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]

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

O_h^1

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: No conditions $0kl$:
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	$\frac{1}{2},y,z;\ z,\frac{1}{2},y;\ y,z,\frac{1}{2};\ \frac{1}{2},z,y;\ y,\frac{1}{2},z;\ z,y,\frac{1}{2};$ $\frac{1}{2},\bar{y},\bar{z};\ \bar{z},\frac{1}{2},\bar{y};\ \bar{y},\bar{z},\frac{1}{2};\ \frac{1}{2},\bar{z},\bar{y};\ \bar{y},\frac{1}{2},\bar{z};\ \bar{z},\bar{y},\frac{1}{2};$ $\frac{1}{2},y,\bar{z};\ \bar{z},\frac{1}{2},y;\ y,\bar{z},\frac{1}{2};\ \frac{1}{2},\bar{z},y;\ y,\frac{1}{2},\bar{z};\ \bar{z},y,\frac{1}{2};$ $\frac{1}{2},\bar{y},z;\ z,\frac{1}{2},\bar{y};\ \bar{y},z,\frac{1}{2};\ \frac{1}{2},z,\bar{y};\ \bar{y},\frac{1}{2},z;\ z,\bar{y},\frac{1}{2}.$	
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	$\frac{1}{2},x,x;\ x,\frac{1}{2},x;\ x,x,\frac{1}{2};\ \frac{1}{2},x,\bar{x};\ \bar{x},\frac{1}{2},x;\ x,\bar{x},\frac{1}{2};$ $\frac{1}{2},\bar{x},\bar{x};\ \bar{x},\frac{1}{2},\bar{x};\ \bar{x},\bar{x},\frac{1}{2};\ \frac{1}{2},\bar{x},x;\ x,\frac{1}{2},\bar{x};\ \bar{x},x,\frac{1}{2}.$	
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	$x,\frac{1}{2},0;\ 0,x,\frac{1}{2};\ \frac{1}{2},0,x;\ x,0,\frac{1}{2};\ \frac{1}{2},x,0;\ 0,\frac{1}{2},x;$ $\bar{x},\frac{1}{2},0;\ 0,\bar{x},\frac{1}{2};\ \frac{1}{2},0,\bar{x};\ \bar{x},0,\frac{1}{2};\ \frac{1}{2},\bar{x},0;\ 0,\frac{1}{2},\bar{x}.$	
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	$4mm$	$x,\frac{1}{2},\frac{1}{2};\ \frac{1}{2},x,\frac{1}{2};\ \frac{1}{2},\frac{1}{2},x;\ \bar{x},\frac{1}{2},\frac{1}{2};\ \frac{1}{2},\bar{x},\frac{1}{2};\ \frac{1}{2},\frac{1}{2},\bar{x}.$	
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	$4/mmm$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}.$	
3	c	$4/mmm$	$0,\frac{1}{2},\frac{1}{2};\ \frac{1}{2},0,\frac{1}{2};\ \frac{1}{2},\frac{1}{2},0.$	
1	b	$m3m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}.$	
1	a	$m3m$	$0,0,0.$	

