International Tables for Crystallography (2010). Vol. B, Appendix 1.4.2, pp. 122–134.

Intuitive proofs follow directly from the restrictions on *hkl*, given in Table 1.4.4.1.

APPENDIX A1.4.1
Comments on the preparation and usage of the tables

By U. Shmueli

The straightforward but rather extensive calculations and text processing related to Tables A1.4.3.1 through A1.4.3.7 and Table A1.4.4.1 in Appendices 1.4.3 and 1.4.4, respectively, were performed with the aid of a combination of FORTRAN and REDUCE (Hearn, 1973) programs, designed so as to enable the author to produce the table entries directly from a space-group symbol and with a minimum amount of intermediate manual intervention. The first stage of the calculation, the generation of a space group (coordinates of the equivalent positions), was accomplished with the program *SPGRGEN*, the algorithm of which was described in some detail elsewhere (Shmueli, 1984). A complete list of computer-adapted space-group symbols, processed by *SPGRGEN* and not given in the latter reference, is presented in Table A1.4.2.1 of Appendix 1.4.2.

The generation of the space group is followed by a construction of symbolic expressions for the scalar products $\mathbf{h}^T(\boldsymbol{P}\mathbf{r}+\mathbf{t})$; *e.g.* for position No. (13) in the space group $P4_132$ (No. 213, *IT* I, 1952, *IT* A, 1983), this scalar product is given by $h(\frac{3}{4}+y)+k(\frac{1}{4}+x)+l(\frac{1}{4}-z)$. The construction of the various table entries consists of expanding the sines and cosines of these scalar products, performing the required summations, and simplifying the result where possible. The construction of the scalar products in a FORTRAN program is fairly easy and the extremely tedious trigonometric calculations required by equations (1.4.2.19) and (1.4.2.20) can be readily performed with the aid of one of several available computer-algebraic languages (for a review, see *Computers in the New Laboratory – a Nature Survey*, 1981); the REDUCE language was employed for the above purpose.

Since the REDUCE programs required for the summations in (1.4.2.19) and (1.4.2.20) for the various space groups were seen to have much in common, it was decided to construct a FORTRAN interface which would process the space-group input and prepare automatically REDUCE programs for the algebraic work. The least straightforward problem encountered during this work was the need to 'convince' the interface to generate *hkl* parity assignments which are appropriate to the space-group information input. This was solved for all the crystal families except the hexagonal by setting up a 'basis' of the form: $h/2, k/2, l/2, (k+l)/2, \ldots, (h+k+l)/4$ and representing the translation parts of the scalar products, $\mathbf{h}^T\mathbf{t}$, as sums of such 'basis functions'. A subsequent construction of an automatic parity routine proved to be easy and the interface could thus produce any number of REDUCE programs for the summations in (1.4.2.19) and (1.4.2.20) using a list of space-group symbols as the sole input. These included trigonal and hexagonal space groups with translation components of $\frac{1}{2}$. This approach seemed to be too awkward for some space groups containing threefold and sixfold screw axes, and these were treated individually.

There is little to say about the REDUCE programs, except that the output they generate is at the same level of trigonometric complexity as the expressions for *A* and *B* appearing in Volume I (*IT* I, 1952). This could have been improved by making use of the pattern-matching capabilities that are incorporated in REDUCE, but it was found more convenient to construct a FORTRAN interpreter which would detect in the REDUCE output the basic building blocks of the trigonometric structure factors (see Section 1.4.3.3) and perform the required transformations.

Tables A1.4.3.1–A1.4.3.7 were thus constructed with the aid of a chain composed of (i) a space-group generating routine, (ii) a FORTRAN interface, which processes the space-group input and 'writes' a complete REDUCE program, (iii) execution of the REDUCE program and (iv) a FORTRAN interpreter of the REDUCE output in terms of the abbreviated symbols to be used in the tables. The computation was at a 'one-group-at-a-time' basis and the automation of its repetition was performed by means of procedural constructs at the operating-system level. The construction of Table A1.4.4.1 involved only the preliminary stage of the processing of the space-group information by the FORTRAN interface. All the computations were carried out on a Cyber 170–855 at the Tel Aviv University Computation Center.

It is of some importance to comment on the recommended usage of the tables included in this chapter in automatic computations. If, for example, we wish to compute the expression: $A=-8(\text{Escs}+\text{Ossc})$, use can be made of the facility provided by most versions of FORTRAN of transferring subprogram names as parameters of a FUNCTION. We thus need only two FUNCTIONs for any calculation of *A* and *B* for a cubic space group, one FUNCTION for the block of even permutations of *x*, *y* and *z*:

```
      FUNCTION E(P,Q,R)
      EXTERNAL SIN,COS
      COMMON/TSF/TPH,TPK,TPL,X,Y,Z
      E = P(TPH * X) * Q(TPK * Y) * R(TPL * Z)
     1 + P(TPH * Z) * Q(TPK * X) * R(TPL * Y)
     2 + P(TPH * Y) * Q(TPK * Z) * R(TPL * X)
      RETURN
      END
```

where TPH, TPK and TPL denote $2\pi h$, $2\pi k$ and $2\pi l$, respectively, and a similar FUNCTION, say O(P,Q,R), for the block of odd permutations of *x*, *y* and *z*. The calling statement in the calling (sub)program can thus be:

```
A = -8 * (E(SIN,COS,SIN) + O(SIN,SIN,COS)).
```

A small number of such FUNCTIONs suffices for all the space-group-specific computations that involve trigonometric structure factors.

APPENDIX A1.4.2
Space-group symbols for numeric and symbolic computations

A1.4.2.1. Introduction

By U. Shmueli, S. R. Hall and R. W. Grosse-Kunstleve

This appendix lists two sets of computer-adapted space-group symbols which are implemented in existing crystallographic software and can be employed in the automated generation of space-group representations. The computer generation of space-group symmetry information is of well known importance in many crystallographic calculations, numeric as well as symbolic. A prerequisite for a computer program that generates this information is a set of computer-adapted space-group symbols which are based on the generating elements of the space group to be derived. The sets of symbols to be presented are:

(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.[1] 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

By U. Shmueli

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:

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

where **P**, **Q** and **R** are point-group operators, and **t**, **u** and **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.*,

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

where **I** is a unit operator and g is the order of the rotation operator **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 (**P**, **t**), (**Q**, **u**) and (**R**, **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

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

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 ith generator is proper or improper, respectively.

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

$\mathrm{t_1t_2t_3}$, $\mathrm{u_1u_2u_3}$, $\mathrm{v_1v_2v_3}$ – 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:

[1] 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.

Table A1.4.2.1. *Explicit symbols*

No.	Short Hermann–Mauguin symbol	Comments	Explicit symbols
1	$P1$		`PAN$P1A000`
2	$P\bar{1}$		`PAC$I1A000`
3	$P2$	$P121$	`PMN$P2B000`
3	$P2$	$P112$	`PMN$P2C000`
4	$P2_1$	$P12_11$	`PMN$P2B060`
4	$P2_1$	$P112_1$	`PMN$P2C006`
5	$C2$	$C121$	`CMN$P2B000`
5	$C2$	$A121$	`AMN$P2B000`
5	$C2$	$I121$	`IMN$P2B000`
5	$C2$	$A112$	`AMN$P2C000`
5	$C2$	$B112$	`BMN$P2C000`
5	$C2$	$I112$	`IMN$P2C000`
6	Pm	$P1m1$	`PMN$I2B000`
6	Pm	$P11m$	`PMN$I2C000`
7	Pc	$P1c1$	`PMN$I2B006`
7	Pc	$P1n1$	`PMN$I2B606`
7	Pc	$P1a1$	`PMN$I2B600`
7	Pc	$P11a$	`PMN$I2C600`
7	Pc	$P11n$	`PMN$I2C660`
7	Pc	$P11b$	`PMN$I2C060`
8	Cm	$C1m1$	`CMN$I2B000`
8	Cm	$A1m1$	`AMN$I2B000`
8	Cm	$I1m1$	`IMN$I2B000`
8	Cm	$A11m$	`AMN$I2C000`
8	Cm	$B11m$	`BMN$I2C000`
8	Cm	$I11m$	`IMN$I2C000`
9	Cc	$C1c1$	`CMN$I2B006`
9	Cc	$A1n1$	`AMN$I2B606`
9	Cc	$I1a1$	`IMN$I2B600`
9	Cc	$A11a$	`AMN$I2C600`
9	Cc	$B11n$	`BMN$I2C660`
9	Cc	$I11b$	`IMN$I2C060`
10	$P2/m$	$P12/m1$	`PMC$I1A000$P2B000`
10	$P2/m$	$P112/m$	`PMC$I1A000$P2C000`
11	$P2_1/m$	$P12_1/m1$	`PMC$I1A000$P2B060`
11	$P2_1/m$	$P112_1/m$	`PMC$I1A000$P2C006`
12	$C2/m$	$C12/m1$	`CMC$I1A000$P2B000`
12	$C2/m$	$A12/m1$	`AMC$I1A000$P2B000`
12	$C2/m$	$I12/m1$	`IMC$I1A000$P2B000`
12	$C2/m$	$A112/m$	`AMC$I1A000$P2C000`
12	$C2/m$	$B112/m$	`BMC$I1A000$P2C000`
12	$C2/m$	$I112/m$	`IMC$I1A000$P2C000`
13	$P2/c$	$P12/c1$	`PMC$I1A000$P2B006`
13	$P2/c$	$P12/n1$	`PMC$I1A000$P2B606`
13	$P2/c$	$P12/a1$	`PMC$I1A000$P2B600`
13	$P2/c$	$P112/a$	`PMC$I1A000$P2C600`
13	$P2/c$	$P112/n$	`PMC$I1A000$P2C660`
13	$P2/c$	$P112/b$	`PMC$I1A000$P2C060`
14	$P2_1/c$	$P12_1/c1$	`PMC$I1A000$P2B066`
14	$P2_1/c$	$P12_1/n1$	`PMC$I1A000$P2B666`
14	$P2_1/c$	$P12_1/a1$	`PMC$I1A000$P2B660`
14	$P2_1/c$	$P112_1/a$	`PMC$I1A000$P2C606`
14	$P2_1/c$	$P112_1/n$	`PMC$I1A000$P2C666`
14	$P2_1/c$	$P112_1/b$	`PMC$I1A000$P2C066`
15	$C2/c$	$C12/c1$	`CMC$I1A000$P2B006`
15	$C2/c$	$A12/n1$	`AMC$I1A000$P2B606`
15	$C2/c$	$I12/a1$	`IMC$I1A000$P2B600`
15	$C2/c$	$A112/a$	`AMC$I1A000$P2C600`
15	$C2/c$	$B112/n$	`BMC$I1A000$P2C660`
15	$C2/c$	$I112/b$	`IMC$I1A000$P2C060`
16	$P222$		`PON$P2C000$P2A000`
17	$P222_1$		`PON$P2C006$P2A000`
18	$P2_12_12$		`PON$P2C000$P2A660`
19	$P2_12_12_1$		`PON$P2C606$P2A660`
20	$C222_1$		`CON$P2C006$P2A000`
21	$C222$		`CON$P2C000$P2A000`
22	$F222$		`FON$P2C000$P2A000`
23	$I222$		`ION$P2C000$P2A000`
24	$I2_12_12_1$		`ION$P2C606$P2A660`
25	$Pmm2$		`PON$P2C000$I2A000`
26	$Pmc2_1$		`PON$P2C006$I2A000`
27	$Pcc2$		`PON$P2C000$I2A006`
28	$Pma2$		`PON$P2C000$I2A600`
29	$Pca2_1$		`PON$P2C006$I2A606`
30	$Pnc2$		`PON$P2C000$I2A066`
31	$Pmn2_1$		`PON$P2C606$I2A000`
32	$Pba2$		`PON$P2C000$I2A660`
33	$Pna2_1$		`PON$P2C006$I2A666`
34	$Pnn2$		`PON$P2C000$I2A666`
35	$Cmm2$		`CON$P2C000$I2A000`
36	$Cmc2_1$		`CON$P2C006$I2A000`
37	$Ccc2$		`CON$P2C000$I2A006`
38	$Amm2$		`AON$P2C000$I2A000`
39	$Abm2$		`AON$P2C000$I2A060`
40	$Ama2$		`AON$P2C000$I2A600`
41	$Aba2$		`AON$P2C000$I2A660`
42	$Fmm2$		`FON$P2C000$I2A000`
43	$Fdd2$		`FON$P2C000$I2A333`
44	$Imm2$		`ION$P2C000$I2A000`
45	$Iba2$		`ION$P2C000$I2A660`
46	$Ima2$		`ION$P2C000$I2A600`
47	$Pmmm$		`POC$I1A000$P2C000$P2A000`
48	$Pnnn$	Origin 1	`POC$I1A666$P2C000$P2A000`
48	$Pnnn$	Origin 2	`POC$I1A000$P2C660$P2A066`
49	$Pccm$		`POC$I1A000$P2C000$P2A006`
50	$Pban$	Origin 1	`POC$I1A660$P2C000$P2A000`
50	$Pban$	Origin 2	`POC$I1A000$P2C660$P2A060`
51	$Pmma$		`POC$I1A000$P2C600$P2A600`
52	$Pnna$		`POC$I1A000$P2C600$P2A066`
53	$Pmna$		`POC$I1A000$P2C606$P2A000`
54	$Pcca$		`POC$I1A000$P2C600$P2A606`
55	$Pbam$		`POC$I1A000$P2C000$P2A660`
56	$Pccn$		`POC$I1A000$P2C660$P2A606`
57	$Pbcm$		`POC$I1A000$P2C006$P2A060`
58	$Pnnm$		`POC$I1A000$P2C000$P2A666`
59	$Pmmn$	Origin 1	`POC$I1A660$P2C000$P2A660`
59	$Pmmn$	Origin 2	`POC$I1A000$P2C660$P2A600`
60	$Pbcn$		`POC$I1A000$P2C666$P2A660`
61	$Pbca$		`POC$I1A000$P2C606$P2A660`
62	$Pnma$		`POC$I1A000$P2C606$P2A666`
63	$Cmcm$		`COC$I1A000$P2C006$P2A000`
64	$Cmca$		`COC$I1A000$P2C066$P2A000`
65	$Cmmm$		`COC$I1A000$P2C000$P2A000`
66	$Cccm$		`COC$I1A000$P2C000$P2A006`
67	$Cmma$		`COC$I1A000$P2C060$P2A000`
68	$Ccca$	Origin 1	`COC$I1A066$P2C660$P2A660`

