

## 1.4. SYMMETRY IN RECIPROCAL SPACE

(i) *Explicit symbols.* These symbols are based on the classification of crystallographic point groups and space groups by Zachariasen (1945). These symbols are termed *explicit* because they contain in an explicit manner the rotation and translation parts of the space-group generators of the space group to be derived and used. These computer-adapted explicit symbols were proposed by Shmueli (1984), who also describes in detail their implementation in the program *SPGRGEN*. This program was used for the automatic preparation of the structure-factor tables for the 17 plane groups and 230 space groups, listed in Appendix 1.4.3, and the 230 space groups in reciprocal space, listed in Appendix 1.4.4. The explicit symbols presented in this appendix are adapted to the 306 representations of the 230 space groups as presented in *IT A* (1983) with regard to the standard settings and choice of space-group origins.

The symmetry-generating algorithm underlying the explicit symbols, and their definition, are given in Section A1.4.2.2 of this appendix and the explicit symbols are listed in Table A1.4.2.1.

(ii) *Hall symbols.* These symbols are based on the implied-origin notation of Hall (1981*a,b*), who also describes in detail the algorithm implemented in the program *SGNAME* (Hall, 1981*a*). In the first edition of *IT B* (1993), the term ‘concise space-group symbols’ was used for this notation. In recent years, however, the term ‘Hall symbols’ has come into use in symmetry papers (Altermatt & Brown, 1987; Grosse-Kunstleve, 1999), software applications (Hovmöller, 1992; Grosse-Kunstleve, 1995; Larine *et al.*, 1995; Dowty, 1997) and data-handling approaches (Bourne *et al.*, 1998). This term has therefore been adopted for the second edition.

The main difference in the definition of the Hall symbols between this edition and the first edition of *IT B* is the generalization of the origin-shift vector to a full change-of-basis matrix. The examples have been expanded to show how this matrix is applied. The notation has also been made more consistent, and a typographical error in a default axis direction has been corrected.<sup>1</sup> The lattice centring symbol ‘H’ has been added to Table A1.4.2.2. In addition, Hall symbols are now provided for 530 settings to include all settings from Table 4.3.1 of *IT A* (1983). Namely, all nonstandard symbols for the monoclinic and orthorhombic space groups are included.

Some of the space-group symbols listed in Table A1.4.2.7 differ from those listed in Table B.6 (p. 119) of the first edition of *IT B*. This is because the symmetry of many space groups can be represented by more than one subset of ‘generator’ elements and these lead to different Hall symbols. The symbols listed in this edition have been selected after first sorting the symmetry elements into a strictly prescribed order based on the shape of their Seitz matrices, whereas those in Table B.6 were selected from symmetry elements in the order of *IT I* (1965). Software for selecting the Hall symbols listed in Table A1.4.2.7 is freely available (Hall, 1997). These symbols and their equivalents in the first edition of *IT B* will generate identical symmetry elements, but the former may be used as a reference table in a strict mapping procedure between different symmetry representations (Hall *et al.*, 2000).

The Hall symbols are defined in Section A1.4.2.3 of this appendix and are listed in Table A1.4.2.7.

A1.4.2.2. *Explicit symbols*

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As shown elsewhere (Shmueli, 1984), the set of representative operators of a crystallographic space group [*i.e.* the set that is

listed for each space group in the symmetry tables of *IT A* (1983) and automatically regenerated for the purpose of compiling the symmetry tables in the present chapter] may have one of the following forms:

$$\begin{aligned} & \{(\mathbf{Q}, \mathbf{u})\}, \\ & \{(\mathbf{Q}, \mathbf{u})\} \times \{(\mathbf{R}, \mathbf{v})\}, \quad \text{or} \\ & \{(\mathbf{P}, \mathbf{t})\} \times [\{(\mathbf{Q}, \mathbf{u})\} \times \{(\mathbf{R}, \mathbf{v})\}], \end{aligned} \quad (\text{A1.4.2.1})$$

where  $\mathbf{P}$ ,  $\mathbf{Q}$  and  $\mathbf{R}$  are point-group operators, and  $\mathbf{t}$ ,  $\mathbf{u}$  and  $\mathbf{v}$  are zero vectors or translations not belonging to the lattice-translations subgroup. Each of the forms in (A1.4.2.1), enclosed in braces, is evaluated as, *e.g.*,

$$\{(\mathbf{P}, \mathbf{t})\} = \{(\mathbf{I}, \mathbf{0}), (\mathbf{P}, \mathbf{t}), (\mathbf{P}, \mathbf{t})^2, \dots, (\mathbf{P}, \mathbf{t})^{g-1}\}, \quad (\text{A1.4.2.2})$$

where  $\mathbf{I}$  is a unit operator and  $g$  is the order of the rotation operator  $\mathbf{P}$  (*i.e.*  $\mathbf{P}^g = \mathbf{I}$ ). The representative operations of the space group are evaluated by expanding the generators into cyclic groups, as in (A1.4.2.2), and forming, as needed, ordered products of the expanded groups as indicated in (A1.4.2.1) and explained in detail in the original article (Shmueli, 1984). The rotation and translation parts of the generators  $(\mathbf{P}, \mathbf{t})$ ,  $(\mathbf{Q}, \mathbf{u})$  and  $(\mathbf{R}, \mathbf{v})$  presented here were adapted to the settings and choices of origin used in the main symmetry tables of *IT A* (1983).

