A

Point Group Character Tables

Appendix A contains Point Group Character (Tables A.1–A.34) to be used throughout the chapters of this book. Pedagogic material to assist the reader in the use of these character tables can be found in Chap. 3. The Schoenflies symmetry (Sect. 3.9) and Hermann–Mauguin notations (Sect. 3.10) for the point groups are also discussed in Chap. 3.

Some of the more novel listings in this appendix are the groups with five-fold symmetry C_5, C_{5h}, C_{5v}, D_5, D_{5d}, D_{5h}, I, I_h. The cubic point group O_h in Table A.31 lists basis functions for all the irreducible representations of O_h and uses the standard solid state physics notation for the irreducible representations.

Table A.1. Character table for group C_1 (triclinic)

C_1 (1)	E
A	1

Table A.2. Character table for group $C_i = S_2$ (triclinic)

S_2 ($\bar{1}$)			E	i
$x^2, y^2, z^2, xy, xz, yz$	R_x, R_y, R_z	A_g	1	1
	x, y, z	A_u	1	−1

Table A.3. Character table for group $C_{1h} = S_1$ (monoclinic)

$C_{1h}(m)$			E	σ_h
x^2, y^2, z^2, xy	R_z, x, y	A'	1	1
xz, yz	R_x, R_y, z	A''	1	−1

Table A.4. Character table for group C_2 (monoclinic)

C_2 (2)			E	C_2
x^2, y^2, z^2, xy	R_z, z	A	1	1
xz, yz	(x, y) (R_x, R_y)	B	1	−1

Table A.5. Character table for group C_{2v} (orthorhombic)

C_{2v} (2mm)			E	C_2	σ_v	σ'_v
x^2, y^2, z^2	z	A_1	1	1	1	1
xy	R_z	A_2	1	1	−1	−1
xz	R_y, x	B_1	1	−1	1	−1
yz	R_x, y	B_2	1	−1	−1	1

Table A.6. Character table for group C_{2h} (monoclinic)

C_{2h} (2/m)			E	C_2	σ_h	i
x^2, y^2, z^2, xy	R_z	A_g	1	1	1	1
	z	A_u	1	1	−1	−1
xz, yz	R_x, R_y	B_g	1	−1	−1	1
	x, y	B_u	1	−1	1	−1

Table A.7. Character table for group $D_2 = V$ (orthorhombic)

D_2 (222)			E	C_2^z	C_2^y	C_2^x
x^2, y^2, z^2		A_1	1	1	1	1
xy	R_z, z	B_1	1	1	−1	−1
xz	R_y, y	B_2	1	−1	1	−1
yz	R_x, x	B_3	1	−1	−1	1

Table A.8. Character table for group $D_{2d} = V_d$ (tetragonal)

D_{2d} ($\bar{4}2m$)			E	C_2	$2S_4$	$2C'_2$	$2\sigma_d$
$x^2 + y^2, z^2$		A_1	1	1	1	1	1
	R_z	A_2	1	1	1	−1	−1
$x^2 - y^2$		B_1	1	1	−1	1	−1
xy	z	B_2	1	1	−1	−1	1
(xz, yz)	(x, y) (R_x, R_y)	E	2	−2	0	0	0

$D_{2h} = D_2 \otimes i$ (mmm) (orthorhombic)

Table A.9. Character table for group C_3 (rhombohedral)

$C_3(3)$			E	C_3	C_3^2
x^2+y^2, z^2	R_z, z	A	1	1	1
(xz, yz), (x^2-y^2, xy)	(x, y), (R_x, R_y)	E	$\begin{cases}1\\1\end{cases}$	ω ω^2	ω^2 ω

$\omega = \mathrm{e}^{2\pi \mathrm{i}/3}$

Table A.10. Character table for group C_{3v} (rhombohedral)

C_{3v} $(3m)$			E	$2C_3$	$3\sigma_v$
x^2+y^2, z^2	z	A_1	1	1	1
	R_z	A_2	1	1	–1
(x^2-y^2, xy), (xz, yz)	(x, y), (R_x, R_y)	E	2	-1	0