Table A1.4.2.1 (*cont.*)

No.	Short Hermann–Mauguin symbol	Comments	Explicit symbols
68	$Ccca$	Origin 2	COC$I1A000$P2C600$P2A606
69	$Fmmm$		FOC$I1A000$P2C000$P2A000
70	$Fddd$	Origin 1	FOC$I1A333$P2C000$P2A000
70	$Fddd$	Origin 2	FOC$I1A000$P2C990$P2A099
71	$Immm$		IOC$I1A000$P2C000$P2A000
72	$Ibam$		IOC$I1A000$P2C000$P2A660
73	$Ibca$		IOC$I1A000$P2C606$P2A660
74	$Imma$		IOC$I1A000$P2C060$P2A000
75	$P4$		PTN$P4C000
76	$P4_1$		PTN$P4C003
77	$P4_2$		PTN$P4C006
78	$P4_3$		PTN$P4C009
79	$I4$		ITN$P4C000
80	$I4_1$		ITN$P4C063
81	$P\bar{4}$		PTN$I4C000
82	$I\bar{4}$		ITN$I4C000
83	$P4/m$		PTC$I1A000$P4C000
84	$P4_2/m$		PTC$I1A000$P4C006
85	$P4/n$	Origin 1	PTC$I1A660$P4C660
85	$P4/n$	Origin 2	PTC$I1A000$P4C600
86	$P4_2/n$	Origin 1	PTC$I1A666$P4C666
86	$P4_2/n$	Origin 2	PTC$I1A000$P4C066
87	$I4/m$		ITC$I1A000$P4C000
88	$I4_1/a$	Origin 1	ITC$I1A063$P4C063
88	$I4_1/a$	Origin 2	ITC$I1A000$P4C933
89	$P422$		PTN$P4C000$P2A000
90	$P42_12$		PTN$P4C660$P2A660
91	$P4_122$		PTN$P4C003$P2A006
92	$P4_12_12$		PTN$P4C663$P2A669
93	$P4_222$		PTN$P4C006$P2A000
94	$P4_22_12$		PTN$P4C666$P2A666
95	$P4_322$		PTN$P4C009$P2A006
96	$P4_32_12$		PTN$P4C669$P2A663
97	$I422$		ITN$P4C000$P2A000
98	$I4_122$		ITN$P4C063$P2A063
99	$P4mm$		PTN$P4C000$I2A000
100	$P4bm$		PTN$P4C000$I2A660
101	$P4_2cm$		PTN$P4C006$I2A006
102	$P4_2nm$		PTN$P4C666$I2A666
103	$P4cc$		PTN$P4C000$I2A006
104	$P4nc$		PTN$P4C000$I2A666
105	$P4_2mc$		PTN$P4C006$I2A000
106	$P4_2bc$		PTN$P4C006$I2A660
107	$I4mm$		ITN$P4C000$I2A000
108	$I4cm$		ITN$P4C000$I2A006
109	$I4_1md$		ITN$P4C063$I2A666
110	$I4_1cd$		ITN$P4C063$I2A660
111	$P\bar{4}2m$		PTN$I4C000$P2A000
112	$P\bar{4}2c$		PTN$I4C000$P2A006
113	$P\bar{4}2_1m$		PTN$I4C000$P2A660
114	$P\bar{4}2_1c$		PTN$I4C000$P2A666
115	$P\bar{4}m2$		PTN$I4C000$P2D000
116	$P\bar{4}c2$		PTN$I4C000$P2D006
117	$P\bar{4}b2$		PTN$I4C000$P2D660
118	$P\bar{4}n2$		PTN$I4C000$P2D666
119	$I\bar{4}m2$		ITN$I4C000$P2D000
120	$I\bar{4}c2$		ITN$I4C000$P2D006
121	$I\bar{4}2m$		ITN$I4C000$P2A000
122	$I\bar{4}2d$		ITN$I4C000$P2A609
123	$P4/mmm$		PTC$I1A000$P4C000$P2A000
124	$P4/mcc$		PTC$I1A000$P4C000$P2A006
125	$P4/nbm$	Origin 1	PTC$I1A660$P4C000$P2A000
125	$P4/nbm$	Origin 2	PTC$I1A000$P4C600$P2A060
126	$P4/nnc$	Origin 1	PTC$I1A666$P4C000$P2A000
126	$P4/nnc$	Origin 2	PTC$I1A000$P4C600$P2A066
127	$P4/mbm$		PTC$I1A000$P4C000$P2A660
128	$P4/mnc$		PTC$I1A000$P4C000$P2A666
129	$P4/nmm$	Origin 1	PTC$I1A660$P4C660$P2A660
129	$P4/nmm$	Origin 2	PTC$I1A000$P4C600$P2A600
130	$P4/ncc$	Origin 1	PTC$I1A660$P4C660$P2A666
130	$P4/ncc$	Origin 2	PTC$I1A000$P4C600$P2A606
131	$P4_2/mmc$		PTC$I1A000$P4C006$P2A000
132	$P4_2/mcm$		PTC$I1A000$P4C006$P2A006
133	$P4_2/nbc$	Origin 1	PTC$I1A666$P4C666$P2A006
133	$P4_2/nbc$	Origin 2	PTC$I1A000$P4C606$P2A060
134	$P4_2/nnm$	Origin 1	PTC$I1A666$P4C666$P2A000
134	$P4_2/nnm$	Origin 2	PTC$I1A000$P4C606$P2A066
135	$P4_2/mbc$		PTC$I1A000$P4C006$P2A660
136	$P4_2/mnm$		PTC$I1A000$P4C666$P2A666
137	$P4_2/nmc$	Origin 1	PTC$I1A666$P4C666$P2A666
137	$P4_2/nmc$	Origin 2	PTC$I1A000$P4C606$P2A600
138	$P4_2/ncm$	Origin 1	PTC$I1A666$P4C666$P2A660
138	$P4_2/ncm$	Origin 2	PTC$I1A000$P4C606$P2A606
139	$I4/mmm$		ITC$I1A000$P4C000$P2A000
140	$I4/mcm$		ITC$I1A000$P4C000$P2A006
141	$I4_1/amd$	Origin 1	ITC$I1A063$P4C063$P2A063
141	$I4_1/amd$	Origin 2	ITC$I1A000$P4C393$P2A000
142	$I4_1/acd$	Origin 1	ITC$I1A063$P4C063$P2A069
142	$I4_1/acd$	Origin 2	ITC$I1A000$P4C393$P2A006
143	$P3$		PRN$P3C000
144	$P3_1$		PRN$P3C004
145	$P3_2$		PRN$P3C008
146	$R3$	Hexagonal axes	RRN$P3C000
146	$R3$	Rhombohedral axes	PRN$P3Q000
147	$P\bar{3}$		PRC$I3C000
148	$R\bar{3}$	Hexagonal axes	RRC$I3C000
148	$R\bar{3}$	Rhombohedral axes	PRC$I3Q000
149	$P312$		PRN$P3C000$P2G000
150	$P321$		PRN$P3C000$P2F000
151	$P3_112$		PRN$P3C004$P2G000
152	$P3_121$		PRN$P3C004$P2F008
153	$P3_212$		PRN$P3C008$P2G000
154	$P3_221$		PRN$P3C008$P2F004
155	$R32$	Hexagonal axes	RRN$P3C000$P2F000
155	$R32$	Rhombohedral axes	PRN$P3Q000$P2E000
156	$P3m1$		PRN$P3C000$I2F000
157	$P31m$		PRN$P3C000$I2G000
158	$P3c1$		PRN$P3C000$I2F006
159	$P31c$		PRN$P3C000$I2G006
160	$R3m$	Hexagonal axes	RRN$P3C000$I2F000
160	$R3m$	Rhombohedral axes	PRN$P3Q000$I2E000
161	$R3c$	Hexagonal axes	RRN$P3C000$I2F006
161	$R3c$	Rhombohedral axes	PRN$P3Q000$I2E666
162	$P\bar{3}1m$		PRC$I3C000$P2G000
163	$P\bar{3}1c$		PRC$I3C000$P2G006
164	$P\bar{3}m1$		PRC$I3C000$P2F000