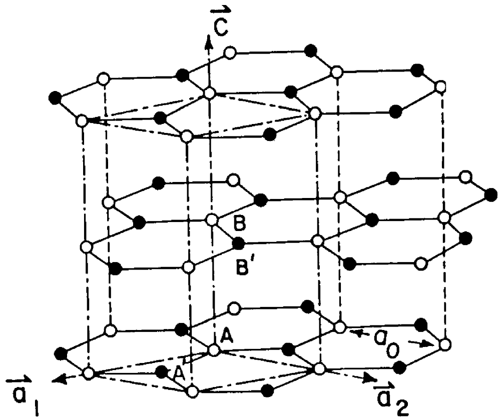


Fig. C.1. Crystal structure of hexagonal graphite, space group #194

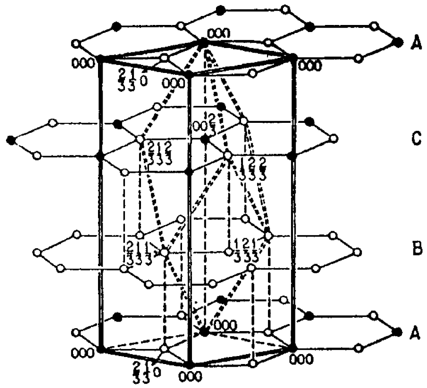
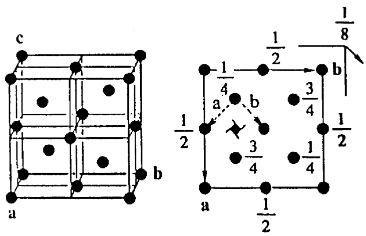


Fig. C.2. Crystal structure of rhombohedral graphite showing *ABC* stacking of the individual sheets, space group #166 $R\bar{3}m$. Also shown with *dashed lines* is the rhombohedral unit cell



(a) (b)

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.