The general structure of a three-generator symbol, corresponding to the last line of (A1.4.2.1), as represented in Table A1.4.2.1, is

$$\text{LSC}\$r_1Pt_1t_2t_3\$r_2Qu_1u_2u_3\$r_3Rv_1v_2v_3, \quad (\text{A1.4.2.3})$$

where

L – lattice type; can be P, A, B, C, I, F, or R. The symbol R is used only for the seven rhombohedral space groups in their representations in rhombohedral and hexagonal axes [obverse setting (*IT I*, 1952)].

S – crystal system; can be A (triclinic), M (monoclinic), O (orthorhombic), T (tetragonal), R (trigonal), H (hexagonal) or C (cubic).

C – status of centrosymmetry; can be C or N according as the space group is centrosymmetric or noncentrosymmetric, respectively.

\$ – this character is followed by six characters that define a generator of the space group.

$r_i$  – indicator of the type of rotation that follows:  $r_i$  is P or I according as the rotation part of the  $i$ th generator is proper or improper, respectively.

P, Q, R – two-character symbols of matrix representations of the point-group rotation operators  $\mathbf{P}$ ,  $\mathbf{Q}$  and  $\mathbf{R}$ , respectively (see below).

$t_1t_2t_3$ ,  $u_1u_2u_3$ ,  $v_1v_2v_3$  – components of the translation parts of the generators, given in units of  $\frac{1}{12}$ ; *e.g.* the translation part  $(0 \frac{1}{2} \frac{3}{4})$  is given in Table A1.4.2.1 as 069. *An exception:*  $(0 0 \frac{5}{6})$  is denoted by 005 and not by 0010.

The two-character symbols for the matrices of rotation, which appear in the explicit space-group symbols in Table A1.4.2.1, are defined as follows:

<sup>1</sup> The correct default axis direction  $\mathbf{a} - \mathbf{b}$  of an N preceded by 3 or 6 replaces  $\mathbf{a} + \mathbf{b}$  on p. 117, right-hand column, line 4, in the first edition of *IT B*.

