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	$\left\{\begin{array}{l}1\\1\end{array}\right.$	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)

$C_{3h} = C_3 \otimes \sigma_h$ $(\bar{6})$			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'	$\left\{\begin{array}{l}1\\1\end{array}\right.$	ω ω^2	ω^2 ω	1 1	ω ω^2	ω^2 ω
(xz, yz)	(R_x, R_y)	E''	$\left\{\begin{array}{l}1\\1\end{array}\right.$	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)

$D_{3d} = D_3 \otimes i$ $(\bar{3}m)$			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), (R_x, R_y)	E	1	−1	i	$-i$
			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^2-y^2, xy)	(x, y), (R_x, R_y)	E	1	−1	i	−i
			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) (R_x, R_y)	E'	$\begin{cases} 1 \\ 1 \end{cases}$	ω ω^5	ω^2 ω^4	ω^3 ω^3	ω^4 ω^2	ω^5 ω
(x^2-y^2, xy)		E''	$\begin{cases} 1 \\ 1 \end{cases}$	ω^2 ω^4	ω^4 ω^2	1 1	ω^2 ω^4	ω^4 ω^2

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

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) (R_x, R_y)	E'	$\begin{cases} 1 \\ 1 \end{cases}$	ω ω^4	ω^2 ω^3	ω^3 ω^2	ω^4 ω
(x^2-y^2, xy)		E''	$\begin{cases} 1 \\ 1 \end{cases}$	ω^2 ω^3	ω^4 ω	ω ω^4	ω^3 ω^2

$\omega = e^{2\pi i/5}$. 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
$z(x,y), z^2(x,y), (x^2+y^2)(x,y)$	(x,y), (R_x,R_y)	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)	(x,y), (R_x,R_y)	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	$\begin{cases} 2z^2-x^2-y^2 \\ x^2-y^2 \\ xy \\ xz \\ yz \end{cases}$

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	$\begin{cases} 2z^2-x^2-y^2 \\ x^2-y^2 \\ xy \\ xz \\ yz \end{cases}$
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	$\begin{cases} 1 \\ 1 \end{cases}$	1 1	ω ω^2	ω^2 ω
$\left.\begin{matrix} (R_x,R_y,R_z) \\ (x,y,z) \\ (yz,zx,xy) \end{matrix}\right\}$	T	3	−1	0	0

$\omega = \mathrm{e}^{2\pi \mathrm{i}/3}$; $T_h = T \otimes i$, $(m3)$ (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
$\left.\begin{array}{l}(R_x, R_y, R_z)\\(x, y, z)\end{array}\right\}$	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^+	$\left\{\begin{array}{l}x^4(y^2-z^2)+\\y^4(z^2-x^2)+\\z^4(x^2-y^2)\end{array}\right.$	1	1	-1	-1	1	1	1	-1	-1	1
E^+	$\left\{\begin{array}{l}x^2-y^2\\2z^2-x^2-y^2\end{array}\right.$	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^-	$\left\{\begin{array}{l}xyz[x^4(y^2-z^2)+\\y^4(z^2-x^2)+\\z^4(x^2-y^2)]\end{array}\right.$	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
$\left.\begin{array}{l}(R_x, R_y, R_z)\\yz, zx, xy)\end{array}\right\}$	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
		$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$

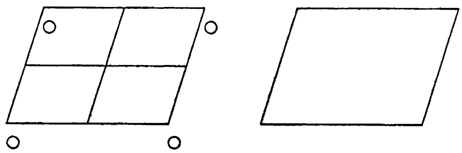
B

Two-Dimensional Space Groups

We include in this appendix a summary of the crystallographic symmetries for all 17 of the 2D space groups, taken from the "International Tables for X-ray Crystallography" [58].

Table B.1. The two-dimensional oblique space group $p1$ or #1 ($p1$)

$p1$	No. 1	$p1$	1 Oblique

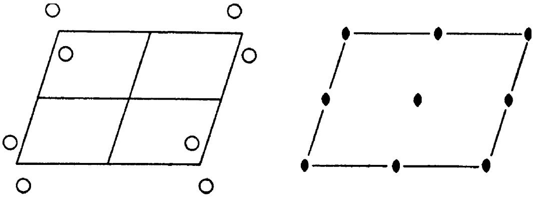


Origin on 1

Number of positions Wyckoff notation, and point symmetry	Co-ordinates of equivalent positions	Conditions limiting possible reflections
1 a 1	x, y	General: No conditions

Table B.2. The two-dimensional oblique space group $p2$ or #2 ($p2111$)

$p2$	No. 2	$p211$	2 Oblique

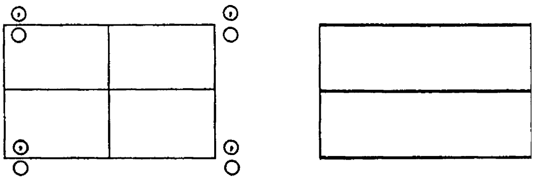


Origin at 2

2	e	1	x, y; $\bar{x}, \bar{y}$	General: No conditions
1	d	2	$\frac{1}{2}, \frac{1}{2}$	Special: No conditions
1	c	2	$\frac{1}{2}, 0$	
1	b	2	$0, \frac{1}{2}$	
1	a	2	$0, 0$	

Table B.3. The two-dimensional rectangular space group pm or #3 ($p1m1$)

pm	No. 3	$p1m1$	m Rectangular

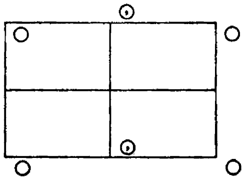
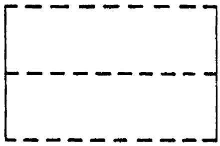


Origin on m

Number of positions Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
2	c	1	x, y; $\bar{x}, y$	General: No conditions
1	b	m	$\frac{1}{2}, y$	Special: No conditions
1	a	m	$0, y$	

Table B.4. The two-dimensional space group pg or #4 ($p1g1$)

pg	No. 4	$p\,1\,g\,1$	m Rectangular

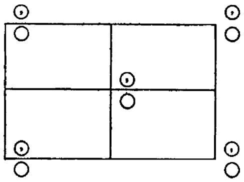
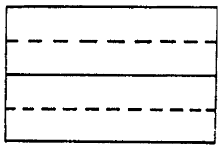



Origin on g

2	a	1	$x, y;\ \bar{x}, \frac{1}{2}+y$	General: hk: No conditions $0k$: $k=2n$

Table B.5. The two-dimensional rectangular space group cm or #5 ($c1m1$)

cm	No. 5	$c\,1\,m\,1$	m Rectangular

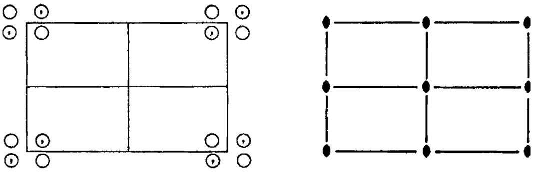



Origin on m

Number of positions Wyckoff notation, and point symmetry				Co-ordinates of equivalent positions $(0,0;\ \frac{1}{2},\frac{1}{2})+$	Conditions limiting possible reflections
4	b	1	$x, y;\ \bar{x}, y$		General: hk: $h+k=2n$
2	a	m	$0, y$		Special: as above only

Table B.6. The two-dimensional rectangular space group *pmm* or #6 (*p*2*mm*)

pmm	No. 6	$p\,2\,m\,m$	$m\,m$ Rectangular

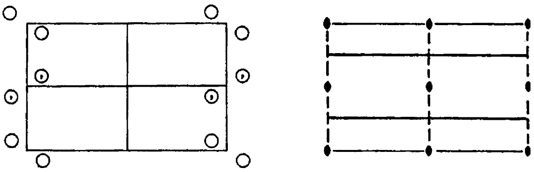


Origin at 2*mm*

Number of positions Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
4	i	1	$x,y;\ \bar{x},y;\ \bar{x},\bar{y};\ x,\bar{y}$	General: no conditions
2	h	m	$\frac{1}{2},y;\ \frac{1}{2},\bar{y}$	Special: No condition
2	g	m	$0,y;\ 0,\bar{y}$	
2	f	m	$x,\frac{1}{2};\ \bar{x},\frac{1}{2}$	
2	e	m	$x,0;\ \bar{x},0$	
1	d	mm	$\frac{1}{2},\frac{1}{2}$	
1	c	mm	$\frac{1}{2},0$	
1	b	mm	$0,\frac{1}{2}$	
1	a	mm	$0,0$	

Table B.7. The two-dimensional rectangular space group *pmg* or #7 (*p*2*mg*)

pmg	No. 7	$p\,2\,m\,g$	$m\,m$ Rectangular

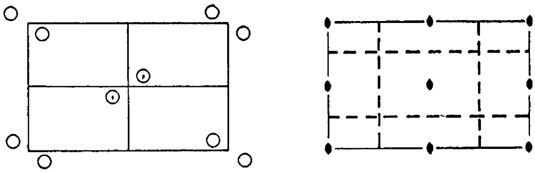


Origin at 2

Number of positions Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
4	d	1	$x,y;\ \bar{x},\bar{y};\ \frac{1}{2}+x,\bar{y};\ \frac{1}{2}-x,y$	General: hk: No conditions $h0$: $h=2n$
2	c	m	$\frac{1}{4},y;\ \frac{3}{4},\bar{y}$	Special: as above, plus no extra conditions
2	b	2	$0,\frac{1}{2};\ \frac{1}{2},\frac{1}{2}$	$\left.\right\}$ hk: $h=2n$
2	a	2	$0,0;\ \frac{1}{2},0$	

Table B.8. The two-dimensional rectangular space group *pgg* or #8 ($p2gg$)

pgg	No. 8	$p\,2\,g\,g$	$m\,m$ Rectangular

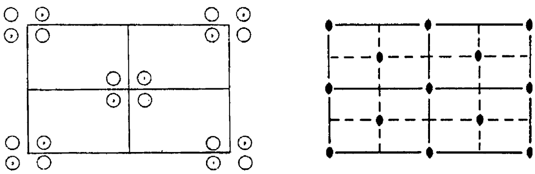


Origin at 2

Number of positions Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
4	c	1	$x,y;\ \bar{x},\bar{y};\ \frac{1}{2}+x,\frac{1}{2}-y;\ \frac{1}{2}-x,\frac{1}{2}+y$	General: hk: no conditions $h0$: $h=2n$ $0l$: $k=2n$ Special: as above, plus
2	b	2	$\frac{1}{2},0;\ 0,\frac{1}{2}$	$\}$ hk: $h+k=2n$
2	a	2	$0,0;\ \frac{1}{2},\frac{1}{2}$	

Table B.9. The two-dimensional rectangular space group *cmm* or #9 ($c2mm$)

cmm	No. 9	$c\,2\,m\,g$	$m\,m$ Rectangular

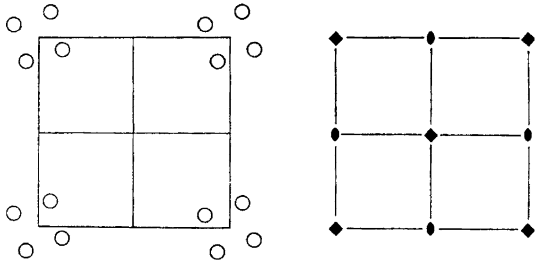


Origin at 2*mm*

Number of positions Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions $(0,0;\ \frac{1}{2},\frac{1}{2})+$	Conditions limiting possible reflections
8	f	1	$x,y;\ \bar{x},y;\ \bar{x},\bar{y};\ x,\bar{y}$	General: hk: $h+k=2n$ Special: as above, plus
4	e	m	$0,y;\ 0,\bar{y}$	$\}$ no extra conditions
4	d	m	$x,0;\ \bar{x},0$	
4	c	2	$\frac{1}{4},\frac{1}{4};\ \frac{1}{4},\frac{3}{4}$	hk: $h=2n$; $(k=2n)$
2	b	mm	$0,\frac{1}{2}$	$\}$ no extra conditions
2	a	mm	$0,0$	

Table B.10. The two-dimensional square space group $p4$ or #10 ($p4$)

$p4$	No. 10	$p4$	4 Square

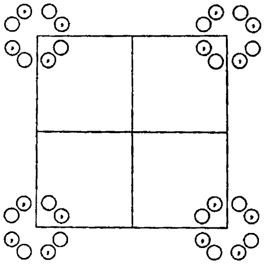


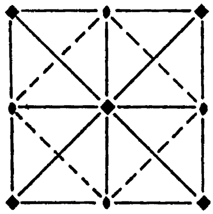
Origin at 4

Number of positions Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
4	d	1	x, y; $\bar{x}, \bar{y}$; $y, \bar{x}$; $\bar{y}, x$	General: No conditions
				Special:
2	c	2	$\frac{1}{2}, 0$; $0, \frac{1}{2}$	hk: $h + k = 2n$
1	b	4	$\frac{1}{2}, \frac{1}{2}$	No conditions
1	a	4	$0, 0$	No conditions

Table B.11. The two-dimensional square space group $p4m$ or #11 ($p4mm$)

$p4m$	No. 11	$p\,4\,m\,m$	$4\,m\,m$ Square



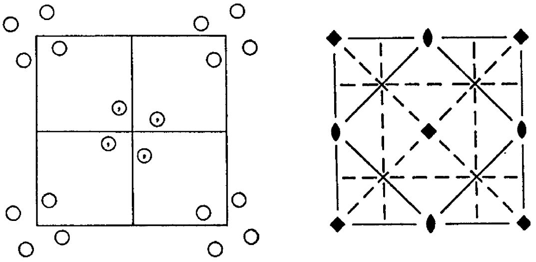


Origin at $4mm$

Number of positions Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
8	g	1	x,y; $\bar{x},\bar{y}$; $y,\bar{x}$; $\bar{y},x$; $\bar{x},y$; $x,\bar{y}$; $\bar{y},\bar{x}$, y,x	General: No conditions
				Special:
4	f	m	x,x; $\bar{x},\bar{x}$; $\bar{x},x$; $x,\bar{x}$	no conditions
4	e	m	$x,\frac{1}{2}$; $\bar{x},\frac{1}{2}$; $\frac{1}{2},x$; $\frac{1}{2},\bar{x}$	no conditions
4	d	m	$x,0$; $\bar{x},0$; $0,x$; $0,\bar{x}$	no conditions
2	c	mm	$\frac{1}{2},0$; $0,\frac{1}{2}$	hk: $h+k=2n$
1	b	$4mm$	$\frac{1}{2},\frac{1}{2}$	no conditions
1	a	$4mm$	$0,0$	no conditions

Table B.12. The two-dimensional square space group $p4g$ or #12 ($p4gm$)

$p4g$	No. 12	$p\,4\,g\,m$	$4mm$ Square

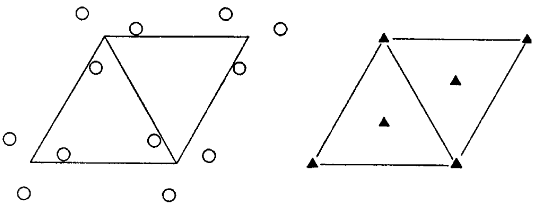


Origin at 4

Number of positions Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			General:	
8	d	1	x,y; $y,\bar{x}$; $\frac{1}{2}-x,\frac{1}{2}+y$; $\frac{1}{2}-y,\frac{1}{2}-x$ $\bar{x},\bar{y}$; $\bar{y},x$; $\frac{1}{2}+x,\frac{1}{2}-y$; $\frac{1}{2}+y,\frac{1}{2}+x$	hk: No conditions $h0$: $h=2n$ ($0k$: $k=2n$) hh: No conditions
				Special: as above, plus
4	c	m	$x,\frac{1}{2}+x$; $\bar{x},\frac{1}{2}-x$; $\frac{1}{2}+x,\bar{x}$; $\frac{1}{2}-x,x$	no extra conditions
2	b	$4mm$	$\frac{1}{2},0$; $0,\frac{1}{2}$	$\left.\right\}$ hk: $h+k=2n$
2	a	4	$0,0$; $\frac{1}{2},\frac{1}{2}$	

Table B.13. The two-dimensional hexagonal space group $p3$ or #13 ($p3$)

$p3$	No. 13	$p\,3$	3 Hexagonal

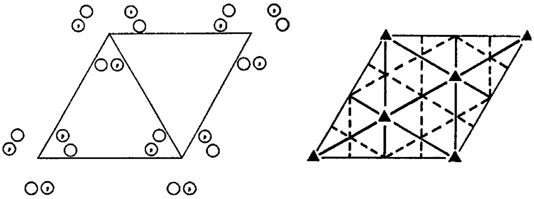


Origin at 3

Number of positions Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
3	d	1	$\bar{y},x-y$; $y-x,\bar{x}$	General: No conditions
				Special:
1	c	3	$\frac{1}{3},\frac{1}{3}$	no conditions
1	b	3	$\frac{1}{3},\frac{1}{3}$	
1	a	3	$0,0$	

Table B.14. The two-dimensional hexagonal space group $p3m1$ or #14 ($p3m1$)

$p3m1$	No. 14	$p3m1$	$3m$ Hexagonal

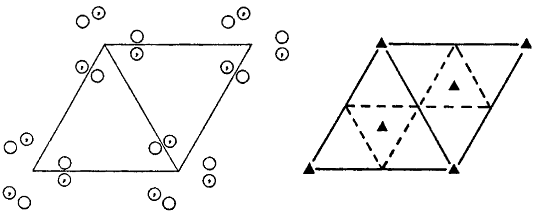


Origin at $3m1$

Number of positions Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
6	e	m	$x, y;\ \bar{y}, x-y;\ y-x, \bar{x}$ $\bar{y}, \bar{x};\ x, x-y;\ y-x, y$	No conditions
				Special:
3	d	m	$x, \bar{x};\ x, 2x;\ 2\bar{x}, x$	No conditions
1	c	$3m$	$\frac{2}{3}, \frac{1}{3}$	
1	b	$3m$	$\frac{1}{3}, \frac{2}{3}$	
1	a	$3m$	$0, 0$	

Table B.15. The two-dimensional hexagonal space group $p31m$ or #15 ($p31m$)