Table A.11. Character table for group $C_{3h} = S_3$ (hexagonal)

$C_{3h} = C_3 \otimes \sigma_h$ $(\overline{6})$			E	C_3	C_3^2	σ_h	S_3	$(\sigma_h C_3^2)$
x^2+y^2, z^2	R_z	A'	1	1	1	1	1	1
	z	A''	1	1	1	-1	-1	-1
(x^2-y^2, xy)	(x, y)	E'	$\begin{cases}1\\1\end{cases}$	ω ω^2	ω^2 ω	1 1	ω ω^2	ω^2 ω
(xz, yz)	(R_x, R_y)	E''	$\begin{cases}1\\1\end{cases}$	ω ω^2	ω^2 ω	-1 -1	$-\omega$ $-\omega^2$	$-\omega^2$ $-\omega$

$\omega = \mathrm{e}^{2\pi \mathrm{i}/3}$

Table A.12. Character table for group D_3 (rhombohedral)

D_3 (32)			E	$2C_3$	$3C_2'$
x^2+y^2, z^2		A_1	1	1	1
	R_z, z	A_2	1	1	-1
(xz, yz), (x^2-y^2, xy)	(x, y), (R_x, R_y)	E	2	-1	0

Table A.13. Character table for group D_{3d} (rhombohedral)

$D_{3d} = D_3 \otimes i$ $(\overline{3}m)$			E	$2C_3$	$3C_2'$	i	$2iC_3$	$3iC_2'$
x^2+y^2, z^2		A_{1g}	1	1	1	1	1	1
	R_z	A_{2g}	1	1	-1	1	1	-1
(xz, yz),(x^2-y^2, xy)	(R_x, R_y)	E_g	2	-1	0	2	-1	0
		A_{1u}	1	1	1	-1	-1	-1
	z	A_{2u}	1	1	-1	-1	-1	1
	(x, y)	E_u	2	-1	0	-2	1	0

Table A.14. Character table for group D_{3h} (hexagonal)

$D_{3h} = D_3 \otimes \sigma_h$ ($\overline{6}m2$)			E	σ_h	$2C_3$	$2S_3$	$3C_2'$	$3\sigma_v$
x^2+y^2, z^2		A_1'	1	1	1	1	1	1
	R_z	A_2'	1	1	1	1	−1	−1
		A_1''	1	−1	1	−1	1	−1
	z	A_2''	1	−1	1	−1	−1	1
(x^2-y^2, xy)	(x, y)	E'	2	2	−1	−1	0	0
(xz, yz)	(R_x, R_y)	E''	2	−2	−1	1	0	0

Table A.15. Character table for group C_4 (tetragonal)

C_4 (4)			E	C_2	C_4	C_4^3
x^2+y^2, z^2	R_z, z	A	1	1	1	1
x^2-y^2, xy		B	1	1	−1	−1
(xz, yz)	(x, y)	E	1	−1	i	$-i$
	(R_x, R_y)		1	−1	$-i$	i

Table A.16. Character table for group C_{4v} (tetragonal)

C_{4v} (4mm)			E	C_2	$2C_4$	$2\sigma_v$	$2\sigma_d$
x^2+y^2, z^2	z	A_1	1	1	1	1	1
	R_z	A_2	1	1	1	−1	−1
x^2-y^2		B_1	1	1	−1	1	−1
xy		B_2	1	1	−1	−1	1
(xz, yz)	(x, y), (R_x, R_y)	E	2	−2	0	0	0

$C_{4h} = C_4 \otimes i$ $(4/m)$ (tetragonal)

Table A.17. Character table for group S_4 (tetragonal)

S_4 ($\overline{4}$)			E	C_2	S_4	S_4^3
x^2+y^2, z^2	R_z	A	1	1	1	1
	z	B	1	1	−1	−1
(xz, yz)	(x, y)	E	1	−1	i	−i
(x^2-y^2, xy)	(R_x, R_y)		1	−1	−i	i

Table A.18. Character table for group D_4 (tetragonal)