# 1. GENERAL RELATIONSHIPS AND TECHNIQUES

Table A1.4.2.1. *Explicit symbols*

No.	Short Hermann–Mauguin symbol	Comments	Explicit symbols	No.	Short Hermann–Mauguin symbol	Comments	Explicit symbols
1	$P1$		PAN\$P1A000	15	$C2/c$	$B112/n$	BMC\$I1A000\$P2C660
2	$P\bar{1}$		PAC\$I1A000	15	$C2/c$	$I112/b$	IMC\$I1A000\$P2C060
3	$P2$	$P121$	PMN\$P2B000	16	$P222$		PON\$P2C000\$P2A000
3	$P2$	$P112$	PMN\$P2C000	17	$P222_1$		PON\$P2C006\$P2A000
4	$P2_1$	$P12_1$	PMN\$P2B060	18	$P2_1,2_1,2$		PON\$P2C000\$P2A660
4	$P2_1$	$P112_1$	PMN\$P2C006	19	$P2_1,2_1,2_1$		PON\$P2C606\$P2A660
5	$C2$	$C121$	CMN\$P2B000	20	$C222_1$		CON\$P2C006\$P2A000
5	$C2$	$A121$	AMN\$P2B000	21	$C222$		CON\$P2C000\$P2A000
5	$C2$	$I121$	IMN\$P2B000	22	$F222$		FON\$P2C000\$P2A000
5	$C2$	$A112$	AMN\$P2C000	23	$I222$		ION\$P2C000\$P2A000
5	$C2$	$B112$	BMN\$P2C000	24	$I2_1,2_1,2_1$		ION\$P2C606\$P2A660
5	$C2$	$I112$	IMN\$P2C000	25	$Pmm2$		PON\$P2C000\$I2A000
6	$Pm$	$P1m1$	PMN\$I2B000	26	$Pmc2_1$		PON\$P2C006\$I2A000
6	$Pm$	$P11m$	PMN\$I2C000	27	$Pcc2$		PON\$P2C000\$I2A006
7	$Pc$	$P1c1$	PMN\$I2B006	28	$Pma2$		PON\$P2C000\$I2A600
7	$Pc$	$P1n1$	PMN\$I2B606	29	$Pca2_1$		PON\$P2C006\$I2A606
7	$Pc$	$P1a1$	PMN\$I2B600	30	$Pnc2$		PON\$P2C000\$I2A066
7	$Pc$	$P11a$	PMN\$I2C600	31	$Pmn2_1$		PON\$P2C606\$I2A000
7	$Pc$	$P11n$	PMN\$I2C660	32	$Pba2$		PON\$P2C000\$I2A660
7	$Pc$	$P11b$	PMN\$I2C060	33	$Pna2_1$		PON\$P2C006\$I2A666
8	$Cm$	$C1m1$	CMN\$I2B000	34	$Pnn2$		PON\$P2C000\$I2A666
8	$Cm$	$A1m1$	AMN\$I2B000	35	$Cmm2$		CON\$P2C000\$I2A000
8	$Cm$	$I1m1$	IMN\$I2B000	36	$Cmc2_1$		CON\$P2C006\$I2A000
8	$Cm$	$A11m$	AMN\$I2C000	37	$Ccc2$		CON\$P2C000\$I2A006
8	$Cm$	$B11m$	BMN\$I2C000	38	$Amm2$		AON\$P2C000\$I2A000
8	$Cm$	$I11m$	IMN\$I2C000	39	$Abm2$		AON\$P2C000\$I2A060
9	$Cc$	$C1c1$	CMN\$I2B006	40	$Ama2$		AON\$P2C000\$I2A600
9	$Cc$	$A1n1$	AMN\$I2B606	41	$Aba2$		AON\$P2C000\$I2A660
9	$Cc$	$I1a1$	IMN\$I2B600	42	$Fmm2$		FON\$P2C000\$I2A000
9	$Cc$	$A11a$	AMN\$I2C600	43	$Fdd2$		FON\$P2C000\$I2A333
9	$Cc$	$B11n$	BMN\$I2C660	44	$Imm2$		ION\$P2C000\$I2A000
9	$Cc$	$I11b$	IMN\$I2C060	45	$Iba2$		ION\$P2C000\$I2A660
10	$P2/m$	$P12/m1$	PMC\$I1A000\$P2B000	46	$Ima2$		ION\$P2C000\$I2A600
10	$P2/m$	$P112/m$	PMC\$I1A000\$P2C000	47	$Pmmm$		POC\$I1A000\$P2C000\$P2A000
11	$P2_1/m$	$P12_1/m1$	PMC\$I1A000\$P2B060	48	$Pnnn$	Origin 1	POC\$I1A666\$P2C000\$P2A000
11	$P2_1/m$	$P112_1/m$	PMC\$I1A000\$P2C006	48	$Pnnn$	Origin 2	POC\$I1A000\$P2C660\$P2A066
12	$C2/m$	$C12/m1$	CMC\$I1A000\$P2B000	49	$Pccm$		POC\$I1A000\$P2C000\$P2A006
12	$C2/m$	$A12/m1$	AMC\$I1A000\$P2B000	50	$Pban$	Origin 1	POC\$I1A660\$P2C000\$P2A000
12	$C2/m$	$I12/m1$	IMC\$I1A000\$P2B000	50	$Pban$	Origin 2	POC\$I1A000\$P2C660\$P2A060
12	$C2/m$	$A112/m$	AMC\$I1A000\$P2C000	51	$Pmma$		POC\$I1A000\$P2C600\$P2A600
12	$C2/m$	$B112/m$	BMC\$I1A000\$P2C000	52	$Pnna$		POC\$I1A000\$P2C600\$P2A066
12	$C2/m$	$I112/m$	IMC\$I1A000\$P2C000	53	$Pmna$		POC\$I1A000\$P2C606\$P2A000
13	$P2/c$	$P12/c1$	PMC\$I1A000\$P2B006	54	$Pcca$		POC\$I1A000\$P2C600\$P2A606
13	$P2/c$	$P12/n1$	PMC\$I1A000\$P2B606	55	$Pbam$		POC\$I1A000\$P2C000\$P2A660
13	$P2/c$	$P12/a1$	PMC\$I1A000\$P2B600	56	$Pccn$		POC\$I1A000\$P2C660\$P2A606
13	$P2/c$	$P112/a$	PMC\$I1A000\$P2C600	57	$Pbcm$		POC\$I1A000\$P2C006\$P2A060
13	$P2/c$	$P112/n$	PMC\$I1A000\$P2C660	58	$Pnmm$		POC\$I1A000\$P2C000\$P2A666
13	$P2/c$	$P112/b$	PMC\$I1A000\$P2C060	59	$Pmmm$	Origin 1	POC\$I1A660\$P2C000\$P2A660
14	$P2_1/c$	$P12_1/c1$	PMC\$I1A000\$P2B066	59	$Pmmm$	Origin 2	POC\$I1A000\$P2C660\$P2A600
14	$P2_1/c$	$P12_1/n1$	PMC\$I1A000\$P2B666	60	$Pbcn$		POC\$I1A000\$P2C666\$P2A660
14	$P2_1/c$	$P12_1/a1$	PMC\$I1A000\$P2B660	61	$Pbca$		POC\$I1A000\$P2C606\$P2A660
14	$P2_1/c$	$P112_1/a$	PMC\$I1A000\$P2C606	62	$Pnma$		POC\$I1A000\$P2C606\$P2A666
14	$P2_1/c$	$P112_1/n$	PMC\$I1A000\$P2C666	63	$Cmcm$		COC\$I1A000\$P2C006\$P2A000
14	$P2_1/c$	$P112_1/b$	PMC\$I1A000\$P2C066	64	$Cmca$		COC\$I1A000\$P2C066\$P2A000
15	$C2/c$	$C12/c1$	CMC\$I1A000\$P2B006	65	$Cmmm$		COC\$I1A000\$P2C000\$P2A000
15	$C2/c$	$A12/n1$	AMC\$I1A000\$P2B606	66	$Cccm$		COC\$I1A000\$P2C000\$P2A006
15	$C2/c$	$I12/a1$	IMC\$I1A000\$P2B600	67	$Cmma$		COC\$I1A000\$P2C060\$P2A000
15	$C2/c$	$A112/a$	AMC\$I1A000\$P2C600	68	$Ccca$	Origin 1	COC\$I1A066\$P2C660\$P2A660

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Table A1.4.2.1 (cont.)