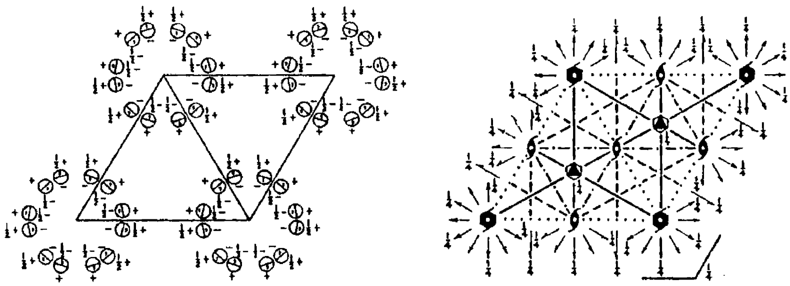
C.2 Reciprocal Space

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

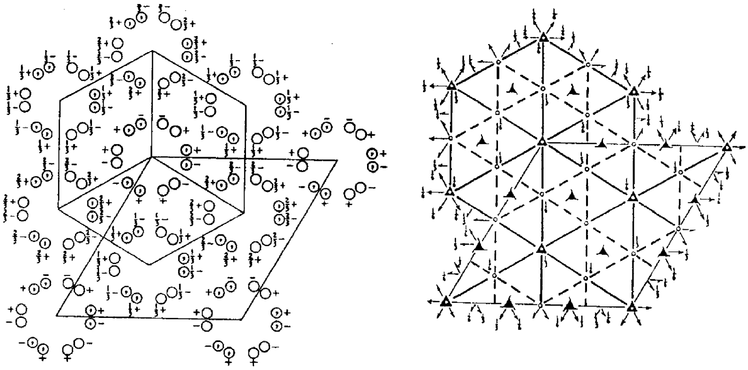
D_{6h}^4



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; $\bar{y},x-y,z$; $y-x,\bar{x},z$; $\bar{y},\bar{x},z$; $x,x-y,z$; $y-x,y,z$; $\bar{x},\bar{y},\bar{z}$; $y,y-x,\bar{z}$; $x-y,x,\bar{z}$; $y,x,\bar{z}$; $\bar{x},y-x,\bar{z}$; $x-y,\bar{y},\bar{z}$; $\bar{x},\bar{y},\frac{1}{2}+z$; $y,y-x,\frac{1}{2}+z$; $x-y,x,\frac{1}{2}+z$; $x,y,\frac{1}{2}-z$; $\bar{y},x-y,\frac{1}{2}-z$; $y-x,\bar{x},\frac{1}{2}-z$; $y,x,\frac{1}{2}+z$; $\bar{x},y-x,\frac{1}{2}+z$; $x-y,\bar{y},\frac{1}{2}+z$; $\bar{y},\bar{x},\frac{1}{2}-z$; $x,x-y,\frac{1}{2}-z$; $y-x,y,\frac{1}{2}-z$.	$hkil$: No conditions $hh\bar{2h}l$: $l=2n$ $h\bar{h}0l$: No conditions
				Special: as above, plus
12	k	m	$x,2x,z$; $2\bar{x},\bar{x},z$; $x,\bar{x},z$; $\bar{x},2\bar{x},\bar{z}$; $2x,x,\bar{z}$; $\bar{x},x,\bar{z}$; $\bar{x},2\bar{x},\frac{1}{2}+z$; $2x,x,\frac{1}{2}+z$; $\bar{x},x,\frac{1}{2}+z$; $x,2x,\frac{1}{2}-z$; $2\bar{x},\bar{x},\frac{1}{2}-z$; $x,\bar{x},\frac{1}{2}-z$.	no extra conditions
12	j	m	$x,y,\frac{1}{4}$; $\bar{y},x-y,\frac{1}{4}$; $y-x,\bar{x},\frac{1}{4}$; $\bar{y},\bar{x},\frac{1}{4}$; $x,x-y,\frac{1}{4}$; $y-x,y,\frac{1}{4}$; $\bar{x},\bar{y},\frac{3}{4}$; $y,y-x,\frac{3}{4}$; $x-y,x,\frac{3}{4}$; $y,x,\frac{3}{4}$; $\bar{x},y-x,\frac{3}{4}$; $x-y,\bar{y},\frac{3}{4}$.	
12	i	2	$x,0,0$; $0,x,0$; $\bar{x},\bar{x},0$; $x,0,\frac{1}{2}$; $0,x,\frac{1}{2}$; $\bar{x},\bar{x},\frac{1}{2}$; $\bar{x},0,0$; $0,\bar{x},0$; $x,x,0$; $\bar{x},0,\frac{1}{2}$; $0,\bar{x},\frac{1}{2}$; $x,x,\frac{1}{2}$.	$hkil$: $l=2n$
6	h	mm	$x,2x,\frac{1}{4}$; $2\bar{x},\bar{x},\frac{1}{4}$; $x,\bar{x},\frac{1}{4}$; $\bar{x},2\bar{x},\frac{3}{4}$; $2x,x,\frac{3}{4}$; $\bar{x},x,\frac{3}{4}$.	no extra conditions
6	g	$2/m$	$\frac{1}{2},0,0$; $0,\frac{1}{2},0$; $\frac{1}{2},\frac{1}{2},0$; $\frac{1}{2},0,\frac{1}{2}$; $0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.	$hkil$: $l=2n$
4	f	$3m$	$\frac{1}{3},\frac{2}{3},z$; $\frac{2}{3},\frac{1}{3},\bar{z}$; $\frac{2}{3},\frac{1}{3},\frac{1}{2}+z$; $\frac{1}{3},\frac{2}{3},\frac{1}{2}-z$.	$hkil$: If $h-k=3n$, then $l=2n$
4	e	$3m$	$0,0,z$; $0,0,\bar{z}$; $0,0,\frac{1}{2}+z$; $0,0,\frac{1}{2}-z$.	$hkil$: $l=2n$
2	d	$\bar{6}m2$	$\frac{1}{3},\frac{2}{3},\frac{3}{4}$; $\frac{2}{3},\frac{1}{3},\frac{1}{4}$.	$hkil$: If $h-k=3n$, then $l=2n$
2	c	$\bar{6}m2$	$\frac{1}{3},\frac{2}{3},\frac{1}{4}$; $\frac{2}{3},\frac{1}{3},\frac{3}{4}$.	
2	b	$\bar{6}m2$	$0,0,\frac{1}{4}$; $0,0,\frac{3}{4}$.	$hkil$: $l=2n$
2	a	$\bar{3}m$	$0,0,0$; $0,0,\frac{1}{2}$.	