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

$$
\mathtt{1A} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad
\mathtt{2A} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix} \quad
\mathtt{2B} = \begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}
$$

$$
\mathtt{2C} = \begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad
\mathtt{2D} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix} \quad
\mathtt{2E} = \begin{pmatrix} 0 & \bar{1} & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}
$$

$$
\mathtt{2F} = \begin{pmatrix} 1 & \bar{1} & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix} \quad
\mathtt{2G} = \begin{pmatrix} 1 & 0 & 0 \\ 1 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix} \quad
\mathtt{3Q} = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}
$$

$$
\mathtt{3C} = \begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad
\mathtt{4C} = \begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad
\mathtt{6C} = \begin{pmatrix} 1 & \bar{1} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix},
$$

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

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

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)

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 *1* (see Table A1.4.2.4). For centrosymmetric lattices the rotation parts are *1* and −*1*. 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		
Symbol	**nS**	Symbol	**nS**	Implied lattice translation(s)
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 $Ia\overline{3}d$, as given in Table A1.4.2.1:

```
ICC$I3Q000$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 $Ia\overline{3}d$, become

$$\left[\begin{pmatrix}0&0&\bar{1}\\ \bar{1}&0&0\\ 0&\bar{1}&0\end{pmatrix}\begin{pmatrix}x\\ y\\ z\end{pmatrix}+\begin{pmatrix}0\\ 0\\ 0\end{pmatrix}\right]=\begin{pmatrix}\bar{z}\\ \bar{x}\\ \bar{y}\end{pmatrix},$$

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

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

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

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

similarly, $[k\overline{h}l:-131/4]$ and $[kh\overline{l}:-311/4]$ are obtained from the second and third generator of $Ia\overline{3}d$, 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* A (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 (1981*a*) 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:

$$\mathbf{L}[\mathbf{N}^{\mathbf{A}}_{\mathbf{T}}]_{\mathbf{1}}\ldots[\mathbf{N}^{\mathbf{A}}_{\mathbf{T}}]_{\mathbf{p}}\mathbf{V}. \qquad \text{(A1.4.2.4)}$$

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
a	$\frac{1}{2}, 0, 0$	*1* in 3_1	$\frac{1}{3}$
b	$0, \frac{1}{2}, 0$	*2* in 3_2	$\frac{2}{3}$
c	$0, 0, \frac{1}{2}$	*1* in 4_1	$\frac{1}{4}$
n	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	*3* in 4_3	$\frac{3}{4}$
u	$\frac{1}{4}, 0, 0$	*1* in 6_1	$\frac{1}{6}$
v	$0, \frac{1}{4}, 0$	*2* in 6_2	$\frac{1}{3}$
w	$0, 0, \frac{1}{4}$	*4* in 6_4	$\frac{2}{3}$
d	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	*5* in 6_5	$\frac{5}{6}$

Table A1.4.2.4. *Rotation matrices for principal axes*

The 3 × 3 matrices for *proper* rotations along the three principal unit-cell directions are given below. The matrices for *improper* rotations (*−1*, *−2*, *−3*, *−4* and *−6*) are identical except that the signs of the elements are reversed.

		Rotation order				
Axis	Symbol A	*1*	*2*	*3*	*4*	*6*
a	*x*	$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}1&0&0\\0&\bar{1}&0\\0&0&\bar{1}\end{pmatrix}$	$\begin{pmatrix}1&0&0\\0&0&\bar{1}\\0&1&\bar{1}\end{pmatrix}$	$\begin{pmatrix}1&0&0\\0&0&\bar{1}\\0&1&0\end{pmatrix}$	$\begin{pmatrix}1&0&0\\0&1&\bar{1}\\0&1&0\end{pmatrix}$
b	*y*	$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}\bar{1}&0&0\\0&1&0\\0&0&\bar{1}\end{pmatrix}$	$\begin{pmatrix}\bar{1}&0&1\\0&1&0\\\bar{1}&0&0\end{pmatrix}$	$\begin{pmatrix}0&0&1\\0&1&0\\\bar{1}&0&0\end{pmatrix}$	$\begin{pmatrix}0&0&1\\0&1&0\\\bar{1}&0&1\end{pmatrix}$
c	*z*	$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}\bar{1}&0&0\\0&\bar{1}&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}0&\bar{1}&0\\1&\bar{1}&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}0&\bar{1}&0\\1&0&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}1&\bar{1}&0\\1&0&0\\0&0&1\end{pmatrix}$

L is the symbol specifying the lattice translational symmetry (see Table A1.4.2.2). The integral translations are implicitly included in the set of generators. If **L** has a leading minus sign, it also specifies an inversion centre at the origin. $[\mathbf{N}_{\mathbf{T}}^{\mathbf{A}}]_{\mathbf{n}}$ specifies the 4 × 4 Seitz matrix $\mathbf{S}_{\mathbf{n}}$ of a symmetry element in the minimum set which defines the space-group symmetry (see Tables A1.4.2.3 to A1.4.2.6), and **p** is the number of elements in the set. **V** is a change-of-basis operator needed for less common descriptions of the space-group symmetry.

The matrix symbol $\mathbf{N}_{\mathbf{T}}^{\mathbf{A}}$ is composed of three parts: **N** is the symbol denoting the |N|-fold order of the rotation matrix (see Tables A1.4.2.4, A1.4.2.5 and A1.4.2.6), **T** is a subscript symbol denoting the *translation* vector (see Table A1.4.2.3) and **A** is a superscript symbol denoting the *axis* of rotation.

The computer-entry format of the Hall notation contains the rotation-order symbol **N** as positive integers *1*, *2*, *3*, *4*, or *6* for proper rotations and as negative integers *−1*, *−2*, *−3*, *−4* or *−6* for improper rotations. The **T** translation symbols *1*, *2*, *3*, *4*, *5*, *6*, *a*, *b*, *c*, *n*, *u*, *v*, *w*, *d* are described in Table A1.4.2.3. These translations apply additively [*e.g.* *ad* signifies a $(\frac{3}{4}, \frac{1}{4}, \frac{1}{4})$ translation]. The **A** axis symbols *x*, *y*, *z* denote rotations about the axes **a**, **b** and **c**, respectively (see Table A1.4.2.4). The axis symbols ″ and ′ signal rotations about the body-diagonal vectors **a** + **b** (or alternatively **b** + **c** or **c** + **a**) and **a** − **b** (or alternatively **b** − **c** or **c** − **a**) (see Table A1.4.2.5). The axis symbol * always refers to a threefold rotation along **a** + **b** + **c** (see Table A1.4.2.6).