No.	Short Hermann–Mauguin symbol	Comments	Explicit symbols	No.	Short Hermann–Mauguin symbol	Comments	Explicit symbols
68	<i>Ccca</i>	Origin 2	COC\$I1A000\$P2C600\$P2A606	122	$\bar{I}4_2d$		ITN\$I4C000\$P2A609
69	<i>Fmmm</i>		FOC\$I1A000\$P2C000\$P2A000	123	<i>P4/mmm</i>		PTC\$I1A000\$P4C000\$P2A000
70	<i>Fddd</i>	Origin 1	FOC\$I1A333\$P2C000\$P2A000	124	<i>P4/mcc</i>		PTC\$I1A000\$P4C000\$P2A006
70	<i>Fddd</i>	Origin 2	FOC\$I1A000\$P2C990\$P2A099	125	<i>P4/nbm</i>	Origin 1	PTC\$I1A660\$P4C000\$P2A000
71	<i>Immm</i>		IOC\$I1A000\$P2C000\$P2A000	125	<i>P4/nbm</i>	Origin 2	PTC\$I1A000\$P4C600\$P2A060
72	<i>Ibam</i>		IOC\$I1A000\$P2C000\$P2A660	126	<i>P4/nnc</i>	Origin 1	PTC\$I1A666\$P4C000\$P2A000
73	<i>Ibca</i>		IOC\$I1A000\$P2C606\$P2A660	126	<i>P4/nnc</i>	Origin 2	PTC\$I1A000\$P4C600\$P2A066
74	<i>Imma</i>		IOC\$I1A000\$P2C060\$P2A000	127	<i>P4/mbm</i>		PTC\$I1A000\$P4C000\$P2A660
75	<i>P4</i>		PTN\$P4C000	128	<i>P4/mnc</i>		PTC\$I1A000\$P4C000\$P2A666
76	<i>P4<sub>1</sub></i>		PTN\$P4C003	129	<i>P4/nmm</i>	Origin 1	PTC\$I1A660\$P4C660\$P2A660
77	<i>P4<sub>2</sub></i>		PTN\$P4C006	129	<i>P4/nmm</i>	Origin 2	PTC\$I1A000\$P4C600\$P2A600
78	<i>P4<sub>3</sub></i>		PTN\$P4C009	130	<i>P4/ncc</i>	Origin 1	PTC\$I1A660\$P4C660\$P2A666
79	<i>I4</i>		ITN\$P4C000	130	<i>P4/ncc</i>	Origin 2	PTC\$I1A000\$P4C600\$P2A606
80	<i>I4<sub>1</sub></i>		ITN\$P4C063	131	<i>P4<sub>2</sub>/mnc</i>		PTC\$I1A000\$P4C006\$P2A000
81	$\bar{P}4$		PTN\$I4C000	132	<i>P4<sub>2</sub>/mcm</i>		PTC\$I1A000\$P4C006\$P2A006
82	$\bar{I}4$		ITN\$I4C000	133	<i>P4<sub>2</sub>/nbc</i>	Origin 1	PTC\$I1A666\$P4C666\$P2A006
83	<i>P4/m</i>		PTC\$I1A000\$P4C000	133	<i>P4<sub>2</sub>/nbc</i>	Origin 2	PTC\$I1A000\$P4C606\$P2A060
84	<i>P4<sub>2</sub>/m</i>		PTC\$I1A000\$P4C006	134	<i>P4<sub>2</sub>/nmm</i>	Origin 1	PTC\$I1A666\$P4C666\$P2A000
85	<i>P4/n</i>	Origin 1	PTC\$I1A660\$P4C660	134	<i>P4<sub>2</sub>/nmm</i>	Origin 2	PTC\$I1A000\$P4C606\$P2A066
85	<i>P4/n</i>	Origin 2	PTC\$I1A000\$P4C600	135	<i>P4<sub>2</sub>/mbc</i>		PTC\$I1A000\$P4C006\$P2A660
86	<i>P4<sub>2</sub>/n</i>	Origin 1	PTC\$I1A666\$P4C666	136	<i>P4<sub>2</sub>/mnm</i>		PTC\$I1A000\$P4C666\$P2A666
86	<i>P4<sub>2</sub>/n</i>	Origin 2	PTC\$I1A000\$P4C066	137	<i>P4<sub>2</sub>/nmc</i>	Origin 1	PTC\$I1A666\$P4C666\$P2A666
87	<i>I4/m</i>		ITC\$I1A000\$P4C000	137	<i>P4<sub>2</sub>/nmc</i>	Origin 2	PTC\$I1A000\$P4C606\$P2A600
88	<i>I4<sub>1</sub>/a</i>	Origin 1	ITC\$I1A063\$P4C063	138	<i>P4<sub>2</sub>/ncm</i>	Origin 1	PTC\$I1A666\$P4C666\$P2A660
88	<i>I4<sub>1</sub>/a</i>	Origin 2	ITC\$I1A000\$P4C933	138	<i>P4<sub>2</sub>/ncm</i>	Origin 2	PTC\$I1A000\$P4C606\$P2A606
89	<i>P422</i>		PTN\$P4C000\$P2A000	139	<i>I4/mmm</i>		ITC\$I1A000\$P4C000\$P2A000
90	<i>P4<sub>2</sub>2</i>		PTN\$P4C660\$P2A660	140	<i>I4/mcm</i>		ITC\$I1A000\$P4C000\$P2A006