$p31m$	No. 15	$p31m$	$3m$ Hexagonal

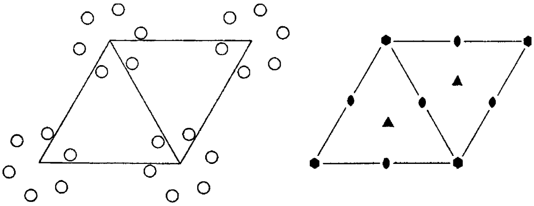


Origin at $31m$

Number of positions Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
6	d	1	$x, y;\ \bar{y}, x-y;\ y-x, \bar{x}$ $y, x;\ \bar{x}, y-x;\ x-y, \bar{y}$	General: No conditions Special:
3	c	m	$x, 0;\ 0, x;\ \bar{x}, \bar{x}$	no conditions
2	b	3	$\frac{1}{3}, \frac{2}{3};\ \frac{2}{3}, \frac{1}{3}$	
1	a	3m	$0, 0$	

Table B.16. The two-dimensional hexagonal space group $p6$ or #16 ($p6$)

$p6$	No. 16	$p6$	Hexagonal 6

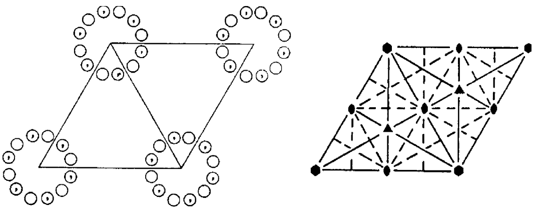


Origin at 6

Number of positions Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
6	d	1	$x,y;\ \bar{y},x-y;\ y-x,\bar{x}$ $\bar{x},\bar{y};\ y,y-x;\ x-y,x$	No conditions
				Special:
3	c	2	$\frac{1}{2},0;\ 0,\frac{1}{2};\ \frac{1}{2},\frac{1}{2}$	No conditions
2	b	3	$\frac{1}{3},\frac{2}{3};\ \frac{2}{3},\frac{1}{3}$	
1	a	6	$0,0$	

Table B.17. The two-dimensional hexagonal space group $p6m$ or #17 ($p6mm$)

$p6m$	No. 17	$p6mm$	$6mm$ Hexagonal



Origin at $6mm$

Number of positions Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
12	f	1	$x,y;\ \bar{y},x-y;\ y-x,\bar{x};\ y,x;\ \bar{x},y-x;\ x-y,\bar{y}$ $\bar{x},\bar{y};\ y,y-x;\ x-y,x;\ \bar{y},\bar{x};\ x,x-y;\ y-x,y$	General: No conditions Special:
6	e	m	$x,\bar{x};\ x,2x;\ 2\bar{x},\bar{x};\ \bar{x},x;\ \bar{x},2\bar{x};\ 2x,x$	No conditions
6	d	m	$x,0;\ 0,x;\ \bar{x},\bar{x};\ \bar{x},0;\ 0,\bar{x};\ x,x$	
3	c	mm	$\frac{1}{2},0;\ 0,\frac{1}{2};\ \frac{1}{2},\frac{1}{2}$	
2	b	$3m$	$\frac{1}{3},\frac{2}{3};\ \frac{2}{3},\frac{1}{3}$	
1	a	$6mm$	$0,0$	

C

Tables for 3D Space Groups

In this appendix, selected tables and figures for 3D space groups in real space and in reciprocal space are presented. The real space tables[1] and figures given in the first part of the appendix (Sect. C.1) pertain mainly to crystallographic information and are used for illustrative purposes in various chapters of this book. The tables which pertain to reciprocal space appear in the second part of the appendix (Sect. C.2) and are mainly for tables for the group of the wave vector for various high symmetry points in the Brillouin zone for various cubic space groups and other space groups selected for illustrative purposes.

C.1 Real Space

A list of the 230 space groups and their Hermann–Mauguin symmetry designations (Sect. 3.10) is given in Table C.1, taken from the web [54]. Most of the current literature presently follows the notation of reference [58]. The reader will find Table C.1 to differ in two ways from entries in the International Tables for X-ray Crystallography [58]. Firstly, a minus sign ($-n$) is used in [54] rather than $\bar{n}$ in [58] to denote improper rotations (see Sect. 3.9) for many of the groups, including #81-82, #111-122, #147-148, #162-167, #174, #187-190, #215-220. Secondly, a minus sign ($-n$) is used in [54], rather than n itself [58] to denote other groups, including #200-206 and #221-230. Some of the special space groups referred to in the book text are the rhombohedral space group #166, the hexagonal space group #194, the simple cubic space group #221, the face-centered cubic space group #225, the space group #227 for the diamond structure, and the body-centered cubic space group #229.

Space groups have in addition to translational symmetry, point group symmetries which single out special high symmetry points. Tables C.2, C.3, and

[1] The notation for these tables is discussed in Chap. 9.

Table C.1. Listing of the Hermann–Mauguin symmetry space group symbol designations for the 230 space groups. The table is taken from the web [54] (see text)

1	$P1$	2	$P-1$	3	$P2$	4	$P2_1$	5	$C2$
6	Pm	7	Pc	8	Cm	9	Cc	10	$P2/m$
11	$P2_1/m$	12	$C2/m$	13	$P2/c$	14	$P2_1/c$	15	$C2/c$
16	$P222$	17	$P222_1$	18	$P2_12_12$	19	$P2_12_12_1$	20	$C222_1$
21	$C222$	22	$F222$	23	$I222$	24	$I2_12_12_1$	25	$Pmm2$
26	$Pmc2_1$	27	$Pcc2$	28	$Pma2$	29	$Pca2_1$	30	$Pnc2$
31	$Pmn2_1$	32	$Pba2$	33	$Pna2_1$	34	$Pmn2$	35	$Cmm2$
36	$Cmc2_1$	37	$Ccc2$	38	$Amm2$	39	$Abm2$	40	$Ama2$
41	$AbA2$	42	$Fmm2$	43	$Fdd2$	44	$Imm2$	45	$Iba2$
46	$Ima2$	47	$Pmmm$	48	$Pnnn$	49	$Pccm$	50	$Pban$
51	$Pmma$	52	$Pnna$	53	$Pnna$	54	$Pcca$	55	$Pbam$
56	$Pccn$	57	$Pbcm$	58	$Pnnm$	59	$Pmmn$	60	$Pbcn$
61	$Pbca$	62	$Pnma$	63	$Cmcm$	64	$Cmca$	65	$Cmmm$
66	$Cccm$	67	$Cmma$	68	$Ccca$	69	$Fmmm$	70	$Fddd$
71	$Immm$	72	$Ibam$	73	$Ibca$	74	$Imma$	75	$P4$
76	$P4_1$	77	$P4_2$	78	$P4_3$	79	$I4$	80	$I4_1$
81	$P-4$	82	$I-4$	83	$P4/m$	84	$P4_2/m$	85	$P4/n$
86	$P4_2/n$	87	$I4/m$	88	$I4_1/a$	89	$P422$	90	$P42_12$
91	$P4_122$	92	$P4_12_12$	93	$P4_222$	94	$P4_22_12$	95	$P4_322$
96	$P4_32_12$	97	$I422$	98	$I4_122$	99	$P4mm$	100	$P4bm$
101	$P4_2cm$	102	$P4_2nm$	103	$P4cc$	104	$P4nc$	105	$P4_2mc$
106	$P4_2bc$	107	$I4mm$	108	$I4cm$	109	$I4_1md$	110	$I4_1cd$
111	$P-42m$	112	$P-42c$	113	$P-42_1m$	114	$P-42_1c$	115	$P-4m2$
116	$P-4c2$	117	$P-4b2$	118	$P-4n2$	119	$I-4m2$	120	$I-4c2$
121	$I-42m$	122	$I-42d$	123	$P4/mmm$	124	$P4/mcc$	125	$P4/nbm$
126	$P4/nnc$	127	$P4/mbm$	128	$P4/mnc$	129	$P4/nmm$	130	$P4/ncc$
131	$P4_2/mmc$	132	$P4_2/mcm$	133	$P4_2/nbc$	134	$P4_2/nmm$	135	$P4_2/mbc$
136	$P4_2/mmm$	137	$P4_2/nmc$	138	$P4_2/ncm$	139	$I4/mmm$	140	$I4/mcm$
141	$I4_1/amd$	142	PI_1/acd	143	$P3$	144	$P3_1$	145	$P3_2$
146	$R3$	147	$P-3$	148	$R-3$	149	$P312$	150	$P321$
151	$P3_112$	152	$P3_121$	153	$P3_212$	154	$P3_221$	155	$R32$
156	$P3m1$	157	$P31m$	158	$P3c1$	159	$P31c$	160	$R3m$
161	$R3c$	162	$P-31m$	163	$P-31c$	164	$P-3m1$	165	$P-3c1$
166	$R-3m$	167	$R-3c$	168	$P6$	169	$P6_1$	170	$P6_5$
171	$P6_2$	172	$P6_4$	173	$P6_3$	174	$P-6$	175	$P6/m$
176	$P6_2/m$	177	$P622$	178	$P6_122$	179	$P6_522$	180	$P6_222$
181	$P6_422$	182	$P6_322$	183	$P6mm$	184	$P6cc$	185	$P6_3cm$
186	$P6_3mc$	187	$P-6m2$	188	$P-6c2$	189	$P-62m$	190	$P-62c$
191	$P6/mmm$	192	$P6/mcc$	193	$P6_3/mcm$	194	$P6_3/mmc$	195	$P23$
196	$F23$	197	$I23$	198	$P2_13$	199	$I2_13$	200	$Pm-3$
201	$Pn-3$	202	$Fm-3$	203	$Fd-3$	204	$Im-3$	205	$Pa-3$
206	$Ia-3$	207	$P432$	208	$P4_232$	209	$F432$	210	$F4_132$
211	$I432$	212	$P4_332$	213	$P4_132$	214	$I4_132$	215	$P-43m$
216	$F-43m$	217	$I-43m$	218	$P-43n$	219	$F-43c$	220	$I-43d$
221	$Pm-3m$	222	$Pn-3n$	223	$Pm-3n$	224	$Pn-3m$	225	$Fm-3m$
226	$Fm-3c$	227	$Fd-3m$	228	$Fd-3c$	229	$Im-3m$	230	$Ia-3d$

Table C.2. Symmetry positions for space group #221 denoted by O_h^1 and ($Pm3m$) using the Schoenflies and Hermann–Mauguin notations, respectively (see Fig. 9.7) [58]

$Pm3m$ O_h^1 No. 221 $P\,4/m\,\bar{3}\,2/m$ $m\,3\,m$ Cubic

Origin at centre ($m3m$)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
48	n	1	$x,y,z;\ z,x,y;\ y,z,x;\ x,z,y;\ y,x,z;\ z,y,x;$ $x,\bar{y},\bar{z};\ z,\bar{x},\bar{y};\ y,\bar{z},\bar{x};\ x,\bar{z},\bar{y};\ y,\bar{x},\bar{z};\ z,\bar{y},\bar{x};$ $\bar{x},y,\bar{z};\ \bar{z},x,\bar{y};\ \bar{y},z,\bar{x};\ \bar{x},z,\bar{y};\ \bar{y},x,\bar{z};\ \bar{z},y,\bar{x};$ $\bar{x},\bar{y},z;\ \bar{z},\bar{x},y;\ \bar{y},\bar{z},x;\ \bar{x},\bar{z},y;\ \bar{y},\bar{x},z;\ \bar{z},\bar{y},x;$ $\bar{x},\bar{y},\bar{z};\ \bar{z},\bar{x},\bar{y};\ \bar{y},\bar{z},\bar{x};\ \bar{x},\bar{z},\bar{y};\ \bar{y},\bar{x},\bar{z};\ \bar{z},\bar{y},\bar{x};$ $\bar{x},y,z;\ \bar{z},x,y;\ \bar{y},z,x;\ \bar{x},z,y;\ \bar{y},x,z;\ \bar{z},y,x;$ $x,\bar{y},z;\ z,\bar{x},y;\ y,\bar{z},x;\ x,\bar{z},y;\ y,\bar{x},z;\ z,\bar{y},x;$ $x,y,\bar{z};\ z,x,\bar{y};\ y,z,\bar{x};\ x,z,\bar{y};\ y,x,\bar{z};\ z,y,\bar{x}.$	General: hkl: hhl: $0kl$: No conditions
24	m	m	$x,x,z;\ z,x,x;\ x,z,x;\ \bar{x},\bar{x},\bar{z};\ \bar{z},\bar{x},\bar{x};\ \bar{x},\bar{z},\bar{x};$ $x,\bar{x},\bar{z};\ z,\bar{x},\bar{x};\ x,\bar{z},\bar{x};\ \bar{x},x,z;\ \bar{z},x,x;\ \bar{x},z,x;$ $\bar{x},x,\bar{z};\ \bar{z},x,\bar{x};\ \bar{x},z,\bar{x};\ x,\bar{x},z;\ z,\bar{x},x;\ x,\bar{z},x;$ $\bar{x},\bar{x},z;\ \bar{z},\bar{x},x;\ \bar{x},\bar{z},x;\ x,x,\bar{z};\ z,x,\bar{x};\ x,z,\bar{x}.$	Special: No conditions
24	l	m	$\tfrac{1}{2},y,z;\ z,\tfrac{1}{2},y;\ y,z,\tfrac{1}{2};\ \tfrac{1}{2},z,y;\ y,\tfrac{1}{2},z;\ z,y,\tfrac{1}{2};$ $\tfrac{1}{2},\bar{y},\bar{z};\ \bar{z},\tfrac{1}{2},\bar{y};\ \bar{y},\bar{z},\tfrac{1}{2};\ \tfrac{1}{2},\bar{z},\bar{y};\ \bar{y},\tfrac{1}{2},\bar{z};\ \bar{z},\bar{y},\tfrac{1}{2};$ $\tfrac{1}{2},y,\bar{z};\ \bar{z},\tfrac{1}{2},y;\ y,\bar{z},\tfrac{1}{2};\ \tfrac{1}{2},\bar{z},y;\ y,\tfrac{1}{2},\bar{z};\ \bar{z},y,\tfrac{1}{2};$ $\tfrac{1}{2},\bar{y},z;\ z,\tfrac{1}{2},\bar{y};\ \bar{y},z,\tfrac{1}{2};\ \tfrac{1}{2},z,\bar{y};\ \bar{y},\tfrac{1}{2},z;\ z,\bar{y},\tfrac{1}{2}.$	
24	k	m	$0,y,z;\ z,0,y;\ y,z,0;\ 0,z,y;\ y,0,z;\ z,y,0;$ $0,\bar{y},\bar{z};\ \bar{z},0,\bar{y};\ \bar{y},\bar{z},0;\ 0,\bar{z},\bar{y};\ \bar{y},0,\bar{z};\ \bar{z},\bar{y},0;$ $0,y,\bar{z};\ \bar{z},0,y;\ y,\bar{z},0;\ 0,\bar{z},y;\ y,0,\bar{z};\ \bar{z},y,0;$ $0,\bar{y},z;\ z,0,\bar{y};\ \bar{y},z,0;\ 0,z,\bar{y};\ \bar{y},0,z;\ z,\bar{y},0.$	
12	j	mm	$\tfrac{1}{2},x,x;\ x,\tfrac{1}{2},x;\ x,x,\tfrac{1}{2};\ \tfrac{1}{2},x,\bar{x};\ \bar{x},\tfrac{1}{2},x;\ x,\bar{x},\tfrac{1}{2};$ $\tfrac{1}{2},\bar{x},\bar{x};\ \bar{x},\tfrac{1}{2},\bar{x};\ \bar{x},\bar{x},\tfrac{1}{2};\ \tfrac{1}{2},\bar{x},x;\ x,\tfrac{1}{2},\bar{x};\ \bar{x},x,\tfrac{1}{2}.$	
12	i	mm	$0,x,x;\ x,0,x;\ x,x,0;\ 0,x,\bar{x};\ \bar{x},0,x;\ x,\bar{x},0;$ $0,\bar{x},\bar{x};\ \bar{x},0,\bar{x};\ \bar{x},\bar{x},0;\ 0,\bar{x},x;\ x,0,\bar{x};\ \bar{x},x,0.$	
12	h	mm	$x,\tfrac{1}{2},0;\ 0,x,\tfrac{1}{2};\ \tfrac{1}{2},0,x;\ x,0,\tfrac{1}{2};\ \tfrac{1}{2},x,0;\ 0,\tfrac{1}{2},x;$ $\bar{x},\tfrac{1}{2},0;\ 0,\bar{x},\tfrac{1}{2};\ \tfrac{1}{2},0,\bar{x};\ \bar{x},0,\tfrac{1}{2};\ \tfrac{1}{2},\bar{x},0;\ 0,\tfrac{1}{2},\bar{x}.$	
8	g	$3m$	$x,x,x;\ x,\bar{x},\bar{x};\ \bar{x},x,\bar{x};\ \bar{x},\bar{x},x;$ $\bar{x},\bar{x},\bar{x};\ \bar{x},x,x;\ x,\bar{x},x;\ x,x,\bar{x}.$	
6	f	$4mm$	$x,\tfrac{1}{2},\tfrac{1}{2};\ \tfrac{1}{2},x,\tfrac{1}{2};\ \tfrac{1}{2},\tfrac{1}{2},x;\ \bar{x},\tfrac{1}{2},\tfrac{1}{2};\ \tfrac{1}{2},\bar{x},\tfrac{1}{2};\ \tfrac{1}{2},\tfrac{1}{2},\bar{x}.$	
6	e	$4mm$	$x,0,0;\ 0,x,0;\ 0,0,x;\ \bar{x},0,0;\ 0,\bar{x},0;\ 0,0,\bar{x}.$	
3	d	$4/mmm$	$\tfrac{1}{2},0,0;\ 0,\tfrac{1}{2},0;\ 0,0,\tfrac{1}{2}.$	
3	c	$4/mmm$	$0,\tfrac{1}{2},\tfrac{1}{2};\ \tfrac{1}{2},0,\tfrac{1}{2};\ \tfrac{1}{2},\tfrac{1}{2},0.$	
1	b	$m3m$	$\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2}.$	
1	a	$m3m$	$0,0,0.$	

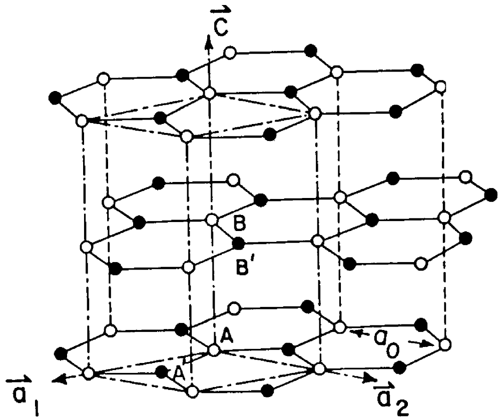


Fig. C.1. Crystal structure of hexagonal graphite, space group #194

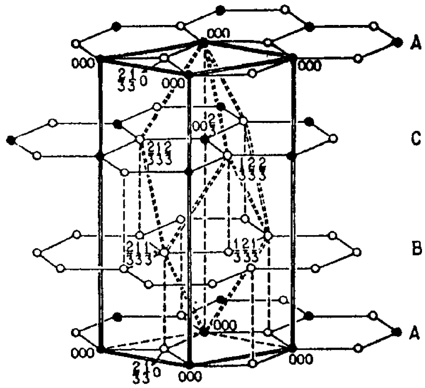


Fig. C.2. Crystal structure of rhombohedral graphite showing *ABC* stacking of the individual sheets, space group #166 $R\bar{3}m$. Also shown with *dashed lines* is the rhombohedral unit cell

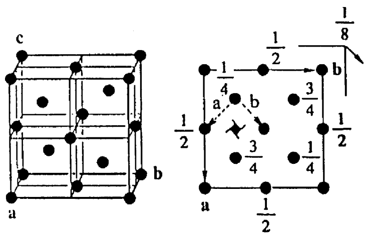


Fig. C.3. (**a**) Diamond structure $Fd3m$ (O_h^7, #227) showing a unit cell with two distinct atom site locations. For the zinc blende structure (see Fig. 10.6) the atoms on the two sites are distinct and belong to group $F\bar{4}3m$ #216. (**b**) The screw axis in the diamond structure shown looking at the projection of the various atoms with their z-axis distances given

C.4 taken from the International Crystallographic Tables [58] list these site symmetries for high symmetry points for a few illustrative 3D space groups in analogy to the Tables in Appendix B which pertain to two-dimensional space groups. For example in Table C.2 for the simple cubic lattice (#221), the general point n has no additional symmetry (C_1), while points a and b have full O_h point group symmetry. The points c through m have more symmetry than the general point n, but less symmetry than points a and b. For each symmetry point a through n, the Wyckoff positions are listed and the corresponding point symmetry for each high symmetry point is given.