Table A1.4.2.5. *Rotation matrices for face-diagonal axes*

The symbols for face-diagonal twofold rotations are *2′* and *2″*. The face-diagonal axis direction is determined by the axis of the preceding rotation N^x, N^y or N^z. Note that the single prime ′ is the default and may be omitted.

Preceding rotation	Rotation	Axis	Matrix
N^x	*2′*	**b** − **c**	$\begin{pmatrix}\bar{1}&0&0\\0&0&\bar{1}\\0&\bar{1}&0\end{pmatrix}$
	2″	**b** + **c**	$\begin{pmatrix}\bar{1}&0&0\\0&0&1\\0&1&0\end{pmatrix}$
N^y	*2′*	**a** − **c**	$\begin{pmatrix}0&0&\bar{1}\\0&\bar{1}&0\\\bar{1}&0&0\end{pmatrix}$
	2″	**a** + **c**	$\begin{pmatrix}0&0&1\\0&\bar{1}&0\\1&0&0\end{pmatrix}$
N^z	*2′*	**a** − **b**	$\begin{pmatrix}0&\bar{1}&0\\\bar{1}&0&0\\0&0&\bar{1}\end{pmatrix}$
	2″	**a** + **b**	$\begin{pmatrix}0&1&0\\1&0&0\\0&0&\bar{1}\end{pmatrix}$

The change-of-basis operator **V** has the general form (v_x, v_y, v_z). The vectors v_x, v_y and v_z are specified by

$$\begin{aligned} v_x &= r_{1,1}X + r_{1,2}Y + r_{1,3}Z + \mathbf{t}_1 \\ v_y &= r_{2,1}X + r_{2,2}Y + r_{2,3}Z + \mathbf{t}_2\,, \\ v_z &= r_{3,1}X + r_{3,2}Y + r_{3,3}Z + \mathbf{t}_3 \end{aligned}$$

where $r_{i,j}$ and $\mathbf{t}_i$ are fractions or real numbers. Terms in which $r_{i,j}$ or $\mathbf{t}_i$ are zero need not be specified. The 4 × 4 change-of-basis matrix operator **V** is defined as

$$\mathbf{V} = \begin{pmatrix} r_{1,1} & r_{1,2} & r_{1,3} & \mathbf{t}_1 \\ r_{2,1} & r_{2,2} & r_{2,3} & \mathbf{t}_2 \\ r_{3,1} & r_{3,2} & r_{3,3} & \mathbf{t}_3 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

The transformed symmetry operations are derived from the specified Seitz matrices $\mathbf{S}_{\mathbf{n}}$ as

$$\mathbf{S}'_{\mathbf{n}} = \mathbf{V} \cdot \mathbf{S}_{\mathbf{n}} \cdot \mathbf{V}^{-1}$$

and from the integral translations **t**(1, 0, 0), **t**(0, 1, 0) and **t**(0, 0, 1) as

$$(\mathbf{t}'_{\mathbf{n}}, \mathbf{1})^T = \mathbf{V} \cdot (\mathbf{t}_{\mathbf{n}}, \mathbf{1})^T.$$

A shorthand form of **V** may be used when the change-of-basis operator only translates the origin of the basis system. In this form v_x, v_y and v_z are specified simply as shifts in twelfths, implying the matrix operator

Table A1.4.2.6. *Rotation matrix for the body-diagonal axis*

The symbol for the threefold rotation in the **a** + **b** + **c** direction is *3**. Note that for cubic space groups the body-diagonal axis is implied and the asterisk * may be omitted.

Axis	Rotation	Matrix
a + **b** + **c**	*3**	$\begin{pmatrix}0&0&1\\1&0&0\\0&1&0\end{pmatrix}$

$$\mathbf{V} = \begin{pmatrix} 1 & 0 & 0 & v_x/12 \\ 0 & 1 & 0 & v_y/12 \\ 0 & 0 & 1 & v_z/12 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

In the shorthand form of **V**, the commas separating the vectors may be omitted.

A1.4.2.3.1. Default axes

For most symbols the rotation axes applicable to each **N** are implied and an explicit axis symbol **A** is not needed. The rules for *default* axis directions are:

(i) the *first* rotation or roto-inversion has an axis direction of **c**;

(ii) the *second* rotation (if |N| is 2) has an axis direction of **a** if preceded by an |N| of 2 or 4, **a**−**b** if preceded by an |N| of 3 or 6;

(iii) the *third* rotation (if |N| is 3) has an axis direction of **a** + **b** + **c**.

A1.4.2.3.2. Example matrices

The following examples show how the notation expands to Seitz matrices.

The notation $\bar{2}^x_c$ represents an improper twofold rotation along **a** and a **c**/2 translation:

$$-2\mathrm{xc} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & \frac{1}{2} \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

The notation 3^* represents a threefold rotation along **a** + **b** + **c**:

$$3^* = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

The notation 4_{vw} represents a fourfold rotation along **c** (implied) and translation of **b**/4 and **c**/4:

$$4\mathrm{vw} = \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & \frac{1}{4} \\ 0 & 0 & 1 & \frac{1}{4} \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

The notation 6_1 2 (0 0 −1) represents a 6_1 screw along **c**, a twofold rotation along **a** − **b** and an origin shift of −**c**/12. Note that the 6_1 matrix is unchanged by the shifted origin whereas the *2* matrix is changed by −**c**/6.

$$61\,2\,(0\,0\,{-1}) = \begin{pmatrix} 1 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & \frac{1}{6} \\ 0 & 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & \frac{5}{6} \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

The change-of-basis vector (0 0 −1) could also be entered as (x, y, z − 1/12).

The *reverse setting of the R-centred lattice* (hexagonal axes) is specified using a change-of-basis transformation applied to the standard *obverse setting* (see Table A1.4.2.2). The obverse Seitz matrices are

$$\mathrm{R}\,3 = \begin{pmatrix} 1 & 0 & 0 & \frac{1}{3} \\ 0 & 1 & 0 & \frac{2}{3} \\ 0 & 0 & 1 & \frac{2}{3} \\ 0 & 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 & \frac{2}{3} \\ 0 & 1 & 0 & \frac{1}{3} \\ 0 & 0 & 1 & \frac{1}{3} \\ 0 & 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

The reverse-setting Seitz matrices are

$$\mathrm{R}\,3\,(-\mathrm{x}, -\mathrm{y}, \mathrm{z}) = \begin{pmatrix} 1 & 0 & 0 & \frac{1}{3} \\ 0 & 1 & 0 & \frac{2}{3} \\ 0 & 0 & 1 & \frac{1}{3} \\ 0 & 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 & \frac{2}{3} \\ 0 & 1 & 0 & \frac{1}{3} \\ 0 & 0 & 1 & \frac{2}{3} \\ 0 & 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

The conventional primitive hexagonal lattice may be transformed to a *C-centred orthohexagonal setting* using the change-of-basis operator

$$\mathrm{P}\,6\,(\mathrm{x} - 1/2\mathrm{y}, 1/2\mathrm{y}, \mathrm{z}) = \begin{pmatrix} \frac{1}{2} & -\frac{3}{2} & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

In this case the lattice translation for the *C* centring is obtained by transforming the integral translation **t**(0, 1, 0):