91	<i>P4<sub>1</sub>22</i>		PTN\$P4C003\$P2A006	141	<i>I4<sub>1</sub>/amd</i>	Origin 1	ITC\$I1A063\$P4C063\$P2A063
92	<i>P4<sub>1</sub>2,2</i>		PTN\$P4C663\$P2A669	141	<i>I4<sub>1</sub>/amd</i>	Origin 2	ITC\$I1A000\$P4C393\$P2A000
93	<i>P4<sub>2</sub>22</i>		PTN\$P4C006\$P2A000	142	<i>I4<sub>1</sub>/acd</i>	Origin 1	ITC\$I1A063\$P4C063\$P2A069
94	<i>P4<sub>2</sub>2,2</i>		PTN\$P4C666\$P2A666	142	<i>I4<sub>1</sub>/acd</i>	Origin 2	ITC\$I1A000\$P4C393\$P2A006
95	<i>P4<sub>3</sub>22</i>		PTN\$P4C009\$P2A006	143	<i>P3</i>		PRN\$P3C000
96	<i>P4<sub>3</sub>2,2</i>		PTN\$P4C669\$P2A663	144	<i>P3<sub>1</sub></i>		PRN\$P3C004
97	<i>I422</i>		ITN\$P4C000\$P2A000	145	<i>P3<sub>2</sub></i>		PRN\$P3C008
98	<i>I4<sub>1</sub>22</i>		ITN\$P4C063\$P2A063	146	<i>R3</i>	Hexagonal axes	RRN\$P3C000
99	<i>P4mm</i>		PTN\$P4C000\$I2A000	146	<i>R3</i>	Rhombohedral axes	PRN\$P3Q000
100	<i>P4bm</i>		PTN\$P4C000\$I2A660	147	$\bar{P}3$		PRC\$I3C000
101	<i>P4<sub>2</sub>cm</i>		PTN\$P4C006\$I2A006	148	$\bar{R}3$	Hexagonal axes	RRC\$I3C000
102	<i>P4<sub>2</sub>nmm</i>		PTN\$P4C666\$I2A666	148	$\bar{R}3$	Rhombohedral axes	PRC\$I3Q000
103	<i>P4cc</i>		PTN\$P4C000\$I2A006	149	<i>P312</i>		PRN\$P3C000\$P2G000
104	<i>P4nc</i>		PTN\$P4C000\$I2A666	150	<i>P321</i>		PRN\$P3C000\$P2F000
105	<i>P4<sub>2</sub>mc</i>		PTN\$P4C006\$I2A000	151	<i>P3<sub>1</sub>12</i>		PRN\$P3C004\$P2G000
106	<i>P4<sub>2</sub>bc</i>		PTN\$P4C006\$I2A660	152	<i>P3<sub>1</sub>21</i>		PRN\$P3C004\$P2F008
107	<i>I4mm</i>		ITN\$P4C000\$I2A000	153	<i>P3<sub>2</sub>12</i>		PRN\$P3C008\$P2G000
108	<i>I4cm</i>		ITN\$P4C000\$I2A006	154	<i>P3<sub>2</sub>21</i>		PRN\$P3C008\$P2F004
109	<i>I4<sub>1</sub>md</i>		ITN\$P4C063\$I2A666	155	<i>R32</i>	Hexagonal axes	RRN\$P3C000\$P2F000
110	<i>I4<sub>1</sub>cd</i>		ITN\$P4C063\$I2A660	155	<i>R32</i>	Rhombohedral axes	PRN\$P3Q000\$P2E000
111	$\bar{P}4_2m$		PTN\$I4C000\$P2A000	156	<i>P3m1</i>		PRN\$P3C000\$I2F000
112	$\bar{P}4_2c$		PTN\$I4C000\$P2A006	157	<i>P31m</i>		PRN\$P3C000\$I2G000
113	$\bar{P}4_2,1m$		PTN\$I4C000\$P2A660	158	<i>P3c1</i>		PRN\$P3C000\$I2F006
114	$\bar{P}4_2,1c$		PTN\$I4C000\$P2A666	159	<i>P31c</i>		PRN\$P3C000\$I2G006
115	$\bar{P}4m2$		PTN\$I4C000\$P2D000	160	<i>R3m</i>	Hexagonal axes	RRN\$P3C000\$I2F000
116	$\bar{P}4c2$		PTN\$I4C000\$P2D006	160	<i>R3m</i>	Rhombohedral axes	PRN\$P3Q000\$I2E000
117	$\bar{P}4b2$		PTN\$I4C000\$P2D660	161	<i>R3c</i>	Hexagonal axes	RRN\$P3C000\$I2F006
118	$\bar{P}4n2$		PTN\$I4C000\$P2D666	161	<i>R3c</i>	Rhombohedral axes	PRN\$P3Q000\$I2E666
119	$\bar{I}4m2$		ITN\$I4C000\$P2D000	162	$\bar{P}31m$		PRC\$I3C000\$P2G000
120	$\bar{I}4c2$		ITN\$I4C000\$P2D006	163	$\bar{P}31c$		PRC\$I3C000\$P2G006
121	$\bar{I}4_2m$		ITN\$I4C000\$P2A000	164	$\bar{P}3m1$		PRC\$I3C000\$P2F000