To better visualize 3D crystal structures, it is important to show ball and stick models when working with specific crystals. Figure C.1 shows such a model for the crystal structure of 3D hexagonal graphite (space group #194), while Fig. C.2 shows the crystal structure of 3D rhombohedral graphite (space group #166). Both hexagonal and rhombohedral graphite are composed of the same individual 2D graphene layers, but hexagonal graphite has an $ABAB$ stacking sequence of these layer planes, while rhombohedral graphite has an $ABCABC$ stacking of these layers. Because of the differences in their stacking sequences, the structure with the $ABAB$ stacking sequence is described by a nonsymmorphic space group #194, while the structure with the $ABCABC$ stacking sequence is described by a symmorphic space group #166. Figure C.3(a) shows the crystal structure for diamond together with a diagram showing the diamond screw axis (Fig. C.3(b)) that explains the non-symmorphic nature of the diamond structure.

Table C.3 gives a listing similar to Table C.2, but now for the hexagonal non-symmorphic space group $P6_3/mmc$ (D_{6h}^4) which is the appropriate space group for 3D graphite, while Table C.4 gives a similar listing for the rhombohedral symmorphic space group #166 which describes rhombohedral graphite. Group #166 is unusual because it can be specified either within a rhombohedral description or a hexagonal description, as seen in Table C.4. The information provided in the International Crystallographic Tables [58], as exemplified by Table C.4 for group #166, can also be found on the web. Table C.5 taken from the web-site [58] gives the same information on the Wyckoff positions and point symmetries as is contained in Table C.4. The notation in Table C.5 which is taken from the web [54] differs from the notation used in the International Tables for X-ray Crystallography [58] insofar as $-x$, $-y$, $-z$ in [54] are used to denote $\bar{x}$, $\bar{y}$, $\bar{z}$ in [58], and some of the entries are given in a different but equivalent order.

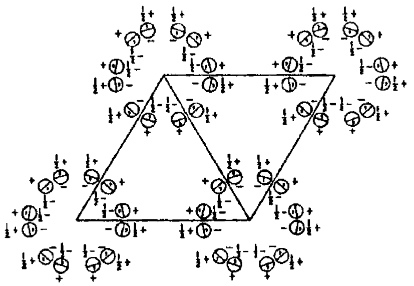
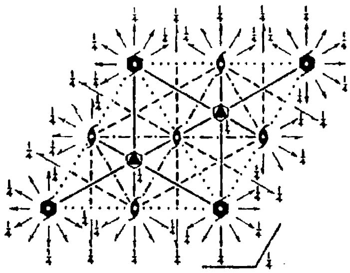
C.2 Reciprocal Space

In this section character tables are presented for the group of the wave vector for a variety of high symmetry points in the Brillouin zone for various space

Table C.3. International Crystallography Table for point group symmetries for the hexagonal space group #194 ($P6_3/mmc$) or D_{6h}^4 (see Fig. C.1)

$P6_3/mmc$ No. 194 $P\,6_3/m\;2/m\;2/c$ $6/m\;m\;m$ Hexagonal

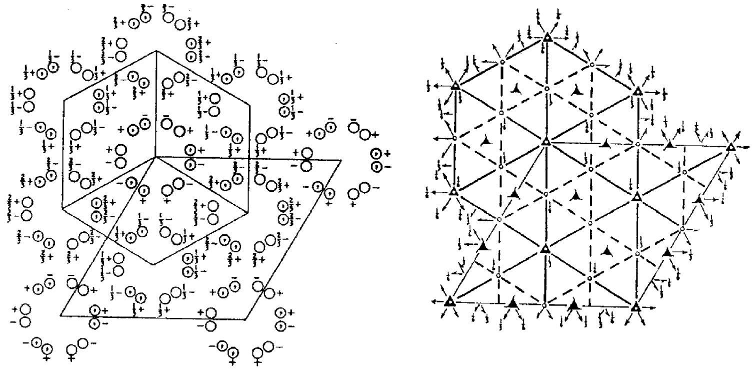
D_{6h}^4

Origin at centre ($\bar{3}m1$)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
24	l	1	$x,y,z;\ \bar{y},x-y,z;\ y-x,\bar{x},z;\ \bar{y},\bar{x},z;\ x,x-y,z;\ y-x,y,z;$ $\bar{x},\bar{y},\bar{z};\ y,y-x,\bar{z};\ x-y,x,\bar{z};\ y,x,\bar{z};\ \bar{x},y-x,\bar{z};\ x-y,\bar{y},\bar{z};$ $\bar{x},\bar{y},\tfrac{1}{2}+z;\ y,y-x,\tfrac{1}{2}+z;\ x-y,x,\tfrac{1}{2}+z;$ $x,y,\tfrac{1}{2}-z;\ \bar{y},x-y,\tfrac{1}{2}-z;\ y-x,\bar{x},\tfrac{1}{2}-z;$ $y,x,\tfrac{1}{2}+z;\ \bar{x},y-x,\tfrac{1}{2}+z;\ x-y,\bar{y},\tfrac{1}{2}+z;$ $\bar{y},\bar{x},\tfrac{1}{2}-z;\ x,x-y,\tfrac{1}{2}-z;\ y-x,y,\tfrac{1}{2}-z.$	$hkil$: No conditions $hh\bar{2h}l$: $l=2n$ $h\bar{h}0l$: No conditions
				Special: as above, plus
12	k	m	$x,2x,z;\ 2\bar{x},\bar{x},z;\ x,\bar{x},z;\ \bar{x},2\bar{x},\bar{z};\ 2x,x,\bar{z};\ \bar{x},x,\bar{z};$ $\bar{x},2\bar{x},\tfrac{1}{2}+z;\ 2x,x,\tfrac{1}{2}+z;\ \bar{x},x,\tfrac{1}{2}+z;$ $x,2x,\tfrac{1}{2}-z;\ 2\bar{x},\bar{x},\tfrac{1}{2}-z;\ x,\bar{x},\tfrac{1}{2}-z.$	no extra conditions
12	j	m	$x,y,\tfrac{1}{4};\ \bar{y},x-y,\tfrac{1}{4};\ y-x,\bar{x},\tfrac{1}{4};\ \bar{y},\bar{x},\tfrac{1}{4};\ x,x-y,\tfrac{1}{4};\ y-x,y,\tfrac{1}{4};$ $\bar{x},\bar{y},\tfrac{3}{4};\ y,y-x,\tfrac{3}{4};\ x-y,x,\tfrac{3}{4};\ y,x,\tfrac{3}{4};\ \bar{x},y-x,\tfrac{3}{4};\ x-y,\bar{y},\tfrac{3}{4}.$	
12	i	2	$x,0,0;\ 0,x,0;\ \bar{x},\bar{x},0;\ x,0,\tfrac{1}{2};\ 0,x,\tfrac{1}{2};\ \bar{x},\bar{x},\tfrac{1}{2};$ $\bar{x},0,0;\ 0,\bar{x},0;\ x,x,0;\ \bar{x},0,\tfrac{1}{2};\ 0,\bar{x},\tfrac{1}{2};\ x,x,\tfrac{1}{2}.$	$hkil$: $l=2n$
6	h	mm	$x,2x,\tfrac{1}{4};\ 2\bar{x},\bar{x},\tfrac{1}{4};\ x,\bar{x},\tfrac{1}{4};\ \bar{x},2\bar{x},\tfrac{3}{4};\ 2x,x,\tfrac{3}{4};\ \bar{x},x,\tfrac{3}{4}.$	no extra conditions
6	g	$2/m$	$\tfrac{1}{2},0,0;\ 0,\tfrac{1}{2},0;\ \tfrac{1}{2},\tfrac{1}{2},0;\ \tfrac{1}{2},0,\tfrac{1}{2};\ 0,\tfrac{1}{2},\tfrac{1}{2};\ \tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2}.$	$hkil$: $l=2n$
4	f	$3m$	$\tfrac{1}{3},\tfrac{2}{3},z;\ \tfrac{2}{3},\tfrac{1}{3},\bar{z};\ \tfrac{2}{3},\tfrac{1}{3},\tfrac{1}{2}+z;\ \tfrac{1}{3},\tfrac{2}{3},\tfrac{1}{2}-z.$	$hkil$: If $h-k=3n$, then $l=2n$
4	e	$3m$	$0,0,z;\ 0,0,\bar{z};\ 0,0,\tfrac{1}{2}+z;\ 0,0,\tfrac{1}{2}-z.$	$hkil$: $l=2n$
2	d	$\bar{6}m2$	$\tfrac{1}{3},\tfrac{2}{3},\tfrac{3}{4};\ \tfrac{2}{3},\tfrac{1}{3},\tfrac{1}{4}.$	$hkil$: If $h-k=3n$, then $l=2n$
2	c	$\bar{6}m2$	$\tfrac{1}{3},\tfrac{2}{3},\tfrac{1}{4};\ \tfrac{2}{3},\tfrac{1}{3},\tfrac{3}{4}.$	
2	b	$\bar{6}m2$	$0,0,\tfrac{1}{4};\ 0,0,\tfrac{3}{4}.$	$hkil$: $l=2n$
2	a	$\bar{3}m$	$0,0,0;\ 0,0,\tfrac{1}{2}.$	

Table C.4. Stereographs for space group #166 R-$3m$, along with the Wyckoff positions and point symmetries for each high symmetry point a through l, listed for both the rhombohedral and hexagonal systems



Origin at centre ($\bar{3}m$)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			(1) RHOMBOHEDRAL AXES:	
				General:
12	i	1	$x,y,z;\ z,x,y;\ y,z,x;\ y,x,z;\ z,y,x;\ x,z,y;$ $\bar{x},\bar{y},\bar{z};\ \bar{z},\bar{x},\bar{y};\ \bar{y},\bar{z},\bar{x};\ \bar{y},\bar{x},\bar{z};\ \bar{z},\bar{y},\bar{x};\ \bar{x},\bar{z},\bar{y}.$	No conditions
				Special:
6	h	m	$x,x,z;\ x,z,x;\ z,x,x;\ \bar{x},\bar{x},\bar{z};\ \bar{x},\bar{z},\bar{x};\ \bar{z},\bar{x},\bar{x}.$	No conditions
6	g	2	$x,\bar{x},\frac{1}{2};\ \bar{x},\frac{1}{2},x;\ \frac{1}{2},x,\bar{x};\ \bar{x},x,\frac{1}{2};\ x,\frac{1}{2},\bar{x};\ \frac{1}{2},\bar{x},x.$	
6	f	2	$x,\bar{x},0;\ \bar{x},0,x;\ 0,x,\bar{x};\ \bar{x},x,0;\ x,0,\bar{x};\ 0,\bar{x},x.$	
3	e	$2/m$	$0,\frac{1}{2},\frac{1}{2};\ \frac{1}{2},0,\frac{1}{2};\ \frac{1}{2},\frac{1}{2},0.$	
3	d	$2/m$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}.$	
2	c	$3m$	$x,x,x;\ \bar{x},\bar{x},\bar{x}.$	
1	b	$\bar{3}m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}.$	
1	a	$\bar{3}m$	$0,0,0.$	
			(2) HEXAGONAL AXES: $(0,0,0;\ \frac{1}{3},\frac{2}{3},\frac{2}{3};\ \frac{2}{3},\frac{1}{3},\frac{1}{3})+$	
				General:
36	i	1	$x,y,z;\ \bar{y},x-y,z;\ y-x,\bar{x},z;$ $\bar{x},\bar{y},\bar{z};\ y,y-x,\bar{z};\ x-y,x,\bar{z};$ $\bar{y},\bar{x},z;\ x,x-y,z;\ y-x,y,z;$ $y,x,\bar{z};\ \bar{x},y-x,\bar{z};\ x-y,\bar{y},\bar{z}.$	$hkil$: $-h+k+l=3n$; $hh2\bar{h}l$: $(l=3n)$; $h\bar{h}0l$: $(h+l=3n)$
				Special: as above only
18	h	m	$x,\bar{x},z;\ x,2x,z;\ 2\bar{x},\bar{x},z;$ $\bar{x},x,\bar{z};\ \bar{x},2\bar{x},\bar{z};\ 2x,x,\bar{z}.$	
18	g	2	$x,0,\frac{1}{2};\ 0,x,\frac{1}{2};\ \bar{x},\bar{x},\frac{1}{2};\ \bar{x},0,\frac{1}{2};\ 0,\bar{x},\frac{1}{2};\ x,x,\frac{1}{2}.$	
18	f	2	$x,0,0;\ 0,x,0;\ \bar{x},\bar{x},0;\ \bar{x},0,0;\ 0,\bar{x},0;\ x,x,0.$	
9	e	$2/m$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ \frac{1}{2},\frac{1}{2},0.$	
9	d	$2/m$	$\frac{1}{2},0,\frac{1}{2};\ 0,\frac{1}{2},\frac{1}{2};\ \frac{1}{2},\frac{1}{2},\frac{1}{2}.$	
6	c	$3m$	$0,0,z;\ 0,0,\bar{z}.$	
3	b	$\bar{3}m$	$0,0,\frac{1}{2}.$	
3	a	$\bar{3}m$	$0,0,0.$	

Table C.5. Wyckoff positions for space group #166 $R\bar{3}m$ (taken from the website given in [54]

Multi-plicity	Wyckoff letter	Site sym-metry	Coordinates $(0,0,0)+$ $(2/3,1/3,1/3)+$ $(1/3,2/3,2/3)+$
36	i	1	(x,y,z) $(-y,x-y,z)$ $(-x+y,-x,z)$ $(y,x,-z)$ $(x-y,-y,-z)$ $(-x,-x+y,-z)$ $(-x,-y,-z)$ $(y,-x+y,-z)$ $(x-y,x,-z)$ $(-y,-x,z)$ $(-x+y,y,z)$ $(x,x-y,z)$
18	h	m	$(x,-x,z)$ $(x,2x,z)$ $(-2x,-x,z)$ $(-x,x,-z)$ $(2x,x,-z)$ $(-x,-2x,-z)$
18	g	2	$(x,0,1/2)$ $(0,x,1/2)$ $(-x,-x,1/2)$ $(-x,0,1/2)$ $(0,-x,1/2)$ $(x,x,1/2)$
18	f	2	$(x,0,0)$ $(0,x,0)$ $(-x,-x,0)$ $(-x,0,0)$ $(0,-x,0)$ $(x,x,0)$
9	e	$2/m$	$(1/2,0,0)$ $(0,1/2,0)$ $(1/2,1/2,0)$
9	d	$2/m$	$(1/2,0,1/2)$ $(0,1/2,1/2)$ $(1/2,1/2,1/2)$
6	c	$3m$	$(0,0,z)$ $(0,0,-z)$
3	b	$-3m$	$(0,0,1/2)$
3	a	$-3m$	$(0,0,0)$

groups. Diagrams for the high symmetry points are also presented for a few representative examples. The high symmetry points of the Brillouin zone for the simple cubic lattice are shown in Fig. C.4, and correspondingly, the high symmetry points for the FCC and BCC space groups #225 and #229 are shown in Fig. C.5(a), C.5(b), respectively. Table C.6 gives a summary of space groups listed in this appendix, together with the high symmetry points for the various groups that are considered in this appendix, giving the road-map for three symmorphic cubic groups (#221 for the simple cubic lattice, #225 for the FCC lattice, and #229 for the BCC lattice). For each high symmetry point and space group that is listed, its symmetry and the table number where the character table appears is given.

When the tables for the group of the wave vector are given (as for example in Tables C.7, C.8 and C.10), the caption cites a specific high symmetry point for a particular space group. Below the table are listed other high symmetry points for the same or other space groups for which the character table applies. Following Table C.8 which applies to point group C_{4v}, the multiplication table for the elements of group C_{4v} is given in Table C.9. Some high symmetry points which pertain to the same group of the wave vector may have classes containing different twofold axes. For this reason, when basis functions are given with the character table, they apply only to the high symmetry point given in the caption to the table. Sometimes a high symmetry point is within the Brillouin zone such as point Λ in Table C.10, while point F for the BCC structure is on the Brillouin zone boundary. Many of these issues are illustrated in Table C.11 which gives the character table for point group C_{2v} (see Table A.5), but the symmetry operations for the twofold axes can refer to different twofold axes, as for example for points Σ and Z. A similar situation applies for Table C.15 for the X and M points for space group #221 regarding their twofold axes. With regard to Table C.12 for the W point for the FCC lattice, we see that the group of the wave vector has C_{4v} symmetry, but in contrast to the symmetry operations for the Δ point in Table C.8 which is an interior point in the Brillouin zone with C_{4v} symmetry, only four of the symmetry operations E, C_4^2, iC_4^2, and $iC_{2'}$ take W into itself while four other symmetry operations $2C_4$, iC_4^2, and $iC_{2'}$ require a reciprocal lattice vector to take W into itself (Table C.12).