$$\boldsymbol{V} \cdot \begin{pmatrix} 0 & 1 & 0 & 1 \end{pmatrix}^T = \begin{pmatrix} 1 & -\frac{1}{2} & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} -\frac{1}{2} & \frac{1}{2} & 0 & 1 \end{pmatrix}^T.$$

The standard setting of an *I*-centred tetragonal space group may be transformed to a primitive setting using the change-of-basis operator

$$\mathrm{I}\,4\,(\mathrm{y} + \mathrm{z}, \mathrm{x} + \mathrm{z}, \mathrm{x} + \mathrm{y}) = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

Note that in the primitive setting, the fourfold axis is along **a** + **b**.

Table A1.4.2.7. *Hall symbols*

The first column, n:c, lists the space-group numbers and axis codes† separated by a colon. The second column lists the Hermann–Mauguin symbols in computer-entry format. The third column lists the Hall symbols in computer-entry format and the fourth column lists the Hall symbols as described in Tables A1.4.2.2–A1.4.2.6.

n:c	H–M entry	Hall entry	Hall symbol
1	P 1	p 1	$P\ 1$
2	P -1	-p 1	$\bar{P}\ 1$
3:b	P 1 2 1	p 2y	$P\ 2^{y}$
3:c	P 1 1 2	p 2	$P\ 2$
3:a	P 2 1 1	p 2x	$P\ 2^{x}$
4:b	P 1 21 1	p 2yb	$P\ 2^{y}_{b}$
4:c	P 1 1 21	p 2c	$P\ 2_{c}$
4:a	P 21 1 1	p 2xa	$P\ 2^{x}_{a}$
5:b1	C 1 2 1	c 2y	$C\ 2^{y}$
5:b2	A 1 2 1	a 2y	$A\ 2^{y}$
5:b3	I 1 2 1	i 2y	$I\ 2^{y}$
5:c1	A 1 1 2	a 2	$A\ 2$
5:c2	B 1 1 2	b 2	$B\ 2$
5:c3	I 1 1 2	i 2	$I\ 2$
5:a1	B 2 1 1	b 2x	$B\ 2^{x}$
5:a2	C 2 1 1	c 2x	$C\ 2^{x}$
5:a3	I 2 1 1	i 2x	$I\ 2^{x}$
6:b	P 1 m 1	p -2y	$P\ \bar{2}^{y}$
6:c	P 1 1 m	p -2	$P\ \bar{2}$
6:a	P m 1 1	p -2x	$P\ \bar{2}^{x}$
7:b1	P 1 c 1	p -2yc	$P\ \bar{2}^{y}_{c}$
7:b2	P 1 n 1	p -2yac	$P\ \bar{2}^{y}_{ac}$
7:b3	P 1 a 1	p -2ya	$P\ \bar{2}^{y}_{a}$
7:c1	P 1 1 a	p -2a	$P\ \bar{2}_{a}$
7:c2	P 1 1 n	p -2ab	$P\ \bar{2}_{ab}$
7:c3	P 1 1 b	p -2b	$P\ \bar{2}_{b}$
7:a1	P b 1 1	p -2xb	$P\ \bar{2}^{x}_{b}$
7:a2	P n 1 1	p -2xbc	$P\ \bar{2}^{x}_{bc}$
7:a3	P c 1 1	p -2xc	$P\ \bar{2}^{x}_{c}$
8:b1	C 1 m 1	c -2y	$C\ \bar{2}^{y}$
8:b2	A 1 m 1	a -2y	$A\ \bar{2}^{y}$
8:b3	I 1 m 1	i -2y	$I\ \bar{2}^{y}$
8:c1	A 1 1 m	a -2	$A\ \bar{2}$
8:c2	B 1 1 m	b -2	$B\ \bar{2}$
8:c3	I 1 1 m	i -2	$I\ \bar{2}$
8:a1	B m 1 1	b -2x	$B\ \bar{2}^{x}$
8:a2	C m 1 1	c -2x	$C\ \bar{2}^{x}$
8:a3	I m 1 1	i -2x	$I\ \bar{2}^{x}$
9:b1	C 1 c 1	c -2yc	$C\ \bar{2}^{y}_{c}$
9:b2	A 1 n 1	a -2yab	$A\ \bar{2}^{y}_{ab}$
9:b3	I 1 a 1	i -2ya	$I\ \bar{2}^{y}_{a}$
9:-b1	A 1 a 1	a -2ya	$A\ \bar{2}^{y}_{a}$
9:-b2	C 1 n 1	c -2yac	$C\ \bar{2}^{y}_{ac}$
9:-b3	I 1 c 1	i -2yc	$I\ \bar{2}^{y}_{c}$
9:c1	A 1 1 a	a -2a	$A\ \bar{2}_{a}$
9:c2	B 1 1 n	b -2ab	$B\ \bar{2}_{ab}$
9:c3	I 1 1 b	i -2b	$I\ \bar{2}_{b}$
9:-c1	B 1 1 b	b -2b	$B\ \bar{2}_{b}$
9:-c2	A 1 1 n	a -2ab	$A\ \bar{2}_{ab}$
9:-c3	I 1 1 a	i -2a	$I\ \bar{2}_{a}$
9:a1	B b 1 1	b -2xb	$B\ \bar{2}^{x}_{b}$
9:a2	C n 1 1	c -2xac	$C\ \bar{2}^{x}_{ac}$
9:a3	I c 1 1	i -2xc	$I\ \bar{2}^{x}_{c}$
9:-a1	C c 1 1	c -2xc	$C\ \bar{2}^{x}_{c}$
9:-a2	B n 1 1	b -2xab	$B\ \bar{2}^{x}_{ab}$
9:-a3	I b 1 1	i -2xb	$I\ \bar{2}^{x}_{b}$
10:b	P 1 2/m 1	-p 2y	$\bar{P}\ 2^{y}$
10:c	P 1 1 2/m	-p 2	$\bar{P}\ 2$
10:a	P 2/m 1 1	-p 2x	$\bar{P}\ 2^{x}$
11:b	P 1 21/m 1	-p 2yb	$\bar{P}\ 2^{y}_{b}$
11:c	P 1 1 21/m	-p 2c	$\bar{P}\ 2_{c}$
11:a	P 21/m 1 1	-p 2xa	$\bar{P}\ 2^{x}_{a}$
12:b1	C 1 2/m 1	-c 2y	$\bar{C}\ 2^{y}$
12:b2	A 1 2/m 1	-a 2y	$\bar{A}\ 2^{y}$
12:b3	I 1 2/m 1	-i 2y	$\bar{I}\ 2^{y}$
12:c1	A 1 1 2/m	-a 2	$\bar{A}\ 2$
12:c2	B 1 1 2/m	-b 2	$\bar{B}\ 2$
12:c3	I 1 1 2/m	-i 2	$\bar{I}\ 2$
12:a1	B 2/m 1 1	-b 2x	$\bar{B}\ 2^{x}$
12:a2	C 2/m 1 1	-c 2x	$\bar{C}\ 2^{x}$
12:a3	I 2/m 1 1	-i 2x	$\bar{I}\ 2^{x}$
13:b1	P 1 2/c 1	-p 2yc	$\bar{P}\ 2^{y}_{c}$
13:b2	P 1 2/n 1	-p 2yac	$\bar{P}\ 2^{y}_{ac}$
13:b3	P 1 2/a 1	-p 2ya	$\bar{P}\ 2^{y}_{a}$
13:c1	P 1 1 2/a	-p 2a	$\bar{P}\ 2_{a}$
13:c2	P 1 1 2/n	-p 2ab	$\bar{P}\ 2_{ab}$
13:c3	P 1 1 2/b	-p 2b	$\bar{P}\ 2_{b}$
13:a1	P 2/b 1 1	-p 2xb	$\bar{P}\ 2^{x}_{b}$
13:a2	P 2/n 1 1	-p 2xbc	$\bar{P}\ 2^{x}_{bc}$
13:a3	P 2/c 1 1	-p 2xc	$\bar{P}\ 2^{x}_{c}$
14:b1	P 1 21/c 1	-p 2ybc	$\bar{P}\ 2^{y}_{bc}$
14:b2	P 1 21/n 1	-p 2yn	$\bar{P}\ 2^{y}_{n}$
14:b3	P 1 21/a 1	-p 2yab	$\bar{P}\ 2^{y}_{ab}$
14:c1	P 1 1 21/a	-p 2ac	$\bar{P}\ 2_{ac}$
14:c2	P 1 1 21/n	-p 2n	$\bar{P}\ 2_{n}$
14:c3	P 1 1 21/b	-p 2bc	$\bar{P}\ 2_{bc}$
14:a1	P 21/b 1 1	-p 2xab	$\bar{P}\ 2^{x}_{ab}$
14:a2	P 21/n 1 1	-p 2xn	$\bar{P}\ 2^{x}_{n}$
14:a3	P 21/c 1 1	-p 2xac	$\bar{P}\ 2^{x}_{ac}$
15:b1	C 1 2/c 1	-c 2yc	$\bar{C}\ 2^{y}_{c}$
15:b2	A 1 2/n 1	-a 2yab	$\bar{A}\ 2^{y}_{ab}$
15:b3	I 1 2/a 1	-i 2ya	$\bar{I}\ 2^{y}_{a}$
15:-b1	A 1 2/a 1	-a 2ya	$\bar{A}\ 2^{y}_{a}$
15:-b2	C 1 2/n 1	-c 2yac	$\bar{C}\ 2^{y}_{ac}$
15:-b3	I 1 2/c 1	-i 2yc	$\bar{I}\ 2^{y}_{c}$
15:c1	A 1 1 2/a	-a 2a	$\bar{A}\ 2_{a}$
15:c2	B 1 1 2/n	-b 2ab	$\bar{B}\ 2_{ab}$
15:c3	I 1 1 2/b	-i 2b	$\bar{I}\ 2_{b}$
15:-c1	B 1 1 2/b	-b 2b	$\bar{B}\ 2_{b}$
15:-c2	A 1 1 2/n	-a 2ab	$\bar{A}\ 2_{ab}$
15:-c3	I 1 1 2/a	-i 2a	$\bar{I}\ 2_{a}$
15:a1	B 2/b 1 1	-b 2xb	$\bar{B}\ 2^{x}_{b}$
15:a2	C 2/n 1 1	-c 2xac	$\bar{C}\ 2^{x}_{ac}$
15:a3	I 2/c 1 1	-i 2xc	$\bar{I}\ 2^{x}_{c}$
15:-a1	C 2/c 1 1	-c 2xc	$\bar{C}\ 2^{x}_{c}$
15:-a2	B 2/n 1 1	-b 2xab	$\bar{B}\ 2^{x}_{ab}$
15:-a3	I 2/b 1 1	-i 2xb	$\bar{I}\ 2^{x}_{b}$
16	P 2 2 2	p 2 2	$P\ 2\ 2$
17	P 2 2 21	p 2c 2	$P\ 2_{c}\ 2$
17:cab	P 21 2 2	p 2a 2a	$P\ 2_{a}\ 2_{a}$
17:bca	P 2 21 2	p 2 2b	$P\ 2\ 2_{b}$
18	P 21 21 2	p 2 2ab	$P\ 2\ 2_{ab}$
18:cab	P 2 21 21	p 2bc 2	$P\ 2_{bc}\ 2$
18:bca	P 21 2 21	p 2ac 2ac	$P\ 2_{ac}\ 2_{ac}$
19	P 21 21 21	p 2ac 2ab	$P\ 2_{ac}\ 2_{ab}$
20	C 2 2 21	c 2c 2	$C\ 2_{c}\ 2$

Table A1.4.2.7 (*cont.*)

n:c	H–M entry	Hall entry	Hall symbol
20:cab	A 21 2 2	a 2a 2a	$A\ 2_{a}\ 2_{a}$
20:bca	B 2 21 2	b 2 2b	$B\ 2\ 2_{b}$
21	C 2 2 2	c 2 2	$C\ 2\ 2$
21:cab	A 2 2 2	a 2 2	$A\ 2\ 2$
21:bca	B 2 2 2	b 2 2	$B\ 2\ 2$
22	F 2 2 2	f 2 2	$F\ 2\ 2$
23	I 2 2 2	i 2 2	$I\ 2\ 2$
24	I 21 21 21	i 2b 2c	$I\ 2_{b}\ 2_{c}$
25	P m m 2	p 2 -2	$P\ 2\ \bar{2}$
25:cab	P 2 m m	p -2 2	$P\ \bar{2}\ 2$
25:bca	P m 2 m	p -2 -2	$P\ \bar{2}\ \bar{2}$
26	P m c 21	p 2c -2	$P\ 2_{c}\ \bar{2}$
26:ba-c	P c m 21	p 2c -2c	$P\ 2_{c}\ \bar{2}_{c}$
26:cab	P 21 m a	p -2a 2a	$P\ \bar{2}_{a}\ 2_{a}$
26:-cba	P 21 a m	p -2 2a	$P\ \bar{2}\ 2_{a}$
26:bca	P b 21 m	p -2 -2b	$P\ \bar{2}\ \bar{2}_{b}$
26:a-cb	P m 21 b	p -2b -2	$P\ \bar{2}_{b}\ \bar{2}$
27	P c c 2	p 2 -2c	$P\ 2\ \bar{2}_{c}$