# 1. GENERAL RELATIONSHIPS AND TECHNIQUES

Table A1.4.2.1 (cont.)

No.	Short Hermann-Mauguin symbol	Comments	Explicit symbols
165	$P\bar{3}c1$		PRC\$I3C000\$P2F006
166	$R\bar{3}m$	Hexagonal axes	RRC\$I3C000\$P2F000
166	$R\bar{3}m$	Rhombohedral axes	PRC\$I3Q000\$P2E000
167	$R\bar{3}c$	Hexagonal axes	RRC\$I3C000\$P2F006
167	$R\bar{3}c$	Rhombohedral axes	PRC\$I3Q000\$P2E666
168	$P6$		PHN\$P6C000
169	$P6_1$		PHN\$P6C002
170	$P6_5$		PHN\$P6C005
171	$P6_2$		PHN\$P6C004
172	$P6_4$		PHN\$P6C008
173	$P6_3$		PHN\$P6C006
174	$P\bar{6}$		PHN\$I6C000
175	$P6/m$		PHC\$I1A000\$P6C000
176	$P6_3/m$		PHC\$I1A000\$P6C006
177	$P622$		PHN\$P6C000\$P2F000
178	$P6_122$		PHN\$P6C002\$P2F000
179	$P6_522$		PHN\$P6C005\$P2F000
180	$P6_222$		PHN\$P6C004\$P2F000
181	$P6_422$		PHN\$P6C008\$P2F000
182	$P6_322$		PHN\$P6C006\$P2F000
183	$P6mm$		PHN\$P6C000\$I2F000
184	$P6cc$		PHN\$P6C000\$I2F006
185	$P6_3cm$		PHN\$P6C006\$I2F006
186	$P6_3mc$		PHN\$P6C006\$I2F000
187	$P\bar{6}m2$		PHN\$I6C000\$P2G000
188	$P\bar{6}c2$		PHN\$I6C006\$P2G000
189	$P\bar{6}2m$		PHN\$I6C000\$P2F000
190	$P\bar{6}2c$		PHN\$I6C006\$P2F000
191	$P6/mmm$		PHC\$I1A000\$P6C000\$P2F000
192	$P6/mcc$		PHC\$I1A000\$P6C000\$P2F006
193	$P6_3/mcm$		PHC\$I1A000\$P6C006\$P2F006
194	$P6_3/mmc$		PHC\$I1A000\$P6C006\$P2F000
195	$P23$		PCN\$P3Q000\$P2C000\$P2A000
196	$F23$		FCN\$P3Q000\$P2C000\$P2A000
197	$I23$		ICN\$P3Q000\$P2C000\$P2A000
198	$P2_13$		PCN\$P3Q000\$P2C606\$P2A660
199	$I2_13$		ICN\$P3Q000\$P2C606\$P2A660

  