D_4 (422)			E	$C_2 = C_4^2$	$2C_4$	$2C_2'$	$2C_2''$
x^2+y^2, z^2		A_1	1	1	1	1	1
	R_z, z	A_2	1	1	1	−1	−1
x^2-y^2		B_1	1	1	−1	1	−1
xy		B_2	1	1	−1	−1	1
(xz, yz)	(x, y), (R_x, R_y)	E	2	−2	0	0	0

$D_{4h} = D_4 \otimes i$ $(4/mmm)$ (tetragonal)

Table A.19. Character table for group C_6 (hexagonal)

C_6 (6)			E	C_6	C_3	C_2	C_3^2	C_6^5
x^2+y^2, z^2	R_z, z	A	1	1	1	1	1	1
		B	1	-1	1	-1	1	-1
(xz, yz)	(x, y)	E'	1	ω	ω^2	ω^3	ω^4	ω^5
	(R_x, R_y)		1	ω^5	ω^4	ω^3	ω^2	ω
(x^2-y^2, xy)		E''	1	ω^2	ω^4	1	ω^2	ω^4
			1	ω^4	ω^2	1	ω^4	ω^2

$\omega = \mathrm{e}^{2\pi \mathrm{i}/6}$

Table A.20. Character table for group C_{6v} (hexagonal)

C_{6v} ($6mm$)			E	C_2	$2C_3$	$2C_6$	$3\sigma_d$	$3\sigma_v$
x^2+y^2, z^2	z	A_1	1	1	1	1	1	1
	R_z	A_2	1	1	1	1	-1	-1
		B_1	1	-1	1	-1	-1	1
		B_2	1	-1	1	-1	1	-1
(xz, yz)	(x, y) (R_x, R_y)	E_1	2	-2	-1	1	0	0
(x^2-y^2, xy)		E_2	2	2	-1	-1	0	0

$C_{6h} = C_6 \otimes i$ $(6/m)$ (hexagonal); $S_6 = C_3 \otimes i$ $(\overline{3})$ (rhombohedral)

Table A.21. Character table for group D_6 (hexagonal)

D_6 (622)			E	C_2	$2C_3$	$2C_6$	$3C_2'$	$3C_2''$
x^2+y^2, z^2		A_1	1	1	1	1	1	1
	R_z, z	A_2	1	1	1	1	-1	-1
		B_1	1	-1	1	-1	1	-1
		B_2	1	-1	1	-1	-1	1
(xz, yz)	(x, y) (R_x, R_y)	E_1	2	-2	-1	1	0	0
(x^2-y^2, xy)		E_2	2	2	-1	-1	0	0

$D_{6h} = D_6 \otimes i$ $(6/mmm)$ (hexagonal)

Table A.22. Character table for group C_5 (icosahedral)

C_5 (5)			E	C_5	C_5^2	C_5^3	C_5^4
x^2+y^2, z^2	R_z, z	A	1	1	1	1	1
(xz, yz)	(x, y)	E'	1	ω	ω^2	ω^3	ω^4
	(R_x, R_y)		1	ω^4	ω^3	ω^2	ω
(x^2-y^2, xy)		E''	1	ω^2	ω^4	ω	ω^3
			1	ω^3	ω	ω^4	ω^2

$\omega = \mathrm{e}^{2\pi \mathrm{i}/5}$. Note group $C_{5h} = C_5 \otimes \sigma_h = S_{10}(\overline{10})$

Table A.23. Character table for group C_{5v} (icosahedral)

C_{5v} (5m)			E	$2C_5$	$2C_5^2$	$5\sigma_v$
$x^2+y^2, z^2, z^3, z(x^2+y^2)$	z	A_1	1	1	1	1
	R_z	A_2	1	1	1	−1
$z(x,y), z^2(x,y), (x^2+y^2)(x,y)$	$\left.\begin{array}{l}(x,y)\\(R_x,R_y)\end{array}\right\}$	E_1	2	$2\cos\alpha$	$2\cos 2\alpha$	0
$(x^2-y^2, xy), z(x^2-y^2, xy)$, $[x(x^2-3y^2), y(3x^2-y^2)]$		E_2	2	$2\cos 2\alpha$	$2\cos 4\alpha$	0