Also included in Table C.6 is a road-map for the character tables provided for the group of the wave vector for the nonsymmorphic diamond structure (#227). For this structure, the symmetry operations of classes that pertain to the O_h point group but are not in the T_d point group, include a translation $\tau_d = (a/4)(1,1,1)$ and the entries for the character tables for these classes includes a phase factor $\exp(\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{\tau}_d)$ (see Table C.17 for the Γ point and Table C.18 for the L point). The special points X, W, and Z on the square face for the diamond structure (#227) do not correspond to Bragg reflections and along this face, and the energy levels stick together (see Sect. 12.5) at these high symmetry points (see Tables C.19 and C.20). Additional character tables for the group of the wave vector at high symmetry points Λ, Σ, Δ, and X for the diamond structure are found in Sect. 10.8 (Tables 10.9–10.12).

Next we consider the group of the wave vector for crystals with hexagonal/rhombohedral symmetry as occurs for graphite with $ABCABC$ stacking (symmorphic space group #166) which has high symmetry points shown in Fig. C.6(a) and (b). Since the space group #166 is symmorphic, the group of the wave vector at high symmetry points is simply found. Explicit examples are given in Tables C.21–C.23 for three points of high symmetry for space group #166. From Figure C.6 it can be seen that the group of the wave vector for the Γ point $k = 0$ has the highest symmetry of D_{3d}, which is shared by point Z at the center of the hexagonal face in Fig. C.6(b) (see Table C.21). The point Δ has a twofold axis with C_2 symmetry (Table C.23) and leads to the point X with C_{3v} point group symmetry at the center of the rectangular face (see Table C.22). The compatibility of the Δ point with the Γ and X points can be verified.

Finally, we present in Tables C.24–C.29 the character tables for the group of the wave vector for selected high symmetry points for the nonsymmorphic hexagonal structure given by space group #194, which is descriptive of 3D graphite with $ABAB$ layer stacking. The high symmetry points in the Brillouin zone for the hexagonal structure are shown in Fig. C.7. Specific character tables are given for the high symmetry points $\Gamma(k = 0)$ in Table C.24, a Δ

Table C.6. Group of the wave vector at various symmetry points in the Brillouin zone for some specific space groups

lattice	point	$\boldsymbol{k}$	symmetry	Table
#221[a]	Γ	(0,0,0)	O_h	C.7
	R	$[(2\pi/a)(1,1,1)]$	O_h	C.7
	X	$[(2\pi/a)(1,0,0)]$	D_{4h}	C.15
	M	$[(2\pi/a)(1,1,0)]$	D_{4h}	C.15
	Λ	$[(2\pi/a)(x,x,x)]$	C_{3v}	C.10
	Σ	$[(2\pi/a)(x,x,0)]$	C_{2v}	C.11
	Δ	$[(2\pi/a)(x,0,0)]$	C_{4v}	C.8
	S	$[(2\pi/a)(1,z,z)]$	C_{2v}	C.11
	T	$[(2\pi/a)(1,1,z)]$	C_{4v}	C.8
	Z	$[(2\pi/a)(1,y,0)]$	C_{2v}	C.11
#225[b]	Γ	(0,0,0)	O_h	C.7
	X	$[(2\pi/a)(1,0,0)]$	D_{4h}	C.15
	W	$[(\pi/a)(2,1,0)]$	C_{4v}	C.12
	L	$[(\pi/a)(1,1,1)]$	D_{3d}	C.16
	Λ	$[(\pi/a)(x,x,x)]$	C_{3v}	C.10
	Σ	$[(2\pi/a)(x,x,0)]$	C_{2v}	C.11
	Δ	$[(2\pi/a)(x,0,0)]$	C_{4v}	C.8
	K	$[(2\pi/a)(0,3/4,3/4)]$	C_{2v}	C.11
	U	$[(2\pi/a)(1,1/4,1/4)]$	C_{2v}	C.11
	Z	$[(2\pi/a)(1,y,0)]$	C_{2v}	C.11
#227[c]	Γ	(0,0,0)	O_h	C.17
	X	$[(2\pi/a)(1,0,0)]$	D_2	10.12
	W	$[(\pi/a)(2,1,0)]$	C_{4v}	C.19
	L	$[(\pi/a)(1,1,1)]$	D_{3d}	C.18
	Λ	$[(2\pi/a)(x,x,x)]$	C_{3v}	10.11
	Σ	$[(2\pi/a)(x,x,0)]$	C_{2v}	10.10
	Δ	$[(2\pi/a)(x,0,0)]$	C_{4v}	10.9
	$Z(V)$	$[(2\pi/a)(1,y,0)]$	C_{2v}	C.20
	Q	$[(4\pi/a)(1/4,1/2-y,y)]$	C_{2v}	A.5
#229[d]	Γ	(0,0,0)	O_h	C.7
	Λ	$[(\pi/a)(x,x,x)]$	C_{3v}	C.10
	Σ	$[(\pi/a)(x,x,0)]$	C_{2v}	C.11
	Δ	$[(2\pi/a)(x,0,0)]$	C_{4v}	C.8
	H	$[(2\pi/a)(1,0,0)]$	D_{4h}	C.15
	P	$[(\pi/a)(1,1,1)]$	T_d	C.13
	F	$[(\pi/a)(1+2x,1-2x,1-2x)]$	C_{3v}	C.10
	G	$[(\pi/a)(1+2x,1-2x,0)]$	C_{2v}	C.11

[a]See Fig. C.4; [b]See Fig. C.5(a); [c]See Figs. C.3 and C.5(a); [d]See Fig. C.5(b)

Table C.6 (continued)

lattice	point	$\boldsymbol{k}$	symmetry	Table
	D	$[(\pi/a)(1,1,z)]$	C_{2v}	C.11
	N	$[(\pi/a)(1,1,0)]$	D_{2h}	C.14
#166[e]	Γ	(0,0,0)	D_{3d}	C.21
	Λ	$[(2\pi/c)(0,0,z)]$	D_3	C.22
	Δ	$[(2\pi/a)(x,0,0)]$	C_2	C.23
	Z	$[(2\pi/c)(0,0,1)]$	D_{3d}	C.21
	X	$[(2\pi/a)(1,0,0)]$	D_3	C.22
#194[f]	Γ	(0,0,0)	D_{6h}	C.24
	A	$[(2\pi/c)(0,0,1)]$	D_{3h}	C.26
	K	$[(2\pi/a)(1/3,1/3,0)]$	D_{3h}	C.27
	H	$[(2\pi)(1/3a,1/3a,1/c)]$	D_{3h}	C.28
	Δ	$[(2\pi/c)(0,0,z)]$	C_{6v}	C.25
	P	$[(2\pi)(1/3a,1/3a,z/c)]$	C_{3v}	C.29
	M	$[(\pi/a)(1,-1,0)]$	D_{2h}	C.30
	T	$[(\pi/a)(1-x,1+x,0)]$	C_{2v}	C.31
	Σ	$[(\pi/a)(x,-x,0)]$	C_{2v}	C.32
	U	$[(2\pi)(1/3a,-1/3a,x/c)]$	C_{1h}	C.33

[e]See Fig. C.6; [f]See Fig. C.7

point in Table C.25, an A point in Table C.26 together with some compatibility relations, a K point in Table C.27, an H point in Table C.28 and a P point in Table C.29.

In the character Table C.24 for the Γ point ($k = 0$), the six classes which are in D_{6h} but not in D_{3d} have a translation vector $\boldsymbol{\tau} = (c/2)(0,0,1)$ in their symmetry operations $\{R|\tau\}$. Phase factors are seen in Table C.25 for the Δ point which is at an interior $k \neq 0$ point in the Brillouin zone. The phase factors $T_\Delta = \exp(\mathrm{i}\boldsymbol{k}_\Delta \cdot \boldsymbol{\tau})$ appear in the character table for the classes containing a translation vector τ. Points A and H are special high symmetry points where energy levels stick together because the points in reciprocal space associated with this plane do not correspond to a true Bragg reflection, i.e., the calculated structure factor for these points is zero. Character Tables for other high symmetry points for group #194 are also given in Table C.30 for point M, Table C.31 for point T, Table C.32 for point Σ, Table C.33 for point U while Table C.34 gives pertinent compatibility relations for group #194. Appendix D gives further character tables for double groups based on group #194 where the spin on the electron is considered in formulating the symmetry for the electronic energy band structure (Tables D.10–D.14).

Table C.7. Character table (for group O_h) for the group of the wave-vector at a Γ point for various cubic space groups

representation	basis functions	E	$3C_4^2$	$6C_4$	$6C_2$	$8C_3$	i	$3iC_4^2$	$6iC_4$	$6iC_2$	$8iC_3$
Γ_1	1	1	1	1	1	1	1	1	1	1	1
Γ_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
Γ_{12}	$\begin{cases} x^2-y^2 \\ 2z^2-x^2-y^2 \end{cases}$	2	2	0	0	−1	2	2	0	0	−1
Γ_{15}	x, y, z	3	−1	1	−1	0	−3	1	−1	1	0
Γ_{25}	$z(x^2-y^2)$, etc.	3	−1	−1	1	0	−3	1	1	−1	0
Γ_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
Γ_2'	xyz	1	1	−1	−1	1	−1	−1	1	1	−1
Γ_{12}'	$xyz(x^2-y^2)$, etc.	2	2	0	0	−1	−2	−2	0	0	1
Γ_{15}'	$xy(x^2-y^2)$, etc.	3	−1	1	−1	0	3	−1	1	−1	0
Γ_{25}'	xy, yz, zx	3	−1	−1	1	0	3	−1	−1	1	0

$\Gamma = (0,0,0)$ [SC (#221), FCC (#225), BCC (#229)]. $R = (2\pi/a)(1,1,1)$ [SC (#221)]. The partners for Γ_{25} are $z(x^2-y^2), x(y^2-z^2), y(z^2-x^2)$, for Γ_{12}' are $xyz(x^2-y^2), xyz(2z^2-x^2-y^2)$, for Γ_{25}' are $xy(x^2-y^2), yz(y^2-z^2), zx(z^2-x^2)$

Table C.8. Character table (for group C_{4v}) for the group of the wave-vector at a Δ point for various cubic space groups

representation	basis functions	E	C_4^2	$2C_4$	$2iC_4^2$	$2iC_2'$
Δ_1	$1; x; 2x^2-y^2-z^2$	1	1	1	1	1
Δ_2	y^2-z^2	1	1	−1	1	−1
Δ_2'	yz	1	1	−1	−1	1
Δ_1'	$yz(y^2-z^2)$	1	1	1	−1	−1
Δ_5	$y, z; xy, xz$	2	−2	0	0	0

$\Delta = (2\pi/a)(x,0,0)$ (SC, FCC, BCC). $T = (2\pi/a)(1,1,z)$ (SC)

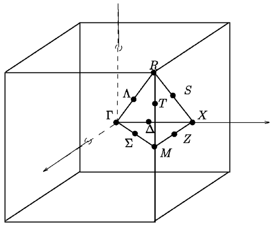


Fig. C.4. Brillouin zone for a simple cubic lattice (#221) showing the high symmetry points and axes

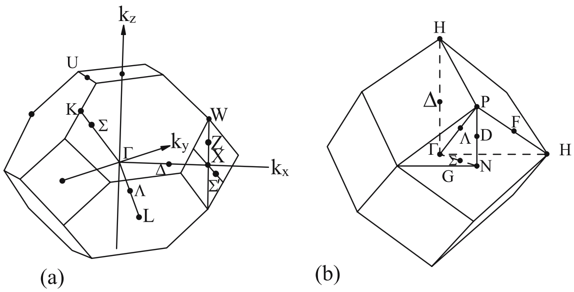
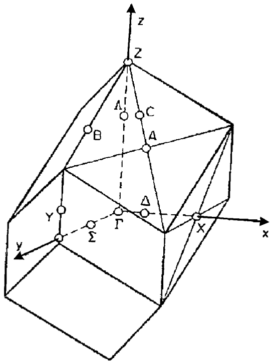


Fig. C.5. Brillouin zones for the (**a**) face-centered (#225) and (**b**) body-centered (#229) cubic lattices. Points and lines of high symmetry are indicated

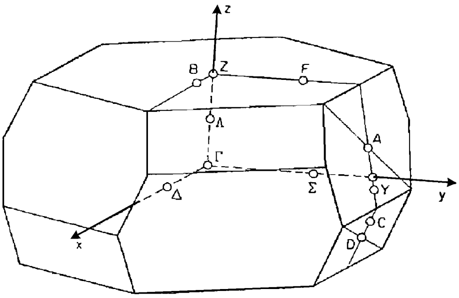
Table C.9. Multiplication table for group C_{4v}

class	operation			designation	E	α	β	γ	δ	ε	ζ	η
E	x	y	z	E	E	α	β	γ	δ	ε	ζ	η
C_4^2	x	$-y$	$-z$	α	α	E	γ	β	ε	δ	η	ζ
$2C_4$	x	$-z$	y	β	β	γ	α	E	ζ	η	ε	δ
	x	z	$-y$	γ	γ	β	E	α	η	ζ	δ	ε
$2iC_4^2$	x	$-y$	z	δ	δ	ε	η	ζ	E	α	γ	β
	x	y	$-z$	ε	ε	δ	ζ	η	α	E	β	γ
$2iC_2$	x	$-z$	$-y$	ζ	ζ	η	δ	ε	β	γ	E	α
	x	z	y	η	η	ζ	ε	δ	γ	β	α	E

The rule for using the multiplication table is $\alpha\beta = (x,-y,-z)(x,-z,y) = [x,-(-z),-(y)] = (x,z,-y) = \gamma$, $\beta\delta = (x,-z,y)(x,-y,z) = (x,z,y) = \eta$, where the right operator (β) designates the row and the left operator (α) designates the column.



(a)



(b)

Fig. C.6. Brillouin zones for a rhombohedral lattice shown in (**a**) for rhombohedral axes and in (**b**) for hexagonal axes as presented in Table C.4 where the site symmetries corresponding to (**a**) and (**b**) are both presented for one of the rhombohedral groups

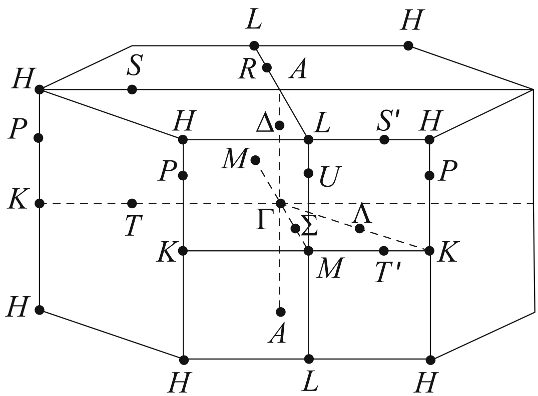


Fig. C.7. Brillouin zone for a hexagonal Bravais lattice showing high symmetry points for hexagonal structures

Table C.10. Character table for group C_{3v} for point Λ for various cubic space groups

representation	basis	E	$2C_3$	$3iC_2$
Λ_1	$1; x+y+z$	1	1	1
Λ_2	$x(y^2-z^2)+y(z^2-x^2)+z(x^2-y^2)$	1	1	-1
Λ_3	$2x-y-z, y-z$	2	-1	0

$\Lambda = (2\pi/a)(x,x,x)$ (SC, FCC, BCC). $F = (\pi/a)(1+2x, 1-2x, 1-2x)$ (BCC)

Table C.11. Character table for the group C_{2v} of the wave vector Σ for various cubic space groups

represen-tation					
	Z	E	C_4^2	iC_4^2	$iC_{4\perp}^2$
	Σ	E	C_2	iC_4^2	iC_2
	G, K, U, S	E	C_2	iC_4^2	iC_2
	D	E	C_4^2	iC_2	$iC_{2\perp}$
Σ_1		1	1	1	1
Σ_2		1	1	-1	-1
Σ_3		1	-1	-1	1
Σ_4		1	-1	1	-1

$\Sigma = (2\pi/a)(x,x,0)$ (SC, FCC, BCC) $G = (\pi/a)(1+2x, 1-2x, 0)$ (BCC). $K = (2\pi/a)(0, \frac{3}{4}, \frac{3}{4})$ (FCC) $U = (2\pi/a)(1, \frac{1}{4}.\frac{1}{4})$ (FCC) $D = (\pi/a)(1,1,z)$ (BCC) $Z = (2\pi/a)(1,y,0)$ (SC, FCC) $S = (2\pi/a)(1,z,z)$ (SC)

Table C.12. Character table for group C_{4v} of the wave vector for W for a symmorphic FCC lattice (#225)

representation	E	C_4^2	$2C_4$	$2iC_4^2$	$2iC_{2'}$
W_1	1	1	1	1	1
W_2	1	1	-1	1	-1
W_3	1	1	-1	-1	1
W_4	1	1	1	-1	-1
W_5	2	-2	0	0	0

$W = (\pi/a)(2,1,0)$ (FCC)

Table C.13. Character table for group T_d for the group of the wave vector for the P point in the BCC lattice

representation	E	$3C_4^2$	$8C_3$	$6iC_4$	$6iC_2$
P_1	1	1	1	1	1
P_2	1	1	1	-1	-1
P_3	2	2	-1	0	0
P_4	3	-1	0	-1	1
P_5	3	-1	0	1	-1

$P = (\pi/a)(1,1,1)$ (BCC)

Table C.14. Character table for group $D_{2h} = D_2 \otimes i$ for the group of the wave vector for point N (BCC)

representation	E	C_4^2	$C_{2\parallel}$	$C_{2\perp}$	i	iC_4^2	$iC_{2\parallel}$	$iC_{2\perp}$
N_1	1	1	1	1	1	1	1	1
N_2	1	−1	1	−1	1	−1	1	−1
N_3	1	−1	−1	1	1	−1	−1	1
N_4	1	1	−1	−1	1	1	−1	−1
N_1'	1	1	1	1	−1	−1	−1	−1
N_2'	1	−1	1	−1	−1	1	−1	1
N_3'	1	1	−1	−1	−1	−1	1	1
N_4'	1	−1	−1	1	−1	1	1	−1

$N = (\pi/a)(1,1,0)$ (BCC)