No.	Short Hermann-Mauguin symbol	Comments	Explicit symbols
200	$Pm\bar{3}$		PCC\$I3Q000\$P2C000\$P2A000
201	$Pn\bar{3}$	Origin 1	PCC\$I3Q666\$P2C000\$P2A000
201	$Pn\bar{3}$	Origin 2	PCC\$I3Q000\$P2C660\$P2A066
202	$Fm\bar{3}$		FCC\$I3Q000\$P2C000\$P2A000
203	$Fd\bar{3}$	Origin 1	FCC\$I3Q333\$P2C000\$P2A000
203	$Fd\bar{3}$	Origin 2	FCC\$I3Q000\$P2C330\$P2A033
204	$Im\bar{3}$		ICC\$I3Q000\$P2C000\$P2A000
205	$Pa\bar{3}$		PCC\$I3Q000\$P2C606\$P2A660
206	$Ia\bar{3}$		ICC\$I3Q000\$P2C606\$P2A660
207	$P432$		PCN\$P3Q000\$P4C000\$P2D000
208	$P4_232$		PCN\$P3Q000\$P4C666\$P2D666
209	$F432$		FCN\$P3Q000\$P4C000\$P2D000
210	$F4_132$		FCN\$P3Q000\$P4C993\$P2D939
211	$I432$		ICN\$P3Q000\$P4C000\$P2D000
212	$P4_332$		PCN\$P3Q000\$P4C939\$P2D399
213	$P4_132$		PCN\$P3Q000\$P4C393\$P2D933
214	$I4_132$		ICN\$P3Q000\$P4C393\$P2D933
215	$P\bar{4}3m$		PCN\$P3Q000\$I4C000\$I2D000
216	$F\bar{4}3m$		FCN\$P3Q000\$I4C000\$I2D000
217	$I\bar{4}3m$		ICN\$P3Q000\$I4C000\$I2D000
218	$P\bar{4}3n$		PCN\$P3Q000\$I4C666\$I2D666
219	$F\bar{4}3c$		FCN\$P3Q000\$I4C666\$I2D666
220	$I\bar{4}3d$		ICN\$P3Q000\$I4C939\$I2D399
221	$Pm\bar{3}m$		PCC\$I3Q000\$P4C000\$P2D000
222	$Pn\bar{3}n$	Origin 1	PCC\$I3Q666\$P4C000\$P2D000
222	$Pn\bar{3}n$	Origin 2	PCC\$I3Q000\$P4C600\$P2D006
223	$Pm\bar{3}n$		PCC\$I3Q000\$P4C666\$P2D666
224	$Pn\bar{3}m$	Origin 1	PCC\$I3Q666\$P4C666\$P2D666
224	$Pn\bar{3}m$	Origin 2	PCC\$I3Q000\$P4C066\$P2D660
225	$Fm\bar{3}m$		FCC\$I3Q000\$P4C000\$P2D000
226	$Fm\bar{3}c$		FCC\$I3Q000\$P4C666\$P2D666
227	$Fd\bar{3}m$	Origin 1	FCC\$I3Q333\$P4C993\$P2D939
227	$Fd\bar{3}m$	Origin 2	FCC\$I3Q000\$P4C693\$P2D936
228	$Fd\bar{3}c$	Origin 1	FCC\$I3Q999\$P4C993\$P2D939
228	$Fd\bar{3}c$	Origin 2	FCC\$I3Q000\$P4C093\$P2D930
229	$Im\bar{3}m$		ICC\$I3Q000\$P4C000\$P2D000
230	$Ia\bar{3}d$		ICC\$I3Q000\$P4C393\$P2D933

$$\begin{aligned}
 1A &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} & 2A &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix} & 2B &= \begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix} \\
 2C &= \begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix} & 2D &= \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix} & 2E &= \begin{pmatrix} 0 & \bar{1} & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix} \\
 2F &= \begin{pmatrix} 1 & \bar{1} & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix} & 2G &= \begin{pmatrix} 1 & 0 & 0 \\ 1 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix} & 3Q &= \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \\
 3C &= \begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix} & 4C &= \begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} & 6C &= \begin{pmatrix} 1 & \bar{1} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix},
 \end{aligned}$$

where only matrices of proper rotation are given (and required), since the corresponding matrices of improper rotation are created by the program for appropriate value of the  $r_i$  indicator.

The first character of a symbol is the order of the axis of rotation and the second character specifies its orientation: in terms of direct-space lattice vectors, we have

$$\begin{aligned}
 A &= [100], B = [010], C = [001], D = [110], \\
 E &= [1\bar{1}0], F = [100], G = [210] \text{ and } Q = [111]
 \end{aligned}$$

for the standard orientations of the axes of rotation. Note that the axes 2F, 2G, 3C and 6C appear in trigonal and hexagonal space groups.

In the above scheme a space group is determined by one, two or at most three generators [see (A1.4.2.1)]. It should be pointed out that a convenient way of achieving a representation of the space group in any setting and relative to any origin is to start from the standard generators in Table A1.4.2.1 and let the computer program perform the appropriate transformation of the generators only, as in equations (1.4.4.4) and (1.4.4.5). The subsequent expansion of the transformed generators and the formation of the required products [see (A1.4.2.1)]

## 1.4. SYMMETRY IN RECIPROCAL SPACE

Table A1.4.2.2. *Lattice symbol L*

The lattice symbol L implies Seitz matrices for the lattice translations. For noncentrosymmetric lattices the rotation parts of the Seitz matrices are for  $I$  (see Table A1.4.2.4). For centrosymmetric lattices the rotation parts are  $I$  and  $-I$ . The translation parts in the fourth columns of the Seitz matrices are listed in the last column of the table. The total number of matrices implied by each symbol is given by  $nS$ .

Noncentrosymmetric		Centrosymmetric		Implied lattice translation(s)
Symbol	$nS$	Symbol	$nS$	
P	1	-P	2	0, 0, 0
A	2	-A	4	0, 0, 0 $0, \frac{1}{2}, \frac{1}{2}$
B	2	-B	4	0, 0, 0 $\frac{1}{2}, 0, \frac{1}{2}$
C	2	-C	4	0, 0, 0 $\frac{1}{2}, \frac{1}{2}, 0$
I	2	-I	4	0, 0, 0 $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$
R	3	-R	6	0, 0, 0 $\frac{2}{3}, \frac{1}{3}, \frac{1}{3}$ $\frac{1}{3}, \frac{2}{3}, \frac{2}{3}$
H	3	-H	6	0, 0, 0 $\frac{2}{3}, \frac{1}{3}, 0$ $\frac{1}{3}, \frac{2}{3}, 0$
F	4	-F	8	0, 0, 0 $0, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, 0$

and (A1.4.2.2)] leads to the new representation of the space group.