$\alpha = 2\pi/5 = 72°$. Note that $\tau = (1+\sqrt{5})/2$ so that $\tau = -2\cos 2\alpha = -2\cos 4\pi/5$ and $\tau - 1 = 2\cos\alpha = 2\cos 2\pi/5$

Table A.24. Character table for group D_5 (icosahedral)

D_5 (52)			E	$2C_5$	$2C_5^2$	$5C_2'$
x^2+y^2, z^2		A_1	1	1	1	1
	R_z, z	A_2	1	1	1	−1
(xz, yz)	$\left.\begin{array}{l}(x,y)\\(R_x,R_y)\end{array}\right\}$	E_1	2	$2\cos\alpha$	$2\cos 2\alpha$	0
(x^2-y^2, xy)		E_2	2	$2\cos 2\alpha$	$2\cos 4\alpha$	0

Table A.25. Character table for D_{5d} (icosahedral)

D_{5d}	E	$2C_5$	$2C_5^2$	$5C_2'$	i	$2S_{10}^{-1}$	$2S_{10}$	$5\sigma_d$	$(h=20)$
A_{1g}	+1	+1	+1	+1	+1	+1	+1	+1	$(x^2+y^2), z^2$
A_{2g}	+1	+1	+1	−1	+1	+1	+1	−1	R_z
E_{1g}	+2	$\tau-1$	$-\tau$	0	+2	$\tau-1$	$-\tau$	0	$z(x+\mathrm{i}y, x-\mathrm{i}y)$
E_{2g}	+2	$-\tau$	$\tau-1$	0	+2	$-\tau$	$\tau-1$	0	$[(x+\mathrm{i}y)^2, (x-\mathrm{i}y)^2]$
A_{1u}	+1	+1	+1	+1	−1	−1	−1	−1	
A_{2u}	+1	+1	+1	−1	−1	−1	−1	+1	z
E_{1u}	+2	$\tau-1$	$-\tau$	0	−2	$1-\tau$	$+\tau$	0	$(x+\mathrm{i}y, x-\mathrm{i}y)$
E_{2u}	+2	$-\tau$	$\tau-1$	0	−2	$+\tau$	$1-\tau$	0	

Note: $D_{5d} = D_5 \otimes i$, $iC_5 = S_{10}^{-1}$ and $iC_5^2 = S_{10}$. Also $iC_2' = \sigma_d$

Table A.26. Character table for D_{5h} (icosahedral)

D_{5h} ($\overline{10}2m$)	E	$2C_5$	$2C_5^2$	$5C_2'$	σ_h	$2S_5$	$2S_5^3$	$5\sigma_v$	$(h=20)$
A_1'	+1	+1	+1	+1	+1	+1	+1	+1	x^2+y^2, z^2
A_2'	+1	+1	+1	−1	+1	+1	+1	−1	R_z
E_1'	+2	$\tau-1$	$-\tau$	0	+2	$\tau-1$	$-\tau$	0	(x,y), (xz^2, yz^2), $[x(x^2+y^2), y(x^2+y^2)]$
E_2'	+2	$-\tau$	$\tau-1$	0	+2	$-\tau$	$\tau-1$	0	(x^2-y^2, xy), $[y(3x^2-y^2), x(x^2-3y^2)]$
A_1''	+1	+1	+1	+1	−1	−1	−1	−1	
A_2''	+1	+1	+1	−1	−1	−1	−1	+1	z, $z^3, z(x^2+y^2)$
E_1''	+2	$\tau-1$	$-\tau$	0	−2	$1-\tau$	$+\tau$	0	(R_x, R_y), (xz, yz)
E_2''	+2	$-\tau$	$\tau-1$	0	−2	$+\tau$	$1-\tau$	0	$[xyz, z(x^2-y^2)]$

$D_{5h} = D_5 \otimes \sigma_h$

Table A.27. Character table for the icosahedral group I (icosahedral)