Table C.15. Character table for D_{4h} for the group of the wave vector for point X for various cubic space groups

representation	basis	E	$2C_{4\perp}^2$	$C_{4\parallel}^2$	$2C_{4\parallel}^2$	$2C_2$	i	$2iC_{4\perp}^2$	$iC_{4\parallel}^2$	$2iC_{4\parallel}$	$2iC_2$
X_1	$1; 2x^2-y^2-z^2$	1	1	1	1	1	1	1	1	1	1
X_2	y^2-z^2	1	1	1	−1	−1	1	1	1	−1	−1
X_3	yz	1	−1	1	−1	1	1	−1	1	−1	1
X_4	$yz(y^2-z^2)$	1	−1	1	1	−1	1	−1	1	1	−1
X_5	xy, xz	2	0	−2	0	0	2	0	−2	0	0
X_1'	$xyz(y^2-z^2)$	1	1	1	1	1	−1	−1	−1	−1	−1
X_2'	xyz	1	1	1	−1	−1	−1	−1	−1	1	1
X_3'	$x(y^2-z^2)$	1	−1	1	−1	1	−1	1	−1	1	−1
X_4'	x	1	−1	1	1	−1	−1	1	−1	−1	1
X_5'	y, z	2	0	−2	0	0	−2	0	2	0	0

$X = (2\pi/a)(1,0,0)$ (SC, FCC). $M = (2\pi/a)(1,1,0)$ (SC). $H = (2\pi/a)(1,0,0)$ (BCC)

Table C.16. Character table for D_{3d} for the group of the wave vector for point L (FCC)

representation	basis	E	$2C_3$	$3C_2$	i	$2iC_3$	$3iC_2$
L_1	$1; xy+yz+xz$	1	1	1	1	1	1
L_2	$yz(y^2-z^2)+xy(x^2-y^2)+xz(z^2-x^2)$	1	1	−1	1	1	−1
L_3	$2x^2-y^2-z^2, y^2-z^2$	2	−1	0	2	−1	0
L_1'	$x(y^2-z^2)+y(z^2-x^2)+z(x^2-y^2)$	1	1	1	−1	−1	−1
L_2'	$x+y+z$	1	1	−1	−1	−1	1
L_3'	$y-z, 2x-y-z$	2	−1	0	−2	1	0

$L = (\pi/a)(1,1,1)$ (FCC)

Table C.17. Character table for group O_h appropriately modified to describe the group of the wave vector for $k = 0$ (the Γ-point) for the diamond structure (#227)

representation	$\{E\|0\}$	$3\{C_4^2\|0\}$	$6\{C_4\|\tau_d\}$	$6\{C_{2'}\|\tau_d\}$	$8\{C_3\|0\}$	$\{i\|\tau_d\}$	$3\{iC_4^2\|\tau_d\}$	$6\{iC_4\|0\}$	$6\{iC_{2'}\|0\}$	$8\{iC_3\|\tau_d\}$
Γ_1	1	1	1	1	1	1	1	1	1	1
Γ_2	1	1	−1	−1	1	1	1	−1	−1	1
Γ_{12}	2	2	0	0	−1	2	2	0	0	−1
Γ_{15}	3	−1	1	−1	0	−3	1	−1	1	0
Γ_{25}	3	−1	−1	1	0	−3	1	1	−1	0
Γ_1'	1	1	1	1	1	−1	−1	−1	−1	−1
Γ_2'	1	1	−1	−1	1	−1	−1	1	1	−1
Γ_{12}'	2	2	0	0	−1	−2	−2	0	0	1
Γ_{15}'	3	−1	1	−1	0	3	−1	1	−1	0
Γ_{25}'	3	−1	−1	1	0	3	−1	−1	1	0

$\tau_d = (a/4)(1,1,1)$. The classes involving τ_d translations are classes in the O_h point group that are not in the T_d point group

Table C.18. Character table for group D_{3d} of the wave vector for point L for the diamond structure (#227)

representation	basis	$\{E\|0\}$	$2\{C_3\|0\}$	$3\{C_{2'}\|0\}$	$\{i\|0\}$	$2\{iC_3\|0\}$	$3\{iC_{2'}\|0\}$
L_1	$1; xy + yz + xz$	1	1	1	1	1	1
L_2	$yz(y^2 - z^2) + xy(x^2 - y^2) + xz(z^2 - x^2)$	1	1	−1	1	1	−1
L_3	$2x^2 - y^2 - z^2, y^2 - z^2$	2	−1	0	2	−1	0
L_1'	$x(y^2 - z^2) + y(z^2 - x^2) + z(x^2 - y^2)$	1	1	1	−1	−1	−1
L_2'	$x + y + z$	1	1	−1	−1	−1	1
L_3'	$y - z, 2x - y - z$	2	−1	0	−2	1	0

For the L point $(\pi/a)(1,1,1)$, the group of the wave vector has no symmetry operations involving the translation vector $\tau_d = (a/4)(1,1,1)$

Table C.19. Character table for group C_{4v} for the group of the wave vector for the W point for the diamond structure (#227)

representation[a]	$\{E\|0\}$	$\{C_4^2\|0\}$	$2\{C_4\|\tau_d\}$	$2\{iC_4^2\|\tau_d\}$	$2\{iC_{2'}\|0\}$
W_1	2	2	0	0	0
W_2	2	−2	0	0	0

[a] Note $\tau_d = (a/4)(1,1,1)$ $W = (\pi/a)(2,1,0)$. Note the W point is not a point with Bragg reflections, so energy levels stick together at this point.

Table C.20. Character table for group C_{2v} of the group of the wave vector for the Z (or V) point for the diamond structure (#227)

representation[a]	$\{E\|0\}$	$\{C_4^2\|0\}$	$\{iC_4^2\|\tau_d\}$	$\{iC_{4\perp}^2\|\tau_d\}$
Z_1	2	2	0	0
Z_2	2	−2	0	0

$Z = (2\pi/a)(1,y,0)$ and $\tau_d = (a/4)(1,1,1)$. Note that the Z (or V) point is not a point with Bragg reflections, so energy bands stick together at this point

Table C.21. Character table with point group symmetry D_{3d} ($\bar{3}m$), for the group of the wave vector at the Γ point ($\boldsymbol{k} = 0$) for the space group #166 $R\bar{3}m$

D_{3d} ($\bar{3}m$)	representation	E	$2C_3$	$3C_{2'}$	i	$2iC_3$	$3iC_{2'}$
	Γ_1^+	1	1	1	1	1	1
	Γ_2^+	1	1	−1	1	1	−1
	Γ_3^+	2	−1	0	2	−1	0
	Γ_1^-	1	1	1	−1	−1	−1
	Γ_2^-	1	1	−1	−1	−1	1
	Γ_3^-	2	−1	0	−2	1	0

$\Gamma = (0,0,0)$. $Z = (2\pi/c)(0,0,1)$

Table C.22. Character table with point group symmetry $C_{3v}(3m)$ for group of the wave vector for a point Λ for the space group #166 $R\bar{3}m$

$C_{3v}(3m)$		E	$2C_3$	$3\sigma_v$
	Λ_1	1	1	1
	Λ_2	1	1	−1
	Λ_3	2	−1	0

$\Lambda = (2\pi/c)(0,0,z)$. $X = (2\pi/a)(1,0,0)$

Table C.23. Character table with point group symmetry $C_2(2)$ for the group of the wave vector for a point Δ for the space group #166 $R\bar{3}m$

C_2 (2)	E	$C_{2'}$
Δ_1	1	1
Δ_2	1	−1

$\Delta = (2\pi/a)(x,0,0)$

Table C.24. Character table with point group symmetry D_{6h} appropriately modified to describe the group of the wave vector for a point Γ $(k=0)$ for the space group #194 D_{6h}^4 $(P6_3/mmc)$[a,b]

	$\{E\|0\}$	$\{C_2\|\tau\}$	$\{C_3^+\|0\}$ $\{C_3^-\|0\}$	$\{C_6^-\|\tau\}$ $\{C_6^+\|\tau\}$	$\{C_2'^A\|0\}$ $\{C_2'^B\|0\}$ $\{C_2'^C\|0\}$	$\{C_2''^A\|\tau\}$ $\{C_2''^B\|\tau\}$ $\{C_2''^C\|\tau\}$	$\{i\|0\}$	$\{\sigma_h\|\tau\}$	$\{S_6^+\|0\}$ $\{S_6^-\|0\}$	$\{S_3^-\|\tau\}$ $\{S^+\|\tau\}$	$\{\sigma_d^A\|0\}$ $\{\sigma_d^B\|0\}$ $\{\sigma_d^C\|0\}$	$\{\sigma_v^A\|\tau\}$ $\{\sigma_v^B\|\tau\}$ $\{\sigma_v^C\|\tau\}$		
Γ_1^+	1	1	1	1	1	1	1	1	1	1	1	1		x^2+y^2 , z^2
Γ_2^+	1	1	1	1	−1	−1	1	1	1	1	−1	−1		R_z
Γ_3^+	1	−1	1	−1	1	−1	1	−1	1	−1	1	−1		
Γ_4^+	1	−1	1	−1	−1	1	1	−1	1	−1	−1	1		
Γ_5^+	2	−2	−1	1	0	0	2	−2	−1	1	0	0		(xz, yz), (R_x, R_y)
Γ_6^+	2	2	−1	−1	0	0	2	2	−1	−1	0	0		(x^2-y^2, xy)
Γ_1^-	1	1	1	1	1	1	−1	−1	−1	−1	−1	−1		
Γ_2^-	1	1	1	1	−1	−1	−1	−1	−1	−1	1	1	z	
Γ_3^-	1	−1	1	−1	1	−1	−1	1	−1	1	−1	1		
Γ_4^-	1	−1	1	−1	−1	1	−1	1	−1	1	1	−1		
Γ_5^-	2	−2	−1	1	0	0	−2	2	1	−1	0	0	(x, y)	
Γ_6^-	2	2	−1	−1	0	0	−2	−2	1	1	0	0		

[a] Since $D_{6h} = D_6 \otimes i$, the group D_{6h} has 12 classes and 12 irreducible representations

[b] Note that the symmetry operations for the nonsymmorphic group of the wave vector at $k = 0$ have translations $\tau = (c/2)(0,0,1)$ if they are elements of group D_{6h} but are not in group D_{3d}

Table C.25. Character table with point group symmetry C_{6v} for the group of the wave vector for a point Δ for the space group #194

C_{6v}	$\{E\|0\}$	$\{C_2\|\boldsymbol{\tau}\}$	$2\{C_3\|0\}$	$2\{C_6\|\boldsymbol{\tau}\}$	$3\{\sigma_d\|0\}$	$3\{\sigma_v\|\boldsymbol{\tau}\}$
Δ_1	1	$1 \cdot T_\Delta$	1	$1 \cdot T_\Delta$	1	$1 \cdot T_\Delta$
Δ_2	1	$1 \cdot T_\Delta$	1	$1 \cdot T_\Delta$	-1	$-1 \cdot T_\Delta$
Δ_3	1	$-1 \cdot T_\Delta$	1	$-1 \cdot T_\Delta$	1	$-1 \cdot T_\Delta$
Δ_4	1	$-1 \cdot T_\Delta$	1	$-1 \cdot T_\Delta$	-1	$1 \cdot T_\Delta$
Δ_5	2	$-2 \cdot T_\Delta$	-1	$1 \cdot T_\Delta$	0	0
Δ_6	2	$2 \cdot T_\Delta$	-1	$-1 \cdot T_\Delta$	0	0

The symmetry operations with translations for point $\Delta = (2\pi/c)(0,0,z)$, where $0 \leq z \leq 1$ are consistent with those in Table C.24 for $k = 0$. The translation here is $\tau = (c/2)(0,0,1)$ and the phase factor is $T_\Delta = \exp(\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{\tau})$ so that at the dimensionless z end points we have $T_\Delta = 1$ at $z = 0$ and $T_\Delta = -1$ at $z = 1$. See Table C.34 for compatibility relations.

Table C.26. Character table with point group symmetry C_{3v} for the group of the wave vector for point A for the space group #194

C_{3v}	$\{E\|0\}$	$\{2C_3\|0\}$	$3\{\sigma_d\|0\}$	compatibility relations
A_1	2	2	2	$A_1 \to \Delta_1 + \Delta_3$
A_2	2	2	-2	$A_2 \to \Delta_2 + \Delta_4$
A_3	4	-2	0	$A_3 \to \Delta_5 + \Delta_6$

Point $A = (2\pi/c)(0,0,1)$. At the A point in the Brillouin zone, the structure factor vanishes so that Bragg reflections do not occur. Therefore the compatibility relations given on the right side of Table C.26 show that at the A point the Δ point bands stick together.

Table C.27. Character table with point group symmetry D_{3h} for the group of the wave vector for a point K for the space group #194

	$\{E\|0\}$	$\{C_3^+\|0\}$ $\{C_3^-\|0\}$	$\{C_2'^A\|0\}$ $\{C_2'^B\|0\}$ $\{C_2'^C\|0\}$	$\{\sigma_h\|\tau\}$	$\{S_3^-\|\tau\}$ $\{S_3^+\|\tau\}$	$\{\sigma_v^A\|\tau\}$ $\{\sigma_v^B\|\tau\}$ $\{\sigma_v^C\|\tau\}$		
K_1^+	1	1	1	1	1	1		$x^2+y^2,\ z^2$
K_2^+	1	1	-1	1	1	-1		R_z
K_3^+	2	-1	0	2	-1	0		(x^2-y^2, xy) (R_x, R_y)
K_1^-	1	1	1	-1	-1	-1		
K_2^-	1	1	-1	-1	-1	1	z	
K_3^-	2	-1	0	-2	1	0	(x,y)	

compatibility relations
$K_1^+ \to P_1;\ K_2^+ \to P_2;\ K_3^+ \to P_3;\ K_1^- \to P_2;\ K_2^- \to P_1;\ K_3^- \to P_3$

$K = (2\pi/a)(1/3, 1/3, 0)$

Table C.28. Character table with point group symmetry D_{3h} for the group of the wave vector for point H for the space group #194

$D_{3h}(\overline{6}m2)$	$\{E\|0\}$	$2\{C_3\|0\}$	$3\{C_{2'}\|0\}$	$\{\sigma_h\|\tau\}$	$2\{S_3\|\tau\}$[a]		$3\{\sigma_v\|\tau\}$	compatibility relations
H_1	2	-1	0	0	$-\sqrt{3}i$	$\sqrt{3}i$	0	$H_1 \to P_3$
H_2	2	-1	0	0	$\sqrt{3}i$	$-\sqrt{3}i$	0	$H_2 \to P_3$
H_3	2	2	0	0	0	0	0	$H_3 \to P_1 + P_2$
H_4	1	-1	i	i	i	$-i$	1	$H_4 \to P_1$
H_5	1	-1	i	$-i$	$-i$	i	-1	$H_5 \to P_1$
H_6	1	-1	$-i$	$-i$	$-i$	i	1	$H_6 \to P_2$

$H = 2\pi(1/3a, 1/3a, 1/c)$

[a] Note that the two columns under class $2\{S_3|\tau\}$ refer to two symmetry operations in this class which have characters that are complex conjugates of one another.

Table C.29. Character table with point group symmetry C_{3v} for the group of the wave vector for point P for the space group #194

C_{3v}	$\{E\|0\}$	$2\{C_3\|0\}$	$3\{\sigma_v\|\tau\}$
P_1	1	1	$1 \cdot T_p$
P_2	1	1	$-1 \cdot T_p$
P_3	2	-1	0

$P = 2\pi(1/3a, 1/3a, z/c)$. $T_p = \exp i\boldsymbol{k}_p \cdot \boldsymbol{\tau}$ where $0 < z < 1$ and $\boldsymbol{\tau} = (c/2)(0, 0, 1)$

Table C.30. Character table with point group symmetry D_{2h} for the group of the wave vector of the M point of space group #194

	$\{E\|0\}$	$\{C_2\|\tau\}$	$\left\{C_2^{'A}\|0\right\}$	$\left\{C_2^{''A}\|\tau\right\}$	$\{i\|0\}$	$\{\sigma_h\|\tau\}$	$\left\{\sigma_d^A\|0\right\}$	$\left\{\sigma_v^A\|\tau\right\}$		
M_1^+	1	1	1	1	1	1	1	1		x^2, y^2, z^2
M_2^+	1	1	-1	-1	1	1	-1	-1		xy
M_3^+	1	-1	1	-1	1	-1	1	-1		xz
M_4^+	1	-1	-1	1	1	-1	-1	1		yz
M_1^-	1	1	1	1	-1	-1	-1	-1		
M_2^-	1	1	-1	-1	-1	-1	1	1	z	
M_3^-	1	-1	1	-1	-1	1	-1	1	y	
M_4^-	1	-1	-1	1	-1	1	1	-1	x	

compatibility relations
$M_1^+ \to \Sigma_1$; $M_2^+ \to \Sigma_3$; $M_3^+ \to \Sigma_4$; $M_4^+ \to \Sigma_2$;
$M_1^- \to \Sigma_2$; $M_2^- \to \Sigma_4$; $M_3^- \to \Sigma_3$; $M_4^- \to \Sigma_1$

$M = (\pi/a)(1, -1, 0)$

Table C.31. Character table for the group of the wave vector for point T for space group #194

	$\{E\|0\}$	$\left\{C_2'^A\|0\right\}$	$\{\sigma_h\|\tau\}$	$\left\{\sigma_v^A\|\tau\right\}$		
T_1	1	1	1	1	y	$x^2,\ y^2,\ z^2$
T_2	1	1	-1	-1		xz
T_3	1	-1	1	-1	x	xy
T_4	1	-1	-1	1	z	yz

$T = (\pi/a)(1-x, 1+x, 0)$

Table C.32. Character table for Σ point for space group #194 (C_s^3, Cm, #8)

	$\{E\|0\}$	$\left\{C_2''^A\|\tau\right\}$	$\{\sigma_h\|\tau\}$	$\left\{\sigma_d^A\|0\right\}$		
Σ_1	1	1	1	1	x	x^2, y^2, z^2
Σ_2	1	1	-1	-1		zy
Σ_3	1	-1	1	-1	y	xy
Σ_4	1	-1	-1	1	z	zx

$\Sigma = (\pi/a)(x, -x, 0)$

Table C.33. Character table with point group C_{1h} for the group of the wave vector for point U for space group #194

	$\{E\|0\}$	$\{\sigma_h\|\tau\}$		
U_1	1	1	$x,\ y$	$x^2,\ y^2,\ z^2,\ xy$
U_2	1	-1	z	$zy,\ zx$

$U = 2\pi(1/3a, -1/3a, p/c)$

Table C.34. Compatibility relations for Γ, Δ, Σ, and T

Γ	Δ	Σ	T
Γ_1^+	Δ_1	Σ_1	T_1
Γ_2^+	Δ_2	Σ_3	T_3
Γ_3^+	Δ_3	Σ_4	T_2
Γ_4^+	Δ_4	Σ_2	T_4
Γ_5^+	Δ_5	$\Sigma_2 + \Sigma_4$	$T_2 + T_4$
Γ_6^+	Δ_6	$\Sigma_1 + \Sigma_3$	$T_1 + T_3$
Γ_1^-	Δ_2	Σ_2	T_2
Γ_2^-	Δ_1	Σ_4	T_4
Γ_3^-	Δ_4	Σ_3	T_1
Γ_4^-	Δ_3	Σ_1	T_3
Γ_5^-	Δ_5	$\Sigma_1 + \Sigma_3$	$T_1 + T_3$
Γ_6^-	Δ_6	$\Sigma_2 + \Sigma_4$	$T_2 + T_4$

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	$S_x S_y S_z$
$\Gamma_3(\Gamma_{12})$	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

	$u_1^3 v_x^4$	$u_1^3 v_y^4$	$u_1^3 v_z^4$	$u_2^3 v_x^4$	$u_2^3 v_y^4$	$u_2^3 v_z^4$
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

	$u_x^4 v_{-1/2}^6$	$u_x^4 v_{1/2}^6$	$u_y^4 v_{-1/2}^6$	$u_y^4 v_{1/2}^6$	$u_z^4 v_{-1/2}^6$	$u_z^4 v_{1/2}^6$
$\psi_{-1/2}^6$	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

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

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

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 $\overline{C}_2$	$2C_3$	$2\overline{C}_3$	$2C_6$	$2\overline{C}_6$	$3C'_2$ $3\overline{C'}_2$	$3C''_2$ $3\overline{C''}_2$	I	$\overline{I}$	σ_h $\overline{\sigma}_h$	$2S_6$	$2\overline{S}_6$	$2S_3$	$2\overline{S}_3$	$3\sigma_d$ $3\overline{\sigma}_d$	$3\sigma_v$ $3\overline{\sigma}_v$	time
			τ			τ	τ		τ			τ			τ	τ		τ	
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)	$\left.\begin{array}{l}(x,y)\\(R_x,R_y)\end{array}\right\}$	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
	$\left.\begin{array}{l}\phi(1/2,1/2)\\\phi(1/2,-1/2)\end{array}\right\}$	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
	$\left.\begin{array}{l}\phi(3/2,3/2)\\\phi(3/2,-3/2)\end{array}\right\}$	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.