27:cab	P 2 a a	p -2a 2	$P\ \bar{2}_{a}\ 2$
27:bca	P b 2 b	p -2b -2b	$P\ \bar{2}_{b}\ \bar{2}_{b}$
28	P m a 2	p 2 -2a	$P\ 2\ \bar{2}_{a}$
28:ba-c	P b m 2	p 2 -2b	$P\ 2\ \bar{2}_{b}$
28:cab	P 2 m b	p -2b 2	$P\ \bar{2}_{b}\ 2$
28:-cba	P 2 c m	p -2c 2	$P\ \bar{2}_{c}\ 2$
28:bca	P c 2 m	p -2c -2c	$P\ \bar{2}_{c}\ \bar{2}_{c}$
28:a-cb	P m 2 a	p -2a -2a	$P\ \bar{2}_{a}\ \bar{2}_{a}$
29	P c a 21	p 2c -2ac	$P\ 2_{c}\ \bar{2}_{ac}$
29:ba-c	P b c 21	p 2c -2b	$P\ 2_{c}\ \bar{2}_{b}$
29:cab	P 21 a b	p -2b 2a	$P\ \bar{2}_{b}\ 2_{a}$
29:-cba	P 21 c a	p -2ac 2a	$P\ \bar{2}_{ac}\ 2_{a}$
29:bca	P c 21 b	p -2bc -2c	$P\ \bar{2}_{bc}\ \bar{2}_{c}$
29:a-cb	P b 21 a	p -2a -2ab	$P\ \bar{2}_{a}\ \bar{2}_{ab}$
30	P n c 2	p 2 -2bc	$P\ 2\ \bar{2}_{bc}$
30:ba-c	P c n 2	p 2 -2ac	$P\ 2\ \bar{2}_{ac}$
30:cab	P 2 n a	p -2ac 2	$P\ \bar{2}_{ac}\ 2$
30:-cba	P 2 a n	p -2ab 2	$P\ \bar{2}_{ab}\ 2$
30:bca	P b 2 n	p -2ab -2ab	$P\ \bar{2}_{ab}\ \bar{2}_{ab}$
30:a-cb	P n 2 b	p -2bc -2bc	$P\ \bar{2}_{bc}\ \bar{2}_{bc}$
31	P m n 21	p 2ac -2	$P\ 2_{ac}\ \bar{2}$
31:ba-c	P n m 21	p 2bc -2bc	$P\ 2_{bc}\ \bar{2}_{bc}$
31:cab	P 21 m n	p -2ab 2ab	$P\ \bar{2}_{ab}\ 2_{ab}$
31:-cba	P 21 n m	p -2 2ac	$P\ \bar{2}\ 2_{ac}$
31:bca	P n 21 m	p -2 -2bc	$P\ \bar{2}\ \bar{2}_{bc}$
31:a-cb	P m 21 n	p -2ab -2	$P\ \bar{2}_{ab}\ \bar{2}$
32	P b a 2	p 2 -2ab	$P\ 2\ \bar{2}_{ab}$
32:cab	P 2 c b	p -2bc 2	$P\ \bar{2}_{bc}\ 2$
32:bca	P c 2 a	p -2ac -2ac	$P\ \bar{2}_{ac}\ \bar{2}_{ac}$
33	P n a 21	p 2c -2n	$P\ 2_{c}\ \bar{2}_{n}$
33:ba-c	P b n 21	p 2c -2ab	$P\ 2_{c}\ \bar{2}_{ab}$
33:cab	P 21 n b	p -2bc 2a	$P\ \bar{2}_{bc}\ 2_{a}$
33:-cba	P 21 c n	p -2n 2a	$P\ \bar{2}_{n}\ 2_{a}$
33:bca	P c 21 n	p -2n -2ac	$P\ \bar{2}_{n}\ \bar{2}_{ac}$
33:a-cb	P n 21 a	p -2ac -2n	$P\ \bar{2}_{ac}\ \bar{2}_{n}$
34	P n n 2	p 2 -2n	$P\ 2\ \bar{2}_{n}$
34:cab	P 2 n n	p -2n 2	$P\ \bar{2}_{n}\ 2$
34:bca	P n 2 n	p -2n -2n	$P\ \bar{2}_{n}\ \bar{2}_{n}$
35	C m m 2	c 2 -2	$C\ 2\ \bar{2}$
35:cab	A 2 m m	a -2 2	$A\ \bar{2}\ 2$
35:bca	B m 2 m	b -2 -2	$B\ \bar{2}\ \bar{2}$
36	C m c 21	c 2c -2	$C\ 2_{c}\ \bar{2}$

n:c	H–M entry	Hall entry	Hall symbol
36:ba-c	C c m 21	c 2c -2c	$C\ 2_{c}\ \bar{2}_{c}$
36:cab	A 21 m a	a -2a 2a	$A\ \bar{2}_{a}\ 2_{a}$
36:-cba	A 21 a m	a -2 2a	$A\ \bar{2}\ 2_{a}$
36:bca	B b 21 m	b -2 -2b	$B\ \bar{2}\ \bar{2}_{b}$
36:a-cb	B m 21 b	b -2b -2	$B\ \bar{2}_{b}\ \bar{2}$
37	C c c 2	c 2 -2c	$C\ 2\ \bar{2}_{c}$
37:cab	A 2 a a	a -2a 2	$A\ \bar{2}_{a}\ 2$
37:bca	B b 2 b	b -2b -2b	$B\ \bar{2}_{b}\ \bar{2}_{b}$
38	A m m 2	a 2 -2	$A\ 2\ \bar{2}$
38:ba-c	B m m 2	b 2 -2	$B\ 2\ \bar{2}$
38:cab	B 2 m m	b -2 2	$B\ \bar{2}\ 2$
38:-cba	C 2 m m	c -2 2	$C\ \bar{2}\ 2$
38:bca	C m 2 m	c -2 -2	$C\ \bar{2}\ \bar{2}$
38:a-cb	A m 2 m	a -2 -2	$A\ \bar{2}\ \bar{2}$
39	A b m 2	a 2 -2b	$A\ 2\ \bar{2}_{b}$
39:ba-c	B m a 2	b 2 -2a	$B\ 2\ \bar{2}_{a}$
39:cab	B 2 c m	b -2a 2	$B\ \bar{2}_{a}\ 2$
39:-cba	C 2 m b	c -2a 2	$C\ \bar{2}_{a}\ 2$
39:bca	C m 2 a	c -2a -2a	$C\ \bar{2}_{a}\ \bar{2}_{a}$
39:a-cb	A c 2 m	a -2b -2b	$A\ \bar{2}_{b}\ \bar{2}_{b}$
40	A m a 2	a 2 -2a	$A\ 2\ \bar{2}_{a}$
40:ba-c	B b m 2	b 2 -2b	$B\ 2\ \bar{2}_{b}$
40:cab	B 2 m b	b -2b 2	$B\ \bar{2}_{b}\ 2$
40:-cba	C 2 c m	c -2c 2	$C\ \bar{2}_{c}\ 2$
40:bca	C c 2 m	c -2c -2c	$C\ \bar{2}_{c}\ \bar{2}_{c}$
40:a-cb	A m 2 a	a -2a -2a	$A\ \bar{2}_{a}\ \bar{2}_{a}$
41	A b a 2	a 2 -2ab	$A\ 2\ \bar{2}_{ab}$
41:ba-c	B b a 2	b 2 -2ab	$B\ 2\ \bar{2}_{ab}$
41:cab	B 2 c b	b -2ab 2	$B\ \bar{2}_{ab}\ 2$
41:-cba	C 2 c b	c -2ac 2	$C\ \bar{2}_{ac}\ 2$
41:bca	C c 2 a	c -2ac -2ac	$C\ \bar{2}_{ac}\ \bar{2}_{ac}$
41:a-cb	A c 2 a	a -2ab -2ab	$A\ \bar{2}_{ab}\ \bar{2}_{ab}$
42	F m m 2	f 2 -2	$F\ 2\ \bar{2}$
42:cab	F 2 m m	f -2 2	$F\ \bar{2}\ 2$
42:bca	F m 2 m	f -2 -2	$F\ \bar{2}\ \bar{2}$
43	F d d 2	f 2 -2d	$F\ 2\ \bar{2}_{d}$
43:cab	F 2 d d	f -2d 2	$F\ \bar{2}_{d}\ 2$
43:bca	F d 2 d	f -2d -2d	$F\ \bar{2}_{d}\ \bar{2}_{d}$
44	I m m 2	i 2 -2	$I\ 2\ \bar{2}$
44:cab	I 2 m m	i -2 2	$I\ \bar{2}\ 2$
44:bca	I m 2 m	i -2 -2	$I\ \bar{2}\ \bar{2}$
45	I b a 2	i 2 -2c	$I\ 2\ \bar{2}_{c}$
45:cab	I 2 c b	i -2a 2	$I\ \bar{2}_{a}\ 2$
45:bca	I c 2 a	i -2b -2b	$I\ \bar{2}_{b}\ \bar{2}_{b}$
46	I m a 2	i 2 -2a	$I\ 2\ \bar{2}_{a}$
46:ba-c	I b m 2	i 2 -2b	$I\ 2\ \bar{2}_{b}$
46:cab	I 2 m b	i -2b 2	$I\ \bar{2}_{b}\ 2$
46:-cba	I 2 c m	i -2c 2	$I\ \bar{2}_{c}\ 2$
46:bca	I c 2 m	i -2c -2c	$I\ \bar{2}_{c}\ \bar{2}_{c}$
46:a-cb	I m 2 a	i -2a -2a	$I\ \bar{2}_{a}\ \bar{2}_{a}$
47	P m m m	-p 2 2	$\bar{P}\ 2\ 2$
48:1	P n n n:1	p 2 2 -1n	$P\ 2\ 2\ \bar{1}_{n}$
48:2	P n n n:2	-p 2ab 2bc	$\bar{P}\ 2_{ab}\ 2_{bc}$
49	P c c m	-p 2 2c	$\bar{P}\ 2\ 2_{c}$
49:cab	P m a a	-p 2a 2	$\bar{P}\ 2_{a}\ 2$
49:bca	P b m b	-p 2b 2b	$\bar{P}\ 2_{b}\ 2_{b}$
50:1	P b a n:1	p 2 2 -1ab	$P\ 2\ 2\ \bar{1}_{ab}$
50:2	P b a n:2	-p 2ab 2b	$\bar{P}\ 2_{ab}\ 2_{b}$
50:1cab	P n c b:1	p 2 2 -1bc	$P\ 2\ 2\ \bar{1}_{bc}$
50:2cab	P n c b:2	-p 2b 2bc	$\bar{P}\ 2_{b}\ 2_{bc}$

Table A1.4.2.7 (*cont.*)

n:c	H–M entry	Hall entry	Hall symbol
50:1bca	P c n a:1	p 2 2 -1ac	$P\ 2\ 2\ \bar{1}_{ac}$
50:2bca	P c n a:2	-p 2a 2c	$\bar{P}\ 2_{a}\ 2_{c}$
51	P m m a	-p 2a 2a	$\bar{P}\ 2_{a}\ 2_{a}$
51:ba-c	P m m b	-p 2b 2	$\bar{P}\ 2_{b}\ 2$
51:cab	P b m m	-p 2 2b	$\bar{P}\ 2\ 2_{b}$
51:-cba	P c m m	-p 2c 2c	$\bar{P}\ 2_{c}\ 2_{c}$
51:bca	P m c m	-p 2c 2	$\bar{P}\ 2_{c}\ 2$
51:a-cb	P m a m	-p 2 2a	$\bar{P}\ 2\ 2_{a}$
52	P n n a	-p 2a 2bc	$\bar{P}\ 2_{a}\ 2_{bc}$
52:ba-c	P n n b	-p 2b 2n	$\bar{P}\ 2_{b}\ 2_{n}$
52:cab	P b n n	-p 2n 2b	$\bar{P}\ 2_{n}\ 2_{b}$
52:-cba	P c n n	-p 2ab 2c	$\bar{P}\ 2_{ab}\ 2_{c}$
52:bca	P n c n	-p 2ab 2n	$\bar{P}\ 2_{ab}\ 2_{n}$
52:a-cb	P n a n	-p 2n 2bc	$\bar{P}\ 2_{n}\ 2_{bc}$
53	P m n a	-p 2ac 2	$\bar{P}\ 2_{ac}\ 2$
53:ba-c	P n m b	-p 2bc 2bc	$\bar{P}\ 2_{bc}\ 2_{bc}$
53:cab	P b m n	-p 2ab 2ab	$\bar{P}\ 2_{ab}\ 2_{ab}$
53:-cba	P c n m	-p 2 2ac	$\bar{P}\ 2\ 2_{ac}$
53:bca	P n c m	-p 2 2bc	$\bar{P}\ 2\ 2_{bc}$
53:a-cb	P m a n	-p 2ab 2	$\bar{P}\ 2_{ab}\ 2$
54	P c c a	-p 2a 2ac	$\bar{P}\ 2_{a}\ 2_{ac}$
54:ba-c	P c c b	-p 2b 2c	$\bar{P}\ 2_{b}\ 2_{c}$
54:cab	P b a a	-p 2a 2b	$\bar{P}\ 2_{a}\ 2_{b}$
54:-cba	P c a a	-p 2ac 2c	$\bar{P}\ 2_{ac}\ 2_{c}$
54:bca	P b c b	-p 2bc 2b	$\bar{P}\ 2_{bc}\ 2_{b}$
54:a-cb	P b a b	-p 2b 2ab	$\bar{P}\ 2_{b}\ 2_{ab}$
55	P b a m	-p 2 2ab	$\bar{P}\ 2\ 2_{ab}$