I (532)	E	$12C_5$	$12C_5^2$	$20C_3$	$15C_2$	($h = 60$)
A	+1	+1	+1	+1	+1	$x^2 + y^2 + z^2$
F_1	+3	$+\tau$	$1-\tau$	0	−1	(x, y, z); (R_x, R_y, R_z)
F_2	+3	$1-\tau$	$+\tau$	0	−1	
G	+4	−1	−1	+1	0	
H	+5	0	0	−1	+1	$\{2z^2 - x^2 - y^2$, $x^2 - y^2$, xy, xz, $yz\}$

Table A.28. Character table for I_h (icosahedral)

I_h	E	$12C_5$	$12C_5^2$	$20C_3$	$15C_2$	i	$12S_{10}^3$	$12S_{10}$	$20S_6$	15σ	($h = 120$)
A_g	+1	+1	+1	+1	+1	+1	+1	+1	+1	+1	$x^2 + y^2 + z^2$
F_{1g}	+3	$+\tau$	$1-\tau$	0	−1	+3	τ	$1-\tau$	0	−1	R_x, R_y, R_z
F_{2g}	+3	$1-\tau$	$+\tau$	0	−1	+3	$1-\tau$	τ	0	−1	
G_g	+4	−1	−1	+1	0	+4	−1	−1	+1	0	
H_g	+5	0	0	−1	+1	+5	0	0	−1	+1	$\{2z^2 - x^2 - y^2$, $x^2 - y^2$, xy, xz, $yz\}$
A_u	+1	+1	+1	+1	+1	−1	−1	−1	−1	−1	
F_{1u}	+3	$+\tau$	$1-\tau$	0	−1	−3	$-\tau$	$\tau-1$	0	+1	(x, y, z)
F_{2u}	+3	$1-\tau$	$+\tau$	0	−1	−3	$\tau-1$	$-\tau$	0	+1	
G_u	+4	−1	−1	+1	0	−4	+1	+1	−1	0	
H_u	+5	0	0	−1	+1	−5	0	0	+1	−1	

$\tau = (1 + \sqrt{5})/2$. Note: C_5 and C_5^{-1} are in different classes, labeled $12C_5$ and $12C_5^2$ in the character table. Then $iC_5 = S_{10}^{-1}$ and $iC_5^{-1} = S_{10}$ are in the classes labeled $12S_{10}^3$ and $12S_{10}$, respectively. Also $iC_2 = \sigma_v$ and $I_h = I \otimes i$

Table A.29. Character table for group T (cubic)

T (23)		E	$3C_2$	$4C_3$	$4C_3'$
$x^2 + y^2 + z^2$	A	1	1	1	1
$(x^2 - y^2, 3z^2 - r^2)$	E	$\{1$	1	ω	ω^2
		1	1	ω^2	ω
$\{(R_x, R_y, R_z)$, (x, y, z), $(yz, zx, xy)\}$	T	3	−1	0	0

$\omega = e^{2\pi i/3}$; $T_h = T \otimes i$, ($m3$) (cubic)

Table A.30. Character table for group O (cubic)

O (432)		E	$8C_3$	$3C_2 = 3C_4^2$	$6C_2'$	$6C_4$
$(x^2+y^2+z^2)$	A_1	1	1	1	1	1
	A_2	1	1	1	−1	−1
$(x^2-y^2, 3z^2-r^2)$	E	2	−1	2	0	0
(R_x, R_y, R_z) (x, y, z)	T_1	3	0	−1	−1	1
(xy, yz, zx)	T_2	3	0	−1	1	−1

$O_h = O \otimes i$, $(m3m)$ (cubic)