E

Group Theory Aspects of Carbon Nanotubes

In this appendix we provide information needed for solving problems related to carbon nanotubes (see Sect. 9.4). Carbon nanotubes in general exhibit compound rotation-translation operations and therefore belong to nonsymmorphic space groups. From the symmetry point of view, there are two types of carbon nanotubes, namely chiral and achiral tubes. We here discuss the structure of carbon nanotubes and provide the character tables for the group of the wavevectors at $k = 0$ and $k \neq 0$, for both chiral and achiral tubes [8].

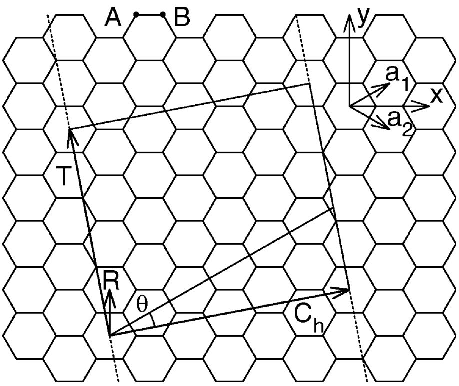


Fig. E.1. An unrolled carbon nanotube projected on a graphene layer (a single layer of crystalline graphite). When the nanotube is rolled up, the chiral vector $\boldsymbol{C}_h$ turns into the circumference of the cylinder, and the translation vector $\boldsymbol{T}$ is aligned along the cylinder axis. $\boldsymbol{R}$ is the symmetry vector (Sect. E.4) and θ is the chiral angle. The unit vectors $(\boldsymbol{a}_1, \boldsymbol{a}_2)$ of the graphene layer are indicated in the figure along with the inequivalent A and B sites within the unit cell of the graphene layer [64]

E.1 Nanotube Geometry and the (n, m) Indices

A single wall carbon nanotube (SWNT) is constructed starting from a graphene layer (see Fig. E.1) by rolling it up into a seamless cylinder. The nanotube structure is uniquely determined by the chiral vector $\boldsymbol{C}_h$ which spans the circumference of the cylinder when the graphene layer is rolled up into a tube. The chiral vector can be written in the form

$$\boldsymbol{C}_h = n\boldsymbol{a}_1 + m\boldsymbol{a}_2 \,, \tag{E.1}$$

where the vectors $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$ bounding the unit cell of the graphene layer contain two distinct carbon atom sites A and B, as shown in Fig. E.1, while n and m are arbitrary integer numbers. In the shortened (n, m) form, the chiral vector is written as a pair of integers. The (n, m) notation is widely used to characterize the geometry of each distinct (n, m) nanotube [63, 64].

The nanotube can also be characterized by its diameter d_t and chiral angle θ, which determine the length $C_h = |\boldsymbol{C}_h| = \pi d_t$ of the chiral vector and its orientation on the graphene layer (see Fig. E.1). Both d_t and θ are expressed in terms of the indices n and m by the relations $d_t = a\sqrt{n^2 + nm + m^2}/\pi$ and $\tan\theta = \sqrt{3}m/(2n+m)$, as one can derive from Fig. E.1, where $a = \sqrt{3}a_{\mathrm{C-C}} = 0.246\,\mathrm{nm}$ is the lattice constant for the graphene layer and $a_{\mathrm{C-C}} = 0.142\,\mathrm{nm}$ is the nearest neighbor C–C distance. As an example, the chiral vector $\boldsymbol{C}_h$ shown in Fig. E.1 is given by $\boldsymbol{C}_h = 4\boldsymbol{a}_1 + 2\boldsymbol{a}_2$, and thus the corresponding nanotube can be identified by the integer pair $(4, 2)$. Due to the sixfold symmetry of the graphene layer, all nonequivalent nanotubes can be characterized by the (n, m) pairs of integers where $0 \le m \le n$. It is also possible to define nanotubes with opposite handedness, for which $0 \le n \le m$ [65]. The nanotubes are classified as chiral $(0 < m < n)$ and achiral ($m = 0$ or $m = n$), which in turn are known as zigzag $(m = 0)$ and armchair $(m = n)$ nanotubes (see Figs. 9.11 and E.1).

E.2 Lattice Vectors in Real Space

To specify the symmetry properties of carbon nanotubes as 1D systems, it is necessary to define the lattice vector or translation vector $\boldsymbol{T}$ along the nanotube axis and normal to the chiral vector $\boldsymbol{C}_h$ defined in Fig. E.1. The vectors $\boldsymbol{T}$ and $\boldsymbol{C}_h$ define the unit cell of the 1D nanotube. The translation vector $\boldsymbol{T}$, of a general chiral nanotube as a function of n and m, can be written as

$$\boldsymbol{T} = (t_1\boldsymbol{a_1} + t_2\boldsymbol{a_2}) = [(2m+n)\boldsymbol{a}_1 - (2n+m)\boldsymbol{a}_2]/d_R \,, \tag{E.2}$$

with a length $T = \sqrt{3}C_h/d_R$, where d is the greatest common divisor of (n, m), and d_R is the greatest common divisor of $2n + m$ and $2m + n$. Then d and d_R are related by

$$d_R = \begin{cases} d & \text{if } n{-}m \text{ is not a multiple of } 3d \\ 3d & \text{if } n{-}m \text{ is a multiple of } 3d\,. \end{cases} \tag{E.3}$$

For the $(4,2)$ nanotube shown in Fig. E.1, we have $d_R = d = 2$ and $(t_1, t_2) = (4, -5)$. For armchair and zigzag achiral tubes, $T = a$ and $T = \sqrt{3}a$, respectively. The unit cell of an unrolled nanotube on a graphene layer is a rectangle bounded by the vectors $\boldsymbol{C}_h$ and $\boldsymbol{T}$ (see the rectangle shown in Fig. E.1 for the $(4,2)$ nanotube). The area of the nanotube unit cell can be easily calculated as a vector product of these two vectors, $|\boldsymbol{C}_h \times \boldsymbol{T}| = \sqrt{3}a^2(n^2+nm+m^2)/d_R$. Dividing this product by the area of the unit cell of a graphene layer $|\boldsymbol{a}_1 \times \boldsymbol{a}_2| = \sqrt{3}a^2/2$, one can get the number of hexagons in the unit cell of a nanotube,

$$N = \frac{2(n^2 + nm + m^2)}{d_R}\,. \tag{E.4}$$

For the $(4,2)$ nanotube we have $N = 28$, so that the unit cell of the $(4,2)$ nanotube (see the rectangle shown in Fig. E.1) contains 28 hexagons, or $2 \times 28 = 56$ carbon atoms. For armchair (n,n) and zigzag $(n,0)$ nanotubes, $N = 2n$.

E.3 Lattice Vectors in Reciprocal Space

The unit cell of a graphene layer is defined by the vectors $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$. The graphene reciprocal lattice unit vectors $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$ can be constructed from $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$ using the standard definition $\boldsymbol{a}_i \cdot \boldsymbol{b}_j = 2\pi\delta_{ij}$, where δ_{ij} is the Kroneker delta symbol. In Fig. E.2, we show a diagram for the real space unit cell of a graphene sheet (Fig. E.2(a)) and its corresponding reciprocal lattice unit cell

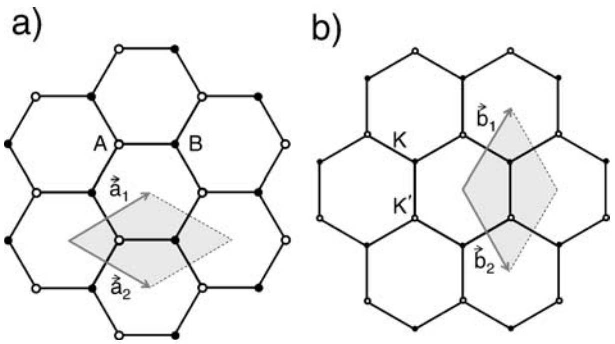


Fig. E.2. (**a**) Real space structure of a graphene layer. The gray rhombus represents the graphene unit cell with the lattice vectors denoted by $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$ delimiting it. Note that this area encloses a total of two atoms, one A atom and one B atom. (**b**) Reciprocal space unit cell of the graphene layer denoted by the unit vectors $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$. Note also that the reciprocal space structure has two inequivalent points K and K' [8]

is shown in Fig. E.2(b). Note the rotation by the angle 30° of the hexagons in real space (Fig. E.2(a)) with respect to those in reciprocal space (Fig. E.2(b)).

In a similar fashion, the reciprocal space of a nanotube can be constructed, if we consider the nanotube as a 1D system with an internal structure that is composed of the $2N$ atoms in its unit cell and with a translational symmetry given by the translation vector $\boldsymbol{T}$. The reciprocal space of the nanotube can be constructed by finding a pair of reciprocal lattice vectors $\boldsymbol{K}_1$ and $\boldsymbol{K}_2$ which satisfy: $\boldsymbol{C}_h \cdot \boldsymbol{K}_1 = \boldsymbol{T} \cdot \boldsymbol{K}_2 = 2\pi$ and $\boldsymbol{C}_h \cdot \boldsymbol{K}_2 = \boldsymbol{T} \cdot \boldsymbol{K}_1 = 0$. Due to the spatial confinement of the nanotube in the radial direction, the vector $\boldsymbol{C}_h$ does not play the role of a translation vector but rather of a generator of pure rotations, and the relation $\boldsymbol{C}_h \cdot \boldsymbol{K}_1 = 2\pi$ can only be satisfied for integer multiples of $2\pi/d_t$, where d_t is the diameter of the nanotube.

E.4 Compound Operations and Tube Helicity

All multiples of the translation vector $\boldsymbol{T}$ will be translational symmetry operations of the nanotube [73]. However, to be more general, it is necessary to consider that any lattice vector

$$\boldsymbol{t}_{p,q} = p\boldsymbol{a}_1 + q\boldsymbol{a}_2\,, \tag{E.5}$$

with p and q integers, of the unfolded graphene layer will also be a symmetry operation of the tube. In fact, the symmetry operation that arises from $\boldsymbol{t}_{p,q}$ will appear as a screw translation of the nanotube. Screw translations are combinations of a rotation (R_ϕ) by an angle ϕ and a small translation of $\boldsymbol{\tau}$ in the axial direction of the nanotube, and can be written as $\{R_\phi|\tau\}$, using the notation common for space group operations [8, 64].

Any lattice vector $\boldsymbol{t}_{p,q}$ can also be written in terms of components of the nanotube lattice vectors, $\boldsymbol{T}$ and $\boldsymbol{C}_h$, as

$$\boldsymbol{t}_{p,q} = \boldsymbol{t}_{u,v} = (u/N)\boldsymbol{C}_h + (v/N)\boldsymbol{T}\,, \tag{E.6}$$

where u and v are negative or positive integers given by

$$u = \frac{(2n+m)p + (2m+n)q}{d_R} \tag{E.7}$$

and

$$v = mp - nq\,. \tag{E.8}$$

The screw translation of the nanotube which is associated with the graphene lattice vector $\boldsymbol{t}_{u,v}$ can then be written as

$$\boldsymbol{t}_{u,v} = \{C_N^u|vT/N\}\,, \tag{E.9}$$

where C_N^u is a rotation of $u(2\pi/N)$ around the nanotube axis, and $\{E|vT/N\}$ is a translation of vT/N along the nanotube axis, with T being the magnitude of the primitive translation vector $\boldsymbol{T}$, and E being the identity operation. It is clear that if a screw vector $\{C_N^u|vT/N\}$ is a symmetry operation of the nanotube, then the vectors $\{C_N^u|vT/N\}^s$, for any integer value of s, are also symmetry operations of the nanotube. The number of hexagons in the unit-cell N assumes the role of the "order" of the screw axis, since the symmetry operation $\{C_N^u|vT/N\}^N = \{E|vT\}$, where E is the identity operator, and $v\boldsymbol{T}$ is a primitive translation of the nanotube.

The nanotube structure can be obtained from a small number of atoms by using any choice of two noncolinear screw vectors $\{C_N^{u_1}|v_1T/N\}$ and $\{C_N^{u_2}|v_2T/N\}$. The two vectors will be colinear if there exists a pair of integers s and l different from 1, for which $lu_1 = su_2 + \lambda N$, and $lv_1 = sv_2 + \gamma T$, where, λ and γ are two arbitrary integers. The area of the nanotube cylindrical surface delimited by these two noncolinear vectors can be regarded as a reduced unit cell. Note that the number of atoms in this reduced unit cell is given by the ratio between the area delimited by these vectors ($|\boldsymbol{t}_{u_1,v_1} \times \boldsymbol{t}_{u_2,v_2}|$) and the area of the unit cell of a graphene sheet ($|\boldsymbol{a}_1 \times \boldsymbol{a}_2|$) multiplied by 2, which is the number of carbon atoms in the graphene unit cell. Thus the number of atoms in the reduced unit cell defined by t_{u_1,v_1} and t_{u_2,v_2} is given by

$$2\frac{|\boldsymbol{t}_{u_1,v_1} \times \boldsymbol{t}_{u_2,v_2}|}{|\boldsymbol{a}_1 \times \boldsymbol{a}_2|} = 2\frac{|v_2u_1 - u_2v_1|}{N} . \tag{E.10}$$

It is important to point out that, in this case, the nanotube ceases to be described as a quasi-1D system, but as a system with two quasitranslational dimensions, which are generated by the two screw vectors.

There are many combinations of screw vectors which can be used to construct the structure of the nanotube. These combinations can be divided into four categories: helical–helical, linear–helical, helical–angular, and linear–angular, as described below. Either one of these constructions can be used to obtain the nanotube structure. The helical–helical construction is characterized by choosing two general screw vectors, for the construction of the nanotube structure (see Fig. E.3(a)). Although this scheme permits the definition of a 2-atom unit cell, the unit cell does not exhibit the full symmetries of the nanotube, and thus is inadequate for representing the nanotube. The linear–helical scheme is characterized by using the translation vector $\boldsymbol{T}$ and a general screw vector as unit vectors (see Fig. E.3(b)). This scheme maintains the translational symmetry of the nanotube, but not the point group operations, and it also permits the definition of a two-atom unit cell. In the helical–angular construction, a general screw vector is used along with a vector in the circumferential direction of the nanotube (see Fig. E.3(c)). This construction also permits the definition of a 2-atom unit cell. However, the 2-atom unit cell does not exhibit many of the symmetries of the nanotube. Instead it is convenient to define a $2d$-atom unit cell, where the integer d is given by $d = gcd(n, m)$, and this unit cell will exhibit all the point group symmetry operations of the nanotube, but not the translational symmetry. The linear–angular construction uses as unit vectors the translational vector

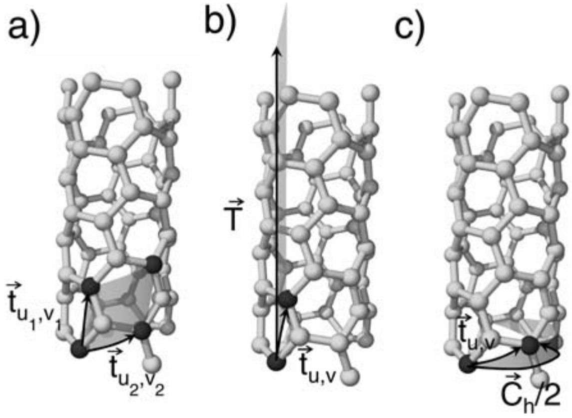


Fig. E.3. The 2-atom reduced unit cell for the: (**a**) helical–helical, (**b**) linear–helical, and (**c**) helical–angular construction for a $(4, 2)$ nanotube. In (**b**) the deformed rhombus, which delimits the reduced unit cell that connects points both inside and outside the nanotube unit cell, had to be truncated to stay within the figure [8]

$\boldsymbol{T}$ and a vector in the circumferential direction, and thus parallel to $\boldsymbol{C}_h$. The linear–angular construction does not permit the definition of a 2-atom unit cell. However, by choosing the vector in the circumferential direction to be $\boldsymbol{C}_h$, the total unit cell of the nanotube, which exhibits all the translational and point symmetries of the nanotube, is restored.