55:cab	P m c b	-p 2bc 2	$\bar{P}\ 2_{bc}\ 2$
55:bca	P c m a	-p 2ac 2ac	$\bar{P}\ 2_{ac}\ 2_{ac}$
56	P c c n	-p 2ab 2ac	$\bar{P}\ 2_{ab}\ 2_{ac}$
56:cab	P n a a	-p 2ac 2bc	$\bar{P}\ 2_{ac}\ 2_{bc}$
56:bca	P b n b	-p 2bc 2ab	$\bar{P}\ 2_{bc}\ 2_{ab}$
57	P b c m	-p 2c 2b	$\bar{P}\ 2_{c}\ 2_{b}$
57:ba-c	P c a m	-p 2c 2ac	$\bar{P}\ 2_{c}\ 2_{ac}$
57:cab	P m c a	-p 2ac 2a	$\bar{P}\ 2_{ac}\ 2_{a}$
57:-cba	P m a b	-p 2b 2a	$\bar{P}\ 2_{b}\ 2_{a}$
57:bca	P b m a	-p 2a 2ab	$\bar{P}\ 2_{a}\ 2_{ab}$
57:a-cb	P c m b	-p 2bc 2c	$\bar{P}\ 2_{bc}\ 2_{c}$
58	P n n m	-p 2 2n	$\bar{P}\ 2\ 2_{n}$
58:cab	P m n n	-p 2n 2	$\bar{P}\ 2_{n}\ 2$
58:bca	P n m n	-p 2n 2n	$\bar{P}\ 2_{n}\ 2_{n}$
59:1	P m m n:1	p 2 2ab -1ab	$P\ 2\ 2_{ab}\ \bar{1}_{ab}$
59:2	P m m n:2	-p 2ab 2a	$\bar{P}\ 2_{ab}\ 2_{a}$
59:1cab	P n m m:1	p 2bc 2 -1bc	$P\ 2_{bc}\ 2\ \bar{1}_{bc}$
59:2cab	P n m m:2	-p 2c 2bc	$\bar{P}\ 2_{c}\ 2_{bc}$
59:1bca	P m n m:1	p 2ac 2ac -1ac	$P\ 2_{ac}\ 2_{ac}\ \bar{1}_{ac}$
59:2bca	P m n m:2	-p 2c 2a	$\bar{P}\ 2_{c}\ 2_{a}$
60	P b c n	-p 2n 2ab	$\bar{P}\ 2_{n}\ 2_{ab}$
60:ba-c	P c a n	-p 2n 2c	$\bar{P}\ 2_{n}\ 2_{c}$
60:cab	P n c a	-p 2a 2n	$\bar{P}\ 2_{a}\ 2_{n}$
60:-cba	P n a b	-p 2bc 2n	$\bar{P}\ 2_{bc}\ 2_{n}$
60:bca	P b n a	-p 2ac 2b	$\bar{P}\ 2_{ac}\ 2_{b}$
60:a-cb	P c n b	-p 2b 2ac	$\bar{P}\ 2_{b}\ 2_{ac}$
61	P b c a	-p 2ac 2ab	$\bar{P}\ 2_{ac}\ 2_{ab}$
61:ba-c	P c a b	-p 2bc 2ac	$\bar{P}\ 2_{bc}\ 2_{ac}$
62	P n m a	-p 2ac 2n	$\bar{P}\ 2_{ac}\ 2_{n}$
62:ba-c	P m n b	-p 2bc 2a	$\bar{P}\ 2_{bc}\ 2_{a}$
62:cab	P b n m	-p 2c 2ab	$\bar{P}\ 2_{c}\ 2_{ab}$
62:-cba	P c m n	-p 2n 2ac	$\bar{P}\ 2_{n}\ 2_{ac}$
62:bca	P m c n	-p 2n 2a	$\bar{P}\ 2_{n}\ 2_{a}$

n:c	H–M entry	Hall entry	Hall symbol
62:a-cb	P n a m	-p 2c 2n	$\bar{P}\ 2_{c}\ 2_{n}$
63	C m c m	-c 2c 2	$\bar{C}\ 2_{c}\ 2$
63:ba-c	C c m m	-c 2c 2c	$\bar{C}\ 2_{c}\ 2_{c}$
63:cab	A m m a	-a 2a 2a	$\bar{A}\ 2_{a}\ 2_{a}$
63:-cba	A m a m	-a 2 2a	$\bar{A}\ 2\ 2_{a}$
63:bca	B b m m	-b 2 2b	$\bar{B}\ 2\ 2_{b}$
63:a-cb	B m m b	-b 2b 2	$\bar{B}\ 2_{b}\ 2$
64	C m c a	-c 2ac 2	$\bar{C}\ 2_{ac}\ 2$
64:ba-c	C c m b	-c 2ac 2ac	$\bar{C}\ 2_{ac}\ 2_{ac}$
64:cab	A b m a	-a 2ab 2ab	$\bar{A}\ 2_{ab}\ 2_{ab}$
64:-cba	A c a m	-a 2 2ab	$\bar{A}\ 2\ 2_{ab}$
64:bca	B b c m	-b 2 2ab	$\bar{B}\ 2\ 2_{ab}$
64:a-cb	B m a b	-b 2ab 2	$\bar{B}\ 2_{ab}\ 2$
65	C m m m	-c 2 2	$\bar{C}\ 2\ 2$
65:cab	A m m m	-a 2 2	$\bar{A}\ 2\ 2$
65:bca	B m m m	-b 2 2	$\bar{B}\ 2\ 2$
66	C c c m	-c 2 2c	$\bar{C}\ 2\ 2_{c}$
66:cab	A m a a	-a 2a 2	$\bar{A}\ 2_{a}\ 2$
66:bca	B b m b	-b 2b 2b	$\bar{B}\ 2_{b}\ 2_{b}$
67	C m m a	-c 2a 2	$\bar{C}\ 2_{a}\ 2$
67:ba-c	C m m b	-c 2a 2a	$\bar{C}\ 2_{a}\ 2_{a}$
67:cab	A b m m	-a 2b 2b	$\bar{A}\ 2_{b}\ 2_{b}$
67:-cba	A c m m	-a 2 2b	$\bar{A}\ 2\ 2_{b}$
67:bca	B m c m	-b 2 2a	$\bar{B}\ 2\ 2_{a}$
67:a-cb	B m a m	-b 2a 2	$\bar{B}\ 2_{a}\ 2$
68:1	C c c a:1	c 2 2 -1ac	$C\ 2\ 2\ \bar{1}_{ac}$
68:2	C c c a:2	-c 2a 2ac	$\bar{C}\ 2_{a}\ 2_{ac}$
68:1ba-c	C c c b:1	c 2 2 -1ac	$C\ 2\ 2\ \bar{1}_{ac}$
68:2ba-c	C c c b:2	-c 2a 2c	$\bar{C}\ 2_{a}\ 2_{c}$
68:1cab	A b a a:1	a 2 2 -1ab	$A\ 2\ 2\ \bar{1}_{ab}$
68:2cab	A b a a:2	-a 2a 2b	$\bar{A}\ 2_{a}\ 2_{b}$
68:1-cba	A c a a:1	a 2 2 -1ab	$A\ 2\ 2\ \bar{1}_{ab}$
68:2-cba	A c a a:2	-a 2ab 2b	$\bar{A}\ 2_{ab}\ 2_{b}$
68:1bca	B b c b:1	b 2 2 -1ab	$B\ 2\ 2\ \bar{1}_{ab}$
68:2bca	B b c b:2	-b 2ab 2b	$\bar{B}\ 2_{ab}\ 2_{b}$
68:1a-cb	B b a b:1	b 2 2 -1ab	$B\ 2\ 2\ \bar{1}_{ab}$
68:2a-cb	B b a b:2	-b 2b 2ab	$\bar{B}\ 2_{b}\ 2_{ab}$
69	F m m m	-f 2 2	$\bar{F}\ 2\ 2$
70:1	F d d d:1	f 2 2 -1d	$F\ 2\ 2\ \bar{1}_{d}$
70:2	F d d d:2	-f 2uv 2vw	$\bar{F}\ 2_{uv}\ 2_{vw}$
71	I m m m	-i 2 2	$\bar{I}\ 2\ 2$
72	I b a m	-i 2 2c	$\bar{I}\ 2\ 2_{c}$
72:cab	I m c b	-i 2a 2	$\bar{I}\ 2_{a}\ 2$
72:bca	I c m a	-i 2b 2b	$\bar{I}\ 2_{b}\ 2_{b}$
73	I b c a	-i 2b 2c	$\bar{I}\ 2_{b}\ 2_{c}$
73:ba-c	I c a b	-i 2a 2b	$\bar{I}\ 2_{a}\ 2_{b}$
74	I m m a	-i 2b 2	$\bar{I}\ 2_{b}\ 2$
74:ba-c	I m m b	-i 2a 2a	$\bar{I}\ 2_{a}\ 2_{a}$
74:cab	I b m m	-i 2c 2c	$\bar{I}\ 2_{c}\ 2_{c}$
74:-cba	I c m m	-i 2 2b	$\bar{I}\ 2\ 2_{b}$
74:bca	I m c m	-i 2 2a	$\bar{I}\ 2\ 2_{a}$
74:a-cb	I m a m	-i 2c 2	$\bar{I}\ 2_{c}\ 2$
75	P 4	p 4	$P\ 4$
76	P 41	p 4w	$P\ 4_{w}$
77	P 42	p 4c	$P\ 4_{c}$
78	P 43	p 4cw	$P\ 4_{cw}$
79	I 4	i 4	$I\ 4$
80	I 41	i 4bw	$I\ 4_{bw}$
81	P -4	p -4	$P\ \bar{4}$
82	I -4	i -4	$I\ \bar{4}$

Table A1.4.2.7 (*cont.*)

n:c	H–M entry	Hall entry	Hall symbol
83	P 4/m	-p 4	$\bar{P}\ 4$
84	P 42/m	-p 4c	$\bar{P}\ 4_c$
85:1	P 4/n:1	p 4ab -1ab	$P\ 4_{ab}\ \bar{1}_{ab}$
85:2	P 4/n:2	-p 4a	$\bar{P}\ 4_a$
86:1	P 42/n:1	p 4n -1n	$P\ 4_n\ \bar{1}_n$
86:2	P 42/n:2	-p 4bc	$\bar{P}\ 4_{bc}$
87	I 4/m	-i 4	$\bar{I}\ 4$
88:1	I 41/a:1	i 4bw -1bw	$I\ 4_{bw}\ \bar{1}_{bw}$
88:2	I 41/a:2	-i 4ad	$\bar{I}\ 4_{ad}$
89	P 4 2 2	p 4 2	P 4 2
90	P 4 21 2	p 4ab 2ab	$P\ 4_{ab}\ 2_{ab}$
91	P 41 2 2	p 4w 2c	$P\ 4_w\ 2_c$
92	P 41 21 2	p 4abw 2nw	$P4_{abw}2_{nw}$
93	P 42 2 2	p 4c 2	$P\ 4_c\ 2$
94	P 42 21 2	p 4n 2n	$P\ 4_n\ 2_n$
95	P 43 2 2	p 4cw 2c	$P\ 4_{cw}\ 2_c$
96	P 43 21 2	p 4nw 2abw	$P\ 4_{nw}\ 2_{abw}$
97	I 4 2 2	i 4 2	I 4 2
98	I 41 2 2	i 4bw 2bw	$I\ 4_{bw}\ 2_{bw}$
99	P 4 m m	p 4 -2	$P\ 4\ \bar{2}$
100	P 4 b m	p 4 -2ab	$P\ 4\ \bar{2}_{ab}$
101	P 42 c m	p 4c -2c	$P\ 4_c\ \bar{2}_c$
102	P 42 n m	p 4n -2n	$P\ 4_n\ \bar{2}_n$
103	P 4 c c	p 4 -2c	$P\ 4\ \bar{2}_c$
104	P 4 n c	p 4 -2n	$P\ 4\ \bar{2}_n$
105	P 42 m c	p 4c -2	$P\ 4_c\ \bar{2}$
106	P 42 b c	p 4c -2ab	$P\ 4_c\ \bar{2}_{ab}$
107	I 4 m m	i 4 -2	$I\ 4\ \bar{2}$
108	I 4 c m	i 4 -2c	$I\ 4\ \bar{2}_c$
109	I 41 m d	i 4bw -2	$I\ 4_{bw}\ \bar{2}$
110	I 41 c d	i 4bw -2c	$I\ 4_{bw}\ \bar{2}_c$
111	P -4 2 m	p -4 2	$P\ \bar{4}\ 2$
112	P -4 2 c	p -4 2c	$P\ \bar{4}\ 2_c$
113	P -4 21 m	p -4 2ab	$P\ \bar{4}\ 2_{ab}$
114	P -4 21 c	p -4 2n	$P\ \bar{4}\ 2_n$
115	P -4 m 2	p -4 -2	$P\ \bar{4}\ \bar{2}$
116	P -4 c 2	p -4 -2c	$P\ \bar{4}\ \bar{2}_c$
117	P -4 b 2	p -4 -2ab	$P\ \bar{4}\ \bar{2}_{ab}$
118	P -4 n 2	p -4 -2n	$P\ \bar{4}\ \bar{2}_n$
119	I -4 m 2	i -4 -2	$I\ \bar{4}\ \bar{2}$
120	I -4 c 2	i -4 -2c	$I\ \bar{4}\ \bar{2}_c$
121	I -4 2 m	i -4 2	$I\ \bar{4}\ 2$
122	I -4 2 d	i -4 2bw	$I\ \bar{4}\ 2_{bw}$
123	P 4/m m m	-p 4 2	$\bar{P}\ 4\ 2$
124	P 4/m c c	-p 4 2c	$\bar{P}\ 4\ 2_c$