Table A.31. Character table for the cubic group O_h (cubic)†

repr.	basis functions	E	$3C_4^2$	$6C_4$	$6C_2'$	$8C_3$	i	$3iC_4^2$	$6iC_4$	$6iC_2'$	$8iC_3$
A_1^+	1	1	1	1	1	1	1	1	1	1	1
A_2^+	$\begin{cases} x^4(y^2-z^2)+ \\ y^4(z^2-x^2)+ \\ z^4(x^2-y^2) \end{cases}$	1	1	−1	−1	1	1	1	−1	−1	1
E^+	$\begin{cases} x^2-y^2 \\ 2z^2-x^2-y^2 \end{cases}$	2	2	0	0	−1	2	2	0	0	−1
T_1^-	x, y, z	3	−1	1	−1	0	−3	1	−1	1	0
T_2^-	$z(x^2-y^2)\ldots$	3	−1	−1	1	0	−3	1	1	−1	0
A_1^-	$\begin{cases} xyz[x^4(y^2-z^2)+ \\ y^4(z^2-x^2)+ \\ z^4(x^2-y^2)] \end{cases}$	1	1	1	1	1	−1	−1	−1	−1	−1
A_2^-	xyz	1	1	−1	−1	1	−1	−1	1	1	−1
E^-	$xyz(x^2-y^2)\ldots$	2	2	0	0	−1	−2	−2	0	0	1
T_1^+	$xy(x^2-y^2)\ldots$	3	−1	1	−1	0	3	−1	1	−1	0
T_2^+	xy, yz, zx	3	−1	−1	1	0	3	−1	−1	1	0

† The basis functions for T_2^- are $z(x^2-y^2)$, $x(y^2-z^2)$, $y(z^2-x^2)$, for E^- are $xyz(x^2-y^2)$, $xyz(3z^2-s^2)$ and for T_1^+ are $xy(x^2-y^2)$, $yz(y^2-z^2)$, $zx(z^2-x^2)$

Table A.32. Character table for group T_d (cubic)[a]

T_d $(\bar{4}3m)$		E	$8C_3$	$3C_2$	$6\sigma_d$	$6S_4$
$x^2+y^2+z^2$	A_1	1	1	1	1	1
	A_2	1	1	1	−1	−1
$(x^2-y^2, 3z^2-r^2)$	E	2	−1	2	0	0
(R_x, R_y, R_z) $yz, zx, xy)$	T_1	3	0	−1	−1	1
(x, y, z)	T_2	3	0	−1	1	−1

[a] Note that (yz, zx, xy) transforms as representation T_1

Table A.33. Character table for group $C_{\infty v}$

$C_{\infty v}$ (∞m)			E	$2C_\phi$	σ_v
(x^2+y^2, z^2)	z	$A_1(\Sigma^+)$	1	1	1
	R_z	$A_2(\Sigma^-)$	1	1	-1
(xz, yz)	$\left.\begin{matrix}(x,y)\\(R_x,R_y)\end{matrix}\right\}$	$E_1(\Pi)$	2	$2\cos\phi$	0
(x^2-y^2, xy)		$E_2(\Delta)$	2	$2\cos 2\phi$	0
		$\vdots$	$\vdots$	$\vdots$	$\vdots$

Table A.34. Character table for group $D_{\infty h}$

$D_{\infty h}$ (∞/mm)			E	$2C_\phi$	C_2'	i	$2iC_\phi$	iC_2'
x^2+y^2, z^2		$A_{1g}(\Sigma_g^+)$	1	1	1	1	1	1
		$A_{1u}(\Sigma_u^-)$	1	1	1	-1	-1	-1
	R_z	$A_{2g}(\Sigma_g^-)$	1	1	-1	1	1	-1
	z	$A_{2u}(\Sigma_u^+)$	1	1	-1	-1	-1	1
(xz, yz)	(R_x, R_y)	$E_{1g}(\Pi_g)$	2	$2\cos\phi$	0	2	$2\cos\phi$	0
	(x, y)	$E_{1u}(\Pi_u)$	2	$2\cos\phi$	0	-2	$-2\cos\phi$	0
(x^2-y^2, xy)		$E_{2g}(\Delta_g)$	2	$2\cos 2\phi$	0	2	$2\cos 2\phi$	0
		$E_{2u}(\Delta_u)$	2	$2\cos 2\phi$	0	-2	$-2\cos 2\phi$	0
		$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$