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)

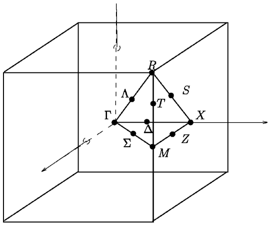


Fig. C.4. Brillouin zone for a simple cubic lattice (#221) showing the high symmetry points and axes

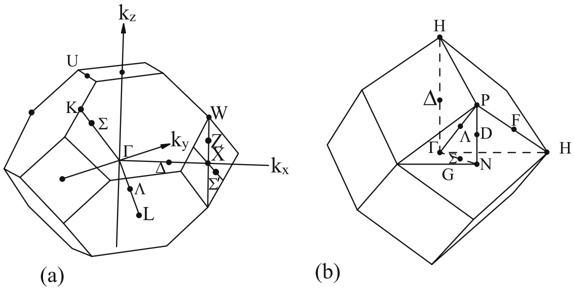


Fig. C.5. Brillouin zones for the (**a**) face-centered (#225) and (**b**) body-centered (#229) cubic lattices. Points and lines of high symmetry are indicated

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.

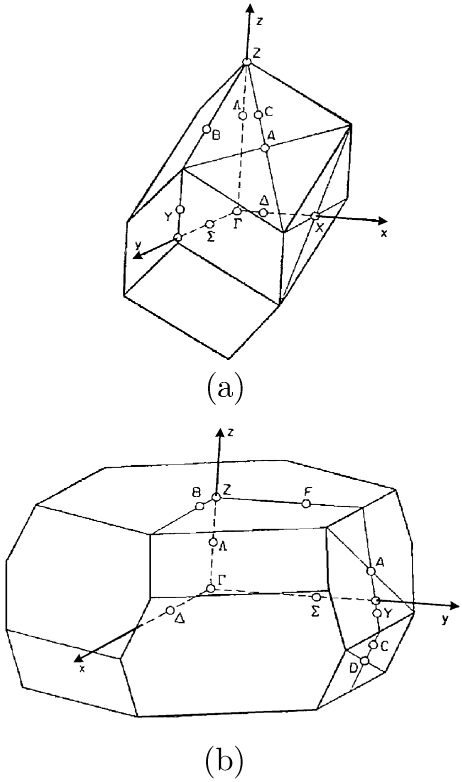


Fig. C.6. Brillouin zones for a rhombohedral lattice shown in (**a**) for rhombohedral axes and in (**b**) for hexagonal axes as presented in Table C.4 where the site symmetries corresponding to (**a**) and (**b**) are both presented for one of the rhombohedral groups

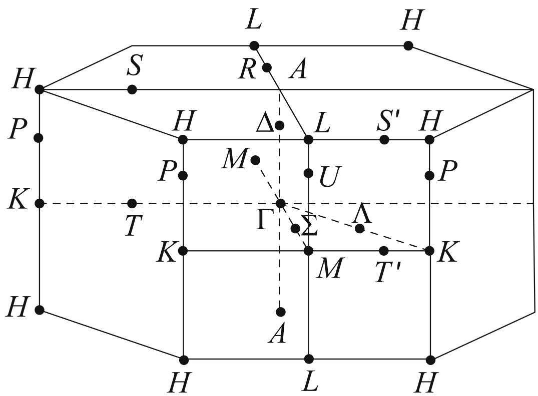


Fig. C.7. Brillouin zone for a hexagonal Bravais lattice showing high symmetry points for hexagonal structures

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}	$\{E\vert 0\}$	$\{C_2\vert\boldsymbol{\tau}\}$	$2\{C_3\vert 0\}$	$2\{C_6\vert\boldsymbol{\tau}\}$	$3\{\sigma_d\vert 0\}$	$3\{\sigma_v\vert\boldsymbol{\tau}\}$
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 $0 \le z \le 1$ 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}	$\{E\vert 0\}$	$\{2C_3\vert 0\}$	$3\{\sigma_d\vert 0\}$	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

	$\{E\vert 0\}$	$\{C_3^+\vert 0\}$ $\{C_3^-\vert 0\}$	$\{C_2'^A\vert 0\}$ $\{C_2'^B\vert 0\}$ $\{C_2'^C\vert 0\}$	$\{\sigma_h\vert\tau\}$	$\{S_3^-\vert\tau\}$ $\{S_3^+\vert\tau\}$	$\{\sigma_v^A\vert\tau\}$ $\{\sigma_v^B\vert\tau\}$ $\{\sigma_v^C\vert\tau\}$		
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	$\Sigma_2 + \Sigma_4$	$T_2 + T_4$