In order to illustrate an explicit space-group symbol consider, for example, the symbol for the space group  $Ia\bar{3}d$ , as given in Table A1.4.2.1:

ICCS\$I3Q000\$P4C393\$P2D933.

The first three characters tell us that the Bravais lattice of this space group is of type I, that the space group is centrosymmetric and that it belongs to the cubic system. We then see that the generators are (i) an improper threefold axis along [111] (I3Q) with a zero translation part, (ii) a proper fourfold axis along [001] (P4C) with translation part (1/4, 3/4, 1/4) and (iii) a proper twofold axis along [110] (P2D) with translation part (3/4, 1/4, 1/4).

If we make use of the above-outlined interpretation of the explicit symbol (A1.4.2.3), the space-group symmetry transformations in direct space, corresponding to these three generators of the space group  $Ia\bar{3}d$ , become

$$\begin{aligned} \left[ \begin{pmatrix} 0 & 0 & \bar{1} \\ \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \right] &= \begin{pmatrix} \bar{z} \\ \bar{x} \\ \bar{y} \end{pmatrix}, \\ \left[ \begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} \frac{1}{4} \\ \frac{3}{4} \\ \frac{1}{4} \end{pmatrix} \right] &= \begin{pmatrix} \frac{1}{4} - y \\ \frac{3}{4} + x \\ \frac{1}{4} + z \end{pmatrix}, \\ \left[ \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} \frac{3}{4} \\ \frac{1}{4} \\ \frac{1}{4} \end{pmatrix} \right] &= \begin{pmatrix} \frac{3}{4} + y \\ \frac{1}{4} + x \\ \frac{1}{4} - z \end{pmatrix}. \end{aligned}$$

The corresponding symmetry transformations in reciprocal space, in the notation of Section 1.4.4, are

$$\left[ (hkl) \begin{pmatrix} 0 & 0 & \bar{1} \\ \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \end{pmatrix} : - (hkl) \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \right] = [\bar{k}\bar{h} : 0];$$

similarly,  $[\bar{k}\bar{h}l : -131/4]$  and  $[k\bar{h}\bar{l} : -311/4]$  are obtained from the second and third generator of  $Ia\bar{3}d$ , respectively.

The first column of Table A1.4.2.1 lists the conventional space-group number. The second column shows the conventional short Hermann-Mauguin or international space-group symbol, and the third column, *Comments*, shows the full international space-group symbol *only* for the different settings of the monoclinic space groups that are given in the main space-group tables of *IT*

(1983). Other comments pertain to the choice of the space-group origin – where there are alternatives – and to axial systems. The fourth column shows the explicit space-group symbols described above for each of the settings considered in *IT A* (1983).

### A1.4.2.3. Hall symbols

BY S. R. HALL AND R. W. GROSSE-KUNSTLEVE

The explicit-origin space-group notation proposed by Hall (1981a) is based on a subset of the symmetry operations, in the form of Seitz matrices, sufficient to uniquely define a space group. The concise unambiguous nature of this notation makes it well suited to handling symmetry in computing and database applications.

Table A1.4.2.7 lists space-group notation in several formats. The first column of Table A1.4.2.7 lists the space-group numbers with axis codes appended to identify the nonstandard settings. The second column lists the Hermann-Mauguin symbols in computer-entry format with appended codes to identify the origin and cell choice when there are alternatives. The general forms of the Hall notation are listed in the fourth column and the computer-entry representations of these symbols are listed in the third column. The computer-entry format is the general notation expressed as case-insensitive ASCII characters with the overline (bar) symbol replaced by a minus sign.

The Hall notation has the general form:

$$\mathbf{L}[\mathbf{N}_T^A]_1 \dots [\mathbf{N}_T^A]_p \mathbf{V}. \quad (\text{A1.4.2.4})$$

Table A1.4.2.3. *Translation symbol T*

The symbol T specifies the translation elements of a Seitz matrix. Alphabetical symbols (given in the first column) specify translations along a fixed direction. Numerical symbols (given in the third column) specify translations as a fraction of the rotation order  $|N|$  and in the direction of the implied or explicitly defined axis.

Translation symbol	Translation vector	Subscript symbol	Fractional translation
<i>a</i>	$\frac{1}{2}, 0, 0$	<i>I</i> in $3_1$	$\frac{1}{2}$
<i>b</i>	$0, \frac{1}{2}, 0$	2 in $3_2$	$\frac{2}{3}$
<i>c</i>	$0, 0, \frac{1}{2}$	<i>I</i> in $4_1$	$\frac{1}{4}$
<i>n</i>	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	3 in $4_3$	$\frac{3}{4}$
<i>u</i>	$\frac{1}{4}, 0, 0$	<i>I</i> in $6_1$	$\frac{1}{6}$
<i>v</i>	$0, \frac{1}{4}, 0$	2 in $6_2$	$\frac{1}{3}$
<i>w</i>	$0, 0, \frac{1}{4}$	4 in $6_4$	$\frac{2}{3}$
<i>d</i>	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	5 in $6_5$	$\frac{5}{6}$