps, which were given in Table 2.2 are included for reference.

(iii) The matrix representatives for the generating elements are given for the degenerate double-valued reps. The matrices of the other elements can be found by using the group multiplication tables in Table 6.2.

(iv) The elements of the point groups can be identified by reference to Figs. 1.1–1.4 and Tables 1.2–1.6.

(v) The scheme used in Table 2.2 for labelling the single-valued reps of the point groups has been extended to cover the double-valued reps as well. Each double-valued point-group rep is labelled either by an extension of the Mulliken (1933) notation or by the Γ notation of Koster, Dimmock, Wheeler, and Statz (1963). In the extended Mulliken notation the symbols labelling the double-valued reps have a bar placed over them.

(vi) We have not given the character tables of those groups that are direct products of some other point group with $\bar{1}$ (C_i); the character tables of these direct product groups can be constructed as follows. If a group G′ is given as a direct product of the form G $\otimes$ $\bar{1}$ then the reps of G′ fall into pairs; each pair M_g and M_u arise out of a single rep M of G and the characters of M_g and M_u obey the following rules. If $R' = RI$ then for all $R \in$ G the character of R in M_g and M_u is equal to the character of R in M; the character of R' in M_g is equal to the character of R in M, but the character of R' in M_u is minus the character of R in M. In the Γ notation of Koster, Dimmock, Wheeler, and Statz (1963), if $\Gamma \equiv M$ in G, then $\Gamma^+ \equiv M_g$ and $\Gamma^- \equiv M_u$ in G′.

(vii) The reality (see Definition 1.3.7) of the double-valued point-group reps is as follows:

non-degenerate, all characters real	first kind
degenerate, all characters real	second kind
non-degenerate, some characters complex degenerate, some characters complex	third kind

In Table 6.6 we give the compatibility tables between the double-valued representations $\mathscr{D}^j\{R(\alpha, \beta, \gamma)\}$ (j = half odd integer) of the 3-dimensional rotation group, $O(3)$, and the double-valued point-group reps. This table, like Table 2.7, is relevant to the study of the splitting of an energy level of a free atom, characterized by a half-odd-integer total angular momentum quantum number j, in the presence of an electrostatic field with the symmetry of any one of the crystallographic point groups