E.5 Character Tables for Carbon Nanotubes

In this section we present the character tables for dealing with carbon nanotubes. Tables E.1 and E.2 give the character tables for the group of the wavevectors for chiral carbon nanotubes, at $k = 0, \pi/T$ and $0 < k < \pi/T$, respectively. Tables E.3 and E.4 give the character tables for the group of the wavevectors for achiral carbon nanotubes, at $k = 0, \pi/T$ and $0 < k < \pi/T$, respectively. Some of the point symmetry operations in these tables are shown in Fig. E.4.

Table E.1. Character table for the group of the wavevectors $k = 0$ and $k = \pi/T$ for chiral tubes

D_N	$\{E\|0\}$	$2\{C_N^u\|vT/N\}$	$2\{C_N^u\|vT/N\}^2$	$\ldots$	$2\{C_N^u\|vT/N\}^{(N/2)-1}$	$2\{C_N^u\|vT/N\}^{N/2}$	$(N/2)\{C_2'\|0\}$	$(N/2)\{C_2''\|0\}$
A_1	1	1	1	$\ldots$	1	1	1	1
A_2	1	1	1	$\ldots$	1	1	−1	−1
B_1	1	−1	1	$\ldots$	$(-1)^{(N/2-1)}$	$(-1)^{N/2}$	1	−1
B_2	1	−1	1	$\ldots$	$(-1)^{(N/2-1)}$	$(-1)^{N/2}$	−1	1
E_1	2	$2\cos 2\pi/N$	$2\cos 4\pi/N$	$\ldots$	$2\cos 2(N/2-1)\pi/N$	−2	0	0
E_2	2	$2\cos 4\pi/N$	$2\cos 8\pi/N$	$\ldots$	$2\cos 4(N/2-1)\pi/N$	2	0	0
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
$E_{(N/2-1)}$	2	$2\cos 2(N/2-1)\pi/N$	$2\cos 4(N/2-1)\pi/N$	$\ldots$	$2\cos 2(N/2-1)^2\pi/N$	$2\cos(N/2-1)\pi$	0	0

This group is isomorphic to the point group D_N

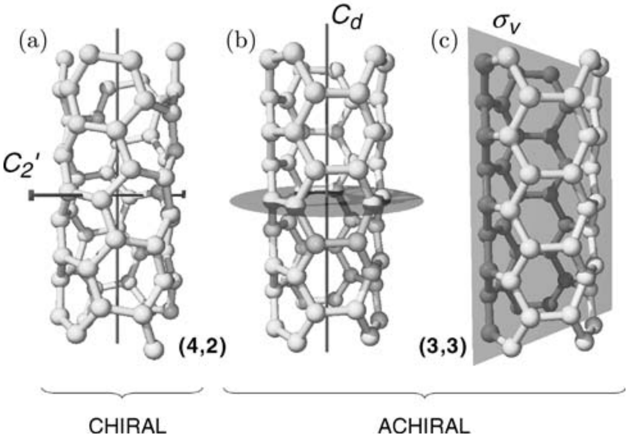


Fig. E.4. (**a**) Unit cell of the chiral (4,2) nanotube, showing the C_d rotation around the nanotube axis, with $d = 2$, and one of the C_2' rotations perpendicular to the nanotube axis. A different class of two-fold rotations (C_2''), which is present for both chiral and achiral nanotubes, is not shown here. (**b**) A section of an achiral armchair (3,3) nanotube is shown emphasizing the horizontal mirror plane σ_h and the symmetry operation C_d, with $d = 3$. (**c**) The same (3,3) armchair nanotube is shown but now emphasizing of the vertical mirror planes σ_v [8]

Table E.2. Character table for the group of the wavevector $0 < k < \pi/T$ for chiral nanotubes

C_N	$\{E\|0\}$	$\{C_N^u\|vT/N\}^1$	$\{C_N^u\|vT/N\}^2$	$\cdots$	$\{C_N^u\|vT/N\}^\ell$	$\cdots$	$\{C_N^u\|vT/N\}^{N-1}$
A	1	1	1	$\cdots$	1	$\cdots$	1
B	1	-1	1	$\cdots$	$(-1)^\ell$	$\cdots$	-1
$E_{\pm 1}$	1	ϵ	ϵ^2	$\cdots$	ϵ^ℓ	$\cdots$	ϵ^{N-1}
	1	ϵ^*	ϵ^{*2}		$\epsilon^{*\ell}$		$\epsilon^{*(N-1)}$
$E_{\pm 2}$	1	ϵ^2	ϵ^4	$\cdots$	$\epsilon^{2\ell}$	$\cdots$	$\epsilon^{2(N-1)}$
	1	ϵ^{*2}	ϵ^{*4}		$\epsilon^{*2\ell}$		$\epsilon^{*2(N-1)}$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
$E_{\pm(\frac{N}{2}-1)}$	1	$\epsilon^{\frac{N}{2}-1}$	$\epsilon^{2(\frac{N}{2}-1)}$	$\cdots$	$\epsilon^{\ell(\frac{N}{2}-1)}$	$\cdots$	$\epsilon^{(N-1)(\frac{N}{2}-1)}$
	1	$\epsilon^{*\frac{N}{2}-1}$	$\epsilon^{*2(\frac{N}{2}-1)}$		$\epsilon^{*\ell(\frac{N}{2}-1)}$		$\epsilon^{*(N-1)(\frac{N}{2}-1)}$

This group is isomorphic to the point group C_N. The $\pm$ signs label the different representations with characters which are complex conjugates of each other. These irreducible representations are degenerate due to time reversal symmetry. The complex number ϵ is $\mathrm{e}^{2\pi\mathrm{i}/N}$.

Table E.3. Character table for the group of the wavevectors $k = 0$ and $k = \pi/T$ for achiral carbon tubes. This group is isomorphic to the point group D_{2nh}

D_{2nh}	$\{E\|0\}$	$\cdots$	$2\{C_{2n}^u\|vT/2n\}^s$	$\cdots$	$\{C_{2n}^u\|vT/2n\}^n$	$n\{C_2'\|0\}$	$n\{C_2''\|0\}$	$\{I\|0\}$	$\cdots$	$2\{IC_{2n}^u\|vT/2n\}^s$	$\cdots$	$\{\sigma_h\|0\}$	$n\{\sigma_v'\|0\}$	$n\{\sigma_v''\|T/2\}$
A_{1g}	1	$\cdots$	1	$\cdots$	1	1	1	1	$\cdots$	1	$\cdots$	1	1	1
A_{2g}	1	$\cdots$	1	$\cdots$	1	–1	–1	1	$\cdots$	1	$\cdots$	1	–1	–1
B_{1g}	1	$\cdots$	$(-1)^s$	$\cdots$	$(-1)^n$	–1	1	1	$\cdots$	$(-1)^s$	$\cdots$	$(-1)^n$	–1	1
B_{2g}	1	$\cdots$	$(-1)^s$	$\cdots$	$(-1)^n$	1	–1	1	$\cdots$	$(-1)^s$	$\cdots$	$(-1)^n$	1	–1
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	
$E_{\mu g}$	2	$\cdots$	$2\cos(\mu s\pi/n)$	$\cdots$	$2(-1)^\mu$	0	0	2	$\cdots$	$2\cos(\mu s\pi/n)$	$\cdots$	$2(-1)^\mu$	0	0
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
A_{1u}	1	$\cdots$	1	$\cdots$	1	1	1	–1	$\cdots$	–1	$\cdots$	–1	–1	–1
A_{2u}	1	$\cdots$	1	$\cdots$	1	–1	–1	–1	$\cdots$	–1	$\cdots$	–1	1	1
B_{1u}	1	$\cdots$	$(-1)^s$	$\cdots$	$(-1)^n$	–1	1	–1	$\cdots$	$-(-1)^s$	$\cdots$	$(-1)^n$	1	–1
B_{2u}	1	$\cdots$	$(-1)^s$	$\cdots$	$(-1)^n$	1	–1	–1	$\cdots$	$-(-1)^s$	$\cdots$	$(-1)^n$	–1	1
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	
$E_{\mu u}$	2	$\cdots$	$2\cos(\mu s\pi/n)$	$\cdots$	$2(-1)^\mu$	0	0	–2	$\cdots$	$-2\cos(\mu s\pi/n)$	$\cdots$	$-2(-1)^\mu$	0	0
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$

The values of s and μ span the integer values between 1 and $n - 1$.

Table E.4. Character table for the group of the wavevectors $0 < k\pi/T$ for achiral carbon nanotubes

C_{2nv}	$\{E\|0\}$	$2\{C_{2n}^u\|vT/2n\}^1$	$\{C_{2n}^u\|vT/2n\}^2$	$\ldots$	$2\{C_{2n}^u\|vT/2n\}^{n-1}$	$\{C_{2n}^u\|vT/2n\}^n$	$n\{\sigma_v'\|\tau'\}$	$n\{\sigma_v''\|\tau''\}$
A'	1	1	1	$\ldots$	1	1	1	1
A''	1	1	1	$\ldots$	1	1	-1	-1
B'	1	-1	1	$\ldots$	$(-1)^{(n-1)}$	$(-1)^n$	1	-1
B''	1	-1	1	$\ldots$	$(-1)^{(n-1)}$	$(-1)^n$	-1	1
E_1	2	$2\cos\pi/n$	$2\cos 2\pi/n$	$\ldots$	$2\cos 2(n-1)\pi/n$	-2	0	0
E_2	2	$2\cos 2\pi/n$	$2\cos 4\pi/n$	$\ldots$	$2\cos 4(n-1)\pi/n$	2	0	0
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
$E_{(n-1)}$	2	$2\cos(n-1)\pi/n$	$2\cos 2(n-1)\pi/n$	$\ldots$	$2\cos(n-1)^2\pi/n$	$2\cos(n-1)\pi$	0	0

This group is isomorphic to the point group C_{2nv}. For zigzag nanotubes with n odd, $\tau' = \tau'' = T/2$, while for armchair nanotubes and zigzag nanotubes with n even, $\tau' = 0$ and $\tau'' = T/2$.

F

Permutation Group Character Tables

In this appendix we provide tables to be used with permutation groups. Tables F.1 and F.2 are the extended character tables for the permutation groups of 3 and 4 objects $P(3)$ and $P(4)$, respectively, and are discussed in Sects. 17.4.2 and 17.4.3, respectively. The discussion in these sections can also be used to understand the extended character tables for the permutation groups $P(5)$, $P(6)$, and $P(7)$ which have many more symmetry elements, namely $5! = 120$, $6! = 720$, and $7! = 5,040$, respectively (see Tables F.3 and F.4). These character tables are sufficient to describe the permutation groups arising for the filling of s, p, d, and f electron states, as discussed in Chap. 17. In Table F.5 for the group $P(7)$ only a few entries are made. The corresponding entries can also be made for permutation groups $P(n)$ of higher order.

When one considers a wave function of n identical particles (e.g., permutation groups in Chap. 17) then the interchange of identical particles is a symmetry operation that must be included. The number of irreducible representations is equal to the number of classes. Table F.6 contains the number of classes and the dimensionalities of the irreducible representations where $P(n)$ labels the permutation group of n objects.

Table F.1. Extended character table for permutation group $P(3)$

	χ(E)	χ(A,B,C)	χ(D,F)	
$P(3)$	(1^3)	$3(2,1)$	$2(3)$	
Γ_1^s	1	1	1	
Γ_1^a	1	–1	1	
Γ_2	2	0	–1	
$\chi_{\text{perm.}}(\psi_1\psi_1\psi_1)$	1	1	1	$\Rightarrow \Gamma_1^s$
$\chi_{\text{perm.}}(\psi_1\psi_1\psi_2)$	3	1	0	$\Rightarrow \Gamma_1^s + \Gamma_2$
$\chi_{\text{perm.}}(\psi_1\psi_2\psi_3)$	6	0	0	$\Rightarrow \Gamma_1^s + \Gamma_1^a + 2\Gamma_2$

Table F.2. Extended character table for the permutation group $P(4)$

$P(4)$	(1^4)	$8(3,1)$	$3(2^2)$	$6(2,1^2)$	$6(4)$	
Γ_1^s	1	1	1	1	1	
Γ_1^a	1	1	1	−1	−1	
Γ_2	2	−1	2	0	0	
Γ_3	3	0	−1	1	−1	
$\Gamma_{3'}$	3	0	−1	−1	1	
$\chi_{\text{perm.}}(\psi_1\psi_1\psi_1\psi_1)$	1	1	1	1	1	$\Rightarrow \Gamma_1^s$
$\chi_{\text{perm.}}(\psi_1\psi_1\psi_1\psi_2)$	4	1	0	2	0	$\Rightarrow \Gamma_1^s + \Gamma_3$
$\chi_{\text{perm.}}(\psi_1\psi_1\psi_2\psi_2)$	6	0	2	2	0	$\Rightarrow \Gamma_1^s + \Gamma_2 + \Gamma_3$
$\chi_{\text{perm.}}(\psi_1\psi_1\psi_2\psi_3)$	12	0	0	2	0	$\Rightarrow \Gamma_1^s + \Gamma_2 + 2\Gamma_3 + \Gamma_{3'}$
$\chi_{\text{perm.}}(\psi_1\psi_2\psi_3\psi_4)$	24	0	0	0	0	$\Rightarrow \Gamma_1^s + \Gamma_1^a + 2\Gamma_2 + 3\Gamma_3 + 3\Gamma_{3'}$

Here the Γ_{n-1} irreducible representation is Γ_3 (see Sect. 17.3)

Table F.3. Extended character table for permutation group $P(5)$

$P(5)$or S_5	(1^5)	$10(2,1^3)$	$15(2^2,1)$	$20(3,1^2)$	$20(3,2)$	$30(4,1)$	$24(5)$
Γ_1^s	1	1	1	1	1	1	1
Γ_1^a	1	–1	1	1	–1	–1	1
Γ_4	4	2	0	1	–1	0	–1
$\Gamma_{4'}$	4	–2	0	1	1	0	–1
Γ_5	5	1	1	–1	1	–1	0
$\Gamma_{5'}$	5	–1	1	–1	–1	1	0
Γ_6	6	0	–2	0	0	0	1
$\chi_{\text{perm.}}(\psi_1\psi_1\psi_1\psi_1\psi_1)$	1	1	1	1	1	1	1
$\chi_{\text{perm.}}(\psi_1\psi_1\psi_1\psi_1\psi_2)$	5	3	1	2	0	1	0
$\chi_{\text{perm.}}(\psi_1\psi_1\psi_1\psi_2\psi_2)$	10	4	2	1	1	0	0
$\chi_{\text{perm.}}(\psi_1\psi_1\psi_1\psi_2\psi_3)$	20	6	0	2	0	0	0
$\chi_{\text{perm.}}(\psi_1\psi_1\psi_2\psi_2\psi_3)$	30	6	2	0	0	0	0
$\chi_{\text{perm.}}(\psi_1\psi_1\psi_2\psi_3\psi_4)$	60	6	0	0	0	0	0
$\chi_{\text{perm.}}(\psi_1\psi_2\psi_3\psi_4\psi_5)$	120	0	0	0	0	0	0

S_5	irreducible representations
$\chi_{\text{perm.}}(\psi_1\psi_1\psi_1\psi_1\psi_1)$	$\Rightarrow \Gamma_1^s$
$\chi_{\text{perm.}}(\psi_1\psi_1\psi_1\psi_1\psi_2)$	$\Rightarrow \Gamma_1^s + \Gamma_4$
$\chi_{\text{perm.}}(\psi_1\psi_1\psi_1\psi_2\psi_2)$	$\Rightarrow \Gamma_1^s + \Gamma_4 + \Gamma_5$
$\chi_{\text{perm.}}(\psi_1\psi_1\psi_1\psi_2\psi_3)$	$\Rightarrow \Gamma_1^s + 2\Gamma_4 + \Gamma_5 + \Gamma_6$
$\chi_{\text{perm.}}(\psi_1\psi_1\psi_2\psi_2\psi_3)$	$\Rightarrow \Gamma_1^s + 2\Gamma_4 + 2\Gamma_5 + \Gamma_{5'} + \Gamma_6$
$\chi_{\text{perm.}}(\psi_1\psi_1\psi_2\psi_3\psi_4)$	$\Rightarrow \Gamma_1^s + 3\Gamma_4 + \Gamma_{4'} + 3\Gamma_5 + 2\Gamma_{5'} + 3\Gamma_6$
$\chi_{\text{perm.}}(\psi_1\psi_2\psi_3\psi_4\psi_5)$	$\Rightarrow \Gamma_1^s + \Gamma_1^a + 4\Gamma_4 + 4\Gamma_{4'} + 5\Gamma_5 + 5\Gamma_{5'} + 6\Gamma_6$

Here the Γ_{n-1} irreducible representation of $P(5)$ is Γ_4”

Table F.4. Extended character table for permutation group $P(6)$

$P(6)$	1 (1^6)	15 $(2,1^4)$	45 $(2^2,1^2)$	15 (2^3)	40 $(3,1^3)$	120 $(3,2,1)$	40 (3^2)	90 $(4,1^2)$	90 $(4,2)$	144 $(5,1)$	120 (6)
Γ_1^s	1	1	1	1	1	1	1	1	1	1	1
Γ_1^a	1	–1	1	–1	1	–1	1	–1	1	1	–1
Γ_5	5	3	1	–1	2	0	–1	1	–1	0	–1
$\Gamma_{5'}$	5	–3	1	1	2	0	–1	–1	–1	0	1
$\Gamma_{5''}$	5	1	1	–3	–1	1	2	–1	–1	0	0
$\Gamma_{5'''}$	5	–1	1	3	–1	–1	2	1	–1	0	0
Γ_9	9	3	1	3	0	0	0	–1	1	–1	0
$\Gamma_{9'}$	9	–3	1	–3	0	0	0	1	1	–1	0
Γ_{10}	10	2	–2	–2	1	–1	1	0	0	0	1
$\Gamma_{10'}$	10	–2	–2	2	1	1	1	0	0	0	–1
Γ_{16}	16	0	0	0	–2	0	–2	0	0	1	0
$\chi_{\text{perm.}}(\psi_1\psi_1\psi_1\psi_1\psi_1\psi_1)$	1	1	1	1	1	1	1	1	1	1	1
$\chi_{\text{perm.}}(\psi_1\psi_1\psi_1\psi_1\psi_1\psi_2)$	6	4	2	0	3	1	0	1	0	1	0
$\vdots$	$\dots$										
$\chi_{\text{perm.}}(\psi_1\psi_2\psi_3\psi_4\psi_5\psi_6)$	720	0	0	0	0	0	0	0	0	0	0

S_6	irreducible representations
$\Gamma_{\text{perm.}}(\psi_1\psi_1\psi_1\psi_1\psi_1\psi_1)$	$\Rightarrow \Gamma_1^s$
$\Gamma_{\text{perm.}}(\psi_1\psi_1\psi_1\psi_1\psi_1\psi_2)$	$\Rightarrow \Gamma_1^s + \Gamma_5$
$\vdots$	$\vdots$
$\Gamma_{\text{perm.}}(\psi_1\psi_2\psi_3\psi_4\psi_5\psi_6)$	$\Rightarrow \Gamma_1^s + \Gamma_1^a + 5\Gamma_5 + 5\Gamma_{5'} + 5\Gamma_{5''} + 5\Gamma_{5'''} +$ $9\Gamma_9 + 9\Gamma_{9'} + 10\Gamma_{10} + 10\Gamma_{10'} + 16\Gamma_{16}$

Here the Γ_{n-1} irreducible representation of $P(6)$ is Γ_{5e}

Table F.5. Character table (schematic) for group $P(7)$

$P(7)$ or S_7	(1^7)	$\cdots$
Γ_1^s	1	$\cdots$
Γ_1^a	1	$\cdots$
Γ_6	6	$\cdots$
$\Gamma_{6'}$	6	$\cdots$
Γ_{14}	14	$\cdots$
$\Gamma_{14'}$	14	$\cdots$
$\Gamma_{14''}$	14	$\cdots$
$\Gamma_{14'''}$	14	$\cdots$
Γ_{15}	15	$\cdots$
$\Gamma_{15'}$	15	$\cdots$
Γ_{21}	21	$\cdots$
$\Gamma_{21'}$	21	$\cdots$
Γ_{35}	35	$\cdots$
$\Gamma_{35'}$	35	$\cdots$
Γ_{20}	20	$\cdots$
$\chi_{\text{perm.}}(\psi_1\psi_1\psi_1\psi_1\psi_1\psi_1\psi_1)$	1	$\cdots$
$\chi_{\text{perm.}}(\psi_1\psi_1\psi_1\psi_1\psi_1\psi_1\psi_2)$	7	$\cdots$
$\vdots$	$\vdots$	$\vdots$
$\chi_{\text{perm.}}(\psi_1\psi_2\psi_3\psi_4\psi_5\psi_6\psi_7)$	5,040	$\cdots$

S_7	irreducible representations
$\Gamma_{\text{perm.}}(\psi_1\psi_1\psi_1\psi_1\psi_1\psi_1\psi_1)$	$\Rightarrow \Gamma_1^s$
$\Gamma_{\text{perm.}}(\psi_1\psi_1\psi_1\psi_1\psi_1\psi_1\psi_2)$	$\Rightarrow \Gamma_1^s + \Gamma_6$
$\vdots$	$\vdots$
$\Gamma_{\text{perm.}}(\psi_1\psi_2\psi_3\psi_4\psi_5\psi_6\psi_7)$	$\Rightarrow \Gamma_1^s + \Gamma_1^a + 6\Gamma_6 + 6\Gamma_{6'} + 14\Gamma_{14}$
	$+14\Gamma_{14'} + 14\Gamma_{14''} + 14\Gamma_{14'''} + 15\Gamma_{15} + 15\Gamma_{15'}$
	$+21\Gamma_{21} + 21\Gamma_{21'} + 35\Gamma_{35} + 35\Gamma_{35'} + 20\Gamma_{20}$

Table F.6. Number of classes and the dimensionalities of the Γ_i in $P(n)$

group	classes	number of group elements $\sum_i \ell_i^2$
$P(1)$	1	$1! = 1^2 = 1$
$P(2)$	2	$2! = 1^2 + 1^2 = 2$
$P(3)$	3	$3! = 1^2 + 1^2 + 2^2 = 6$
$P(4)$	5	$4! = 1^2 + 1^2 + 2^2 + 3^2 + 3^2 = 24$
$P(5)$	7	$5! = 1^2 + 1^2 + 4^2 + 4^2 + 5^2 + 5^2 + 6^2 = 120$
$P(6)$	11	$6! = 1^2 + 1^2 + 5^2 + 5^2 + 5^2 + 5^2 + 9^2 + 9^2 + 10^2 + 10^2 + 16^2 = 720$
$P(7)$	15	$7! = 1^2 + 1^2 + 6^2 + 6^2 + 14^2 + 14^2 + 14^2 + 14^2 + 15^2 + 15^2 + 21^2 + 21^2 +$
		$+35^2 + 35^2 + 20^2 = 5,040$
$P(8)$	22	$8! = 1^2 + 1^2 + 7^2 + 7^2 + 14^2 + 14^2 + 20^2 + 20^2 + 21^2 + 21^2 + 28^2 + 28^2 +$
		$+35^2 + 35^2 + 56^2 + 56^2 + 64^2 + 64^2 + 70^2 + 70^2 + 42^2 + 90^2 = 40{,}320$
$P(9)$	31	$9! = 1^2 + 1^2 + 8^2 + 8^2 + \ldots = 362{,}880$
$P(10)$	37	$10! = 1^2 + 1^2 + 9^2 + 9^2 + \ldots = 3{,}628{,}800$
$P(11)$	52	$11! = 1^2 + 1^2 + 10^2 + 10^2 + \ldots = 39{,}916{,}800$
$P(12)$	67	$12! = 1^2 + 1^2 + 11^2 + 11^2 + \ldots = 479{,}001{,}600$
$\vdots$	$\vdots$	$\vdots$
$P(n)$		$n! = 1^2 + 1^2 + (n-1)^2 + (n-1)^2 + \ldots = n!$

References

1. L.P. Bouckaert, R. Smoluchowski, and E. Wigner, *Theory of Brillouin zones and symmetry properties of wave functions in crystals*. Phys. Rev. **50**, 58 (1936)
2. E. Wigner, *Gruppentheorie und ihre Anwendung auf die Quantenmechanik der Atomspektren*. (Vieweg, Braunschweig 1931)
3. A. Abragam and B. Bleaney, *Electron Paramagnetic Resonance of Transition Ions*. (Clarendon Press, Oxford 1970)
4. R.L. Aggarwal and A.K. Ramdas, *Optical determination of the symmetry of the ground states of group-V donors in silicon*. Phys. Rev. **140**, A1246 (1965)
5. G.B. Arfken and H.J. Weber, *Mathematical Methods for Physicists*. 5th Edn. (Academic Press, New York 2000)
6. N.W. Ashcroft and N.D. Mermin, *Solid State Physics*. (Holt, Rinehart and Winston, New York 1976)
7. C.S. Barrett, *Structure of Metals: Crystallographic Methods, Principles and Data*. (McGraw-Hill, New York 1952) p. 14
8. E.B. Barros, A. Jorio, Ge.G. Samsonidze, R.B. Capaz, A.G. Souza Filho, J. Mendes Filho, G. Dresselhaus, and M.S. Dresselhaus, *Review on the symmetry-related properties of carbon nanotubes*. Phys. Reports **431**, 261–302 (2006)
9. J.-L. Basdevant and J. Dalibard, *The Quantum Mechanics Solver: How to Apply Quantum Theory to Modern Physics*. (Springer, Berlin Heidelberg New York Tokyo 2000)
10. F. Bassani and G. Pastori Parravicini, *Electronic States and Optical Transitions in Solids*. (Pergamon Press, Oxford 1975)
11. H.A. Bethe, *Term-splitting in crystals*. Ann. Phys. **3**, 133–208 (1959)
12. B.N. Brockhouse, *Inelastic Scattering of Neutrons in Solids and Liquids*. (IAEA, Vienna 1961) p. 113
13. B.N. Brockhouse, L.M. Corliss, and J.M. Hastings, *Multiple scattering of slow neutrons by flat specimens and magnetic scattering by zinc ferrite*. Phys. Rev. **98**, 1721–1727 (1955)
14. B. Brockhouse and P. Iyengar, Phys. Rev. **111**, 747 (1958)
15. H.A. Buckmaster, Can. J. Phys. **40**, 11670 (1962)
16. G. Burns and A.M. Glaser, *Space Groups for Solid State Physicists*. (Academic Press, New York 1978)
17. M. Cardona and F.H. Pollack, *Energy band structure of Ge and Si: the $k \cdot p$ method*. Phys. Rev. **142**, 530 (1966)

18. Clebsch and Gordon, *Tables of Clebsch–Gordon Coefficients.* http://pdg.lbl.gov/2005/reviews/sclebrpp.pdf
19. M.H. Cohen and E.I. Blount, *The g-factor and de Haas–van Alphen effect of electrons in bismuth.* Phil. Mag. **5**, 115–126 (1960)
20. E.U. Condon and G.Shortley, *Theory of Atomic Spectra.* (Cambridge University Press, Cambridge 1951) pp. 56–78
21. J.B. Conklin, Jr., L.E. Johnson, and G.W. Pratt, Jr., *Energy bands in PbTe.* Phys. Rev. **137**, A1282 (1965)
22. M. Damnjanović and M. Vujicić, *Magnetic line groups.* Phys. Rev. B **25**, 6987 (1982)
23. M. Damnjanović, I. Milosević, M. Vujicić, and R. Sredanović, *Full symmetry, optical activity and potentials of single- and multi-wall nanotubes.* Phys. Rev. B **60**, 2728 (1999)
24. M. Damnjanović, I. Milosević, M. Vujicić, and R. Sredanović, *Symmetry and lattices of single wall nanotubes.* J. Phys. A: Math. Gen. **32**, 4097–4104 (1999)
25. G. Dresselhaus, *Spin–orbit interaction in zinc-blende structures.* Phys. Rev. **100**, 580–586 (1955)
26. G. Dresselhaus and M.S. Dresselhaus, *Spin–orbit interaction in graphite.* Phys. Rev. **140**, A401–A412 (1965)
27. G. Dresselhaus and M.S. Dresselhaus, *Magneto-optical effects in solids.* (XXXIV Corso) (Academic Press, New York 1966) pp. 198–256
28. G. Dresselhaus and M.S. Dresselhaus, *An effective hamiltonian for the optical properties of silicon and germanium.* Int. J. Quant. Chem. **IS**, 595 (1967)
29. G. Dresselhaus and M.S. Dresselhaus, *Fourier expansion for the electronic energy bands in silicon and germanium.* Phys. Rev. **160**, 649–679 (1967)
30. G. Dresselhaus and M.S. Dresselhaus, *Interpolation methods for phonon spectra in crystals.* Int. J. Quant. Chem. **IIS**, 333–345 (1968)
31. G. Dresselhaus, A.F. Kip, and C. Kittel, *Cyclotron resonance of electrons and holes in silicon and germanium crystals.* Phys. Rev. **98**, 368–384 (1955)
32. M.S. Dresselhaus, G. Dresselhaus and P. C. Eklund, *Science of Fullerenes and Carbon Nanotubes.* (Academic Press, New York, San Diego, 1996)
33. R.J. Elliott, *Theory of the effect of spin–orbit coupling on magnetic resonance in some semiconductors.* Phys. Rev. **96**, 266–279 (1954)
34. R.J. Elliott and K.W.H. Stevens, Proc. Roy. Soc. A **215**, 437 (1952)
35. G. Feher, *Electron spin resonance experiments on donors in silicon.* i. electronic structure of donors by the electron nuclear double resonance technique (ENDOR). Phys. Rev. **114**, 1219–1244 (1959)
36. E. Guadagnini, M. Martellini, and M. Mintchev, *Braids aand quantum group symmetry in Chern–Simons theory.* Nuclear Phys. B **336**, 581–609 (1990)
37. V. Heine, *Group Theory in Quantum Mechanics.* (Pergamon Press, Oxford 1960)
38. F. Herman and S. Skillman, *Atomic Structure Calculations.* (Prentice-Hall, Englewood Cliffs 1963)
39. C. Herring, *Effect of time reversal symmetry on energy levels of crystals.* Phys. Rev. **52**, 361 (1937)
40. G.F. Herzberg, *Infrared and Raman Spectra of Polyatomic Molecules, Molecular Spectra and Molecular Structure II.* (Van Nostrand Reinhold, New York 1949)
41. M.T. Hutchings, Sol. State Phys. **16**, 227 (1964)
42. H.A. Jahn and E.R. Teller, *Stability of polyatomic molecules in degenerate electronic states.* Part I – orbital degeneracy. Proc. Roy. Soc. A **161**, 220–235 (1937)

43. C.K. Johnson, *Crystallographic Topology 2: Overview and Work in Progress.* (International Press, Cambridge 1999)
44. H. Kamimura, *Theoretical aspects of band structures and electronic properties of pseudo-one-dimensional solids.* (Kluwer, Hingham 1985)
45. C. Kittel, *Introduction to Solid State Physics.* (Wiley, New York 1996)
46. W. Kohn and J.M.G. Luttinger, *Hyperfine splitting of donor states in silicon.* Phys. Rev. **97**, 883 (1955)
47. G.F. Koster, *Space groups and their representations.* (Solid State Physics, vol. 5) (Academic Press, New York 1957) p. 173
48. G.F. Koster, J.O. Dimmock, R.G. Wheeler, and H. Statz, *Properties of the Thirty-Two Point Groups.* (MIT Press, Cambridge 1964)
49. O.V. Kovalev, *Irreducible Representations of the Space Groups.* (Gordon and Breach, New York 1965) [Academy of Sciences USSR Press, Kiev 1961]
50. M. Lax, *Symmetry Principles in Solid State and Molecular Physics.* (Wiley, New York 1974)
51. D.B. Litvin, *Magnetic space-group types.* Act. Crystall. A **57(6)**, 729–730 (2001)
52. J.M. Luttinger, *Quantum theory of cyclotron resonance in semiconductors: general theory.* Phys. Rev. **102**, 1030 (1956)
53. G.Ya. Lyubarskii, *Application of Group Theory in Physics.* (Pergamon, New York 1960)
54. S.C. Miller and W.H. Love, *Tables of Irreducible Representations of Space Groups and Co-Representations of Magnetic Space Groups.* (Pruett Press, Denver 1967) Much of this material is also available on the web: http://www.cryst.ehu.es/ (Bilbao Crystallographic Server, University of the Basque Country, Bilbao, Basque Country, Spain)
55. C.E. Moore, *Atomic Energy Levels (National Bureau of Standards, Circular #467).* (NBS Press, Washington, 1949 [Vol. 1], 1952 [Vol. 2], 1958 [Vol. 3]). See http://physicslnist.gov/PhysRefData/DFTdata/ as well as http://physicslnist.gov/PhysRefData/ASD/
56. A. Nussbaum, *Applied Group Theory for Chemists, Physicists and Engineers.* (Prentice-Hall, Englewood Cliffs 1971)
57. J.F. Nye, *Physical Properties of Crystals: Their Representation by Tensors and Matrices.* (Oxford University Press, Oxford 1985)
58. International Union of Crystallography, *International Tables for X-Ray Crystallography.* (Kynoch Press, Birmingham 1952) See http://www.crystallography.net/ as well as http://www.cryst.ehu.es/
59. G.E. Pake and T.L. Estle, *The Physical Principles of Electron Paramagnetic Resonance.* (W.A. Benjamin, Cambridge 1973)
60. Yu.E. Perlin and M.Wagner, *Modern Problems in Condensed Matter Sciences.* Vol. 7: The dynamical Jahn–Teller Effect in Localized Systems. (North-Holland Physics Publishing, Amsterdam 1984)
61. B.M. Powell and P. Martel, *Crystal dynamics of tellurium.* Proc. 10th Int. Conf on Physics of Semiconductors 1970, pp. 851–855
62. L.M. Roth, *g factor and donor spin–lattice relaxation for electrons in germanium and silicon.* Phys. Rev. **118**, 1534–1540 (1960)
63. R. Saito, G. Dresselhaus, and M.S. Dresselhaus, *Physical Properties of Carbon Nanotubes.* (Imperial College Press, London 1998)
64. E.B. Barros, R.B. Capaz, A. Jorio, Ge.G. Samsonidze, A.G. Souza-Filho, S. Ismail-Beigi, C.D. Spataru, S.G. Louie, G. Dresselhaus, and M.S. Dresselhaus,

Selection rules for one and two-photon absorption for excitons in carbon nanotubes. Phys. Rev. **B73**, 242406 (R) (2006)
65. Ge.G. Samsonidze, A. Grüneis, R. Saito, A. Jorio, A.G. Souza Filho, G. Dresselhaus, and M.S. Dresselhaus, *Interband optical transitions in left- and right-handed single-wall carbon nanotubes.* Phys. Rev. B **69**, 205402–(1–11) (2004)
66. J. Slater and G. Koster, *Simplified LCAO method for the periodic potential problem.* Phys. Rev. **94**, 1498–1524 (1959)
67. V.J. Tekippe, H.R. Chandrasekhar, P. Fisher, and A.K. Ramdas, *Determination of the deformation-potential constant of the conduction band of silicon from the piezospectroscopy of donors.* Phys. Rev. B **6**, 2348–2356 (1972)
68. The International Tables for X-Ray Crystallographers, Vol. A, published by the International Union of Crystallography (1987) (also check web site)
69. The Optical Properties of Solids, Proceedings of the International School of Physics, Enrico Fermi Course XXXIV (Academic Press, 1966) p. 198–256
70. M. Tinkham, *Group Theory and Quantum Mechanics.* (McGraw-Hill, New York 1964)
71. M. Vujicić, I.B. Bozović, and F. Herbut, *Construction of the symmetry groups of polymer molecules.* J. Phys. A: Math. Gen. **10**, 1271 (1977)
72. S.A. Werner, R. Colella, A.W. Overhauser, and C.F. Eagen, *Observation of the phase shift of a neutron due to precession in a magnetic field.* Phys. Rev. Lett. **35**, 1053 (1975)
73. C.T. White, D.H. Roberston, and J.W. Mintmire, *Helical and rotational symmetries of nanoscale graphite tubules.* Phys. Rev. B **47**, 5485 (1993)
74. P.A. Wolff, *Matrix elements and selection rules for the two-band model of bismuth.* J. Phys. Chem. Solids **25**, 1057–1068 (1964)
75. W.A. Wooster, *Tensors and Group Theory for Physical Properties of Crystals.* (Clarendon Press, Oxford 1973)
76. R.W.G. Wyckoff, *Crystal Structures.* 2nd Edn. (Krieger, New York 1981) Also available on the web: http://www.cryst.ehu.es/ and http://www.crystallography.net/
77. Y. Yafet, *Space groups and their representations.* (Solid State Physics, vol. 14) (Academic Press, New York 1963) pp. 1–98

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