125:1	P 4/n b m:1	p 4 2 -1ab	$P\ 4\ 2\ \bar{1}_{ab}$
125:2	P 4/n b m:2	-p 4a 2b	$\bar{P}\ 4_a\ 2_b$
126:1	P 4/n n c:1	p 4 2 -1n	$P\ 4\ 2\ \bar{1}_n$
126:2	P 4/n n c:2	-p 4a 2bc	$\bar{P}\ 4_a\ 2_{bc}$
127	P 4/m b m	-p 4 2ab	$\bar{P}\ 4\ 2_{ab}$
128	P 4/m n c	-p 4 2n	$\bar{P}\ 4\ 2_n$
129:1	P 4/n m m:1	p 4ab 2ab -1ab	$P\ 4_{ab}\ 2_{ab}\ \bar{1}_{ab}$
129:2	P 4/n m m:2	-p 4a 2a	$\bar{P}\ 4_a\ 2_a$
130:1	P 4/n c c:1	p 4ab 2n -1ab	$P\ 4_{ab}\ 2_n\ \bar{1}_{ab}$
130:2	P 4/n c c:2	-p 4a 2ac	$\bar{P}\ 4_a\ 2_{ac}$
131	P 42/m m c	-p 4c 2	$\bar{P}\ 4_c\ 2$
132	P 42/m c m	-p 4c 2c	$\bar{P}\ 4_c\ 2_c$
133:1	P 42/n b c:1	p 4n 2c -1n	$P\ 4_n\ 2_c\ \bar{1}_n$
133:2	P 42/n b c:2	-p 4ac 2b	$\bar{P}\ 4_{ac}\ 2_b$
134:1	P 42/n n m:1	p 4n 2 -1n	$P\ 4_n\ 2\ \bar{1}_n$
134:2	P 42/n n m:2	-p 4ac 2bc	$\bar{P}\ 4_{ac}\ 2_{bc}$
135	P 42/m b c	-p 4c 2ab	$\bar{P}\ 4_c\ 2_{ab}$
136	P 42/m n m	-p 4n 2n	$\bar{P}\ 4_n\ 2_n$
137:1	P 42/n m c:1	p 4n 2n -1n	$P\ 4_n\ 2_n\ \bar{1}_n$
137:2	P 42/n m c:2	-p 4ac 2a	$\bar{P}\ 4_{ac}\ 2_a$
138:1	P 42/n c m:1	p 4n 2ab -1n	$P\ 4_n\ 2_{ab}\ \bar{1}_n$
138:2	P 42/n c m:2	-p 4ac 2ac	$\bar{P}\ 4_{ac}\ 2_{ac}$
139	I 4/m m m	-i 4 2	$\bar{I}\ 4\ 2$
140	I 4/m c m	-i 4 2c	$\bar{I}\ 4\ 2_c$
141:1	I 41/a m d:1	i 4bw 2bw -1bw	$I\ 4_{bw}\ 2_{bw}\ \bar{1}_{bw}$
141:2	I 41/a m d:2	-i 4bd 2	$\bar{I}\ 4_{bd}\ 2$
142:1	I 41/a c d:1	i 4bw 2aw -1bw	$I\ 4_{bw}\ 2_{aw}\ \bar{1}_{bw}$
142:2	I 41/a c d:2	-i 4bd 2c	$\bar{I}\ 4_{bd}\ 2_c$
143	P 3	p 3	P 3
144	P 31	p 31	$P\ 3_1$
145	P 32	p 32	$P\ 3_2$
146:h	R 3:h	r 3	R 3
146:r	R 3:r	p 3*	P 3*
147	P -3	-p 3	$\bar{P}\ 3$
148:h	R -3:h	-r 3	$\bar{R}\ 3$
148:r	R -3:r	-p 3*	$\bar{P}\ 3^*$
149	P 3 1 2	p 3 2	P 3 2
150	P 3 2 1	p 3 2"	P 3 2"
151	P 31 1 2	p 31 2 (0 0 4)	$P\ 3_1\ 2\ (0\ 0\ 4)$
152	P 31 2 1	p 31 2"	$P\ 3_1\ 2''$
153	P 32 1 2	p 32 2 (0 0 2)	$P\ 3_2\ 2\ (0\ 0\ 2)$
154	P 32 2 1	p 32 2"	$P\ 3_2\ 2''$
155:h	R 3 2:h	r 3 2"	R 3 2"
155:r	R 3 2:r	p 3* 2	P 3* 2
156	P 3 m 1	p 3 -2"	$P\ 3\ \bar{2}''$
157	P 3 1 m	p 3 -2	$P\ 3\ \bar{2}$
158	P 3 c 1	p 3 -2"c	$P\ 3\ \bar{2}''_c$
159	P 3 1 c	p 3 -2c	$P\ 3\ \bar{2}_c$
160:h	R 3 m:h	r 3 -2"	$R\ 3\ \bar{2}''$
160:r	R 3 m:r	p 3* -2	$P\ 3^*\ \bar{2}$
161:h	R 3 c:h	r 3 -2"c	$R\ 3\ \bar{2}''_c$
161:r	R 3 c:r	p 3* -2n	$P\ 3^*\ \bar{2}_n$
162	P -3 1 m	-p 3 2	$\bar{P}\ 3\ 2$
163	P -3 1 c	-p 3 2c	$\bar{P}\ 3\ 2_c$
164	P -3 m 1	-p 3 2"	$\bar{P}\ 3\ 2''$
165	P -3 c 1	-p 3 2"c	$\bar{P}\ 3\ 2''_c$
166:h	R -3 m:h	-r 3 2"	$\bar{R}\ 3\ 2''$
166:r	R -3 m:r	-p 3* 2	$\bar{P}\ 3^*\ 2$
167:h	R -3 c:h	-r 3 2"c	$\bar{R}\ 3\ 2''_c$
167:r	R -3 c:r	-p 3* 2n	$\bar{P}\ 3^*\ 2_n$
168	P 6	p 6	P 6
169	P 61	p 61	$P\ 6_1$
170	P 65	p 65	$P\ 6_5$
171	P 62	p 62	$P\ 6_2$
172	P 64	p 64	$P\ 6_4$
173	P 63	p 6c	$P\ 6_c$
174	P -6	p -6	$P\ \bar{6}$
175	P 6/m	-p 6	$\bar{P}\ 6$
176	P 63/m	-p 6c	$\bar{P}\ 6_c$
177	P 6 2 2	p 6 2	P 6 2
178	P 61 2 2	p 61 2 (0 0 5)	$P\ 6_1\ 2\ (0\ 0\ 5)$
179	P 65 2 2	p 65 2 (0 0 1)	$P\ 6_5\ 2\ (0\ 0\ 1)$
180	P 62 2 2	p 62 2 (0 0 4)	$P\ 6_2\ 2\ (0\ 0\ 4)$
181	P 64 2 2	p 64 2 (0 0 2)	$P\ 6_4\ 2\ (0\ 0\ 2)$
182	P 63 2 2	p 6c 2c	$P\ 6_c\ 2_c$

Table A1.4.2.7 (*cont.*)

n:c	H–M entry	Hall entry	Hall symbol
183	P 6 m m	p 6 -2	$P\ 6\ \bar{2}$
184	P 6 c c	p 6 -2c	$P\ 6\ \bar{2}_c$
185	P 63 c m	p 6c -2	$P\ 6_c\ \bar{2}$
186	P 63 m c	p 6c -2c	$P\ 6_c\ \bar{2}_c$
187	P -6 m 2	p -6 2	$P\ \bar{6}\ 2$
188	P -6 c 2	p -6c 2	$P\ \bar{6}_c\ 2$
189	P -6 2 m	p -6 -2	$P\ \bar{6}\ \bar{2}$
190	P -6 2 c	p -6c -2c	$P\ \bar{6}_c\ \bar{2}_c$
191	P 6/m m m	-p 6 2	$\bar{P}\ 6\ 2$
192	P 6/m c c	-p 6 2c	$\bar{P}\ 6\ 2_c$
193	P 63/m c m	-p 6c 2	$\bar{P}\ 6_c\ 2$
194	P 63/m m c	-p 6c 2c	$\bar{P}\ 6_c\ 2_c$
195	P 2 3	p 2 2 3	$P\ 2\ 2\ 3$
196	F 2 3	f 2 2 3	$F\ 2\ 2\ 3$
197	I 2 3	i 2 2 3	$I\ 2\ 2\ 3$
198	P 21 3	p 2ac 2ab 3	$P\ 2_{ac}\ 2_{ab}\ 3$
199	I 21 3	i 2b 2c 3	$I\ 2_b\ 2_c\ 3$
200	P m -3	-p 2 2 3	$\bar{P}\ 2\ 2\ 3$
201:1	P n -3:1	p 2 2 3 -1n	$P\ 2\ 2\ 3\ \bar{1}_n$
201:2	P n -3:2	-p 2ab 2bc 3	$\bar{P}\ 2_{ab}\ 2_{bc}\ 3$
202	F m -3	-f 2 2 3	$\bar{F}\ 2\ 2\ 3$
203:1	F d -3:1	f 2 2 3 -1d	$F\ 2\ 2\ 3\ \bar{1}_d$
203:2	F d -3:2	-f 2uv 2vw 3	$\bar{F}\ 2_{uv}\ 2_{vw}\ 3$
204	I m -3	-i 2 2 3	$\bar{I}\ 2\ 2\ 3$
205	P a -3	-p 2ac 2ab 3	$\bar{P}\ 2_{ac}\ 2_{ab}\ 3$
206	I a -3	-i 2b 2c 3	$\bar{I}\ 2_b\ 2_c\ 3$
207	P 4 3 2	p 4 2 3	$P\ 4\ 2\ 3$
208	P 42 3 2	p 4n 2 3	$P\ 4_n\ 2\ 3$
209	F 4 3 2	f 4 2 3	$F\ 4\ 2\ 3$
210	F 41 3 2	f 4d 2 3	$F\ 4_d\ 2\ 3$
211	I 4 3 2	i 4 2 3	$I\ 4\ 2\ 3$
212	P 43 3 2	p 4acd 2ab 3	$P\ 4_{acd}\ 2_{ab}\ 3$
213	P 41 3 2	p 4bd 2ab 3	$P\ 4_{bd}\ 2_{ab}\ 3$
214	I 41 3 2	i 4bd 2c 3	$I\ 4_{bd}\ 2_c\ 3$
215	P -4 3 m	p -4 2 3	$P\ \bar{4}\ 2\ 3$
216	F -4 3 m	f -4 2 3	$F\ \bar{4}\ 2\ 3$
217	I -4 3 m	i -4 2 3	$I\ \bar{4}\ 2\ 3$
218	P -4 3 n	p -4n 2 3	$P\ \bar{4}_n\ 2\ 3$
219	F -4 3 c	f -4a 2 3	$F\ \bar{4}_a\ 2\ 3$
220	I -4 3 d	i -4bd 2c 3	$I\ \bar{4}_{bd}\ 2_c\ 3$
221	P m -3 m	-p 4 2 3	$\bar{P}\ 4\ 2\ 3$
222:1	P n -3 n:1	p 4 2 3 -1n	$P\ 4\ 2\ 3\ \bar{1}_n$
222:2	P n -3 n:2	-p 4a 2bc 3	$\bar{P}\ 4_a\ 2_{bc}\ 3$
223	P m -3 n	-p 4n 2 3	$\bar{P}\ 4_n\ 2\ 3$
224:1	P n -3 m:1	p 4n 2 3 -1n	$P\ 4_n\ 2\ 3\ \bar{1}_n$
224:2	P n -3 m:2	-p 4bc 2bc 3	$\bar{P}\ 4_{bc}\ 2_{bc}\ 3$
225	F m -3 m	-f 4 2 3	$\bar{F}\ 4\ 2\ 3$
226	F m -3 c	-f 4a 2 3	$\bar{F}\ 4_a\ 2\ 3$
227:1	F d -3 m:1	f 4d 2 3 -1d	$F\ 4_d\ 2\ 3\ \bar{1}_d$
227:2	F d -3 m:2	-f 4vw 2vw 3	$\bar{F}\ 4_{vw}\ 2_{vw}\ 3$
228:1	F d -3 c:1	f 4d 2 3 -1ad	$F\ 4_d\ 2\ 3\ \bar{1}_{ad}$
228:2	F d -3 c:2	-f 4ud 2vw 3	$\bar{F}\ 4_{ud}\ 2_{vw}\ 3$
229	I m -3 m	-i 4 2 3	$\bar{I}\ 4\ 2\ 3$
230	I a -3 d	-i 4bd 2c 3	$\bar{I}\ 4_{bd}\ 2_c\ 3$

The codes appended to the space-group numbers listed in the first column identify the relationship between the symmetry elements and the crystal cell. Where no code is given the first choice listed below applies. *Monoclinic*. Code = <*unique axis*><*cell choice*>: unique axis choices [*cf. IT* A (2005) Table 4.3.2.1] b, -b, c, -c, a, -a; cell choices [*cf. IT* A (2005) Table 4.3.2.1] 1, 2, 3. *Orthorhombic*. Code = <*origin choice*><*setting*>: origin choices 1, 2; setting choices [*cf. IT* A (2005) Table 4.3.2.1] abc, ba-c, cab, -cba, bca, a-cb. *Tetragonal, cubic*. Code = <*origin choice*>: origin choices 1, 2. *Trigonal*. Code = <*cell choice*>: cell choices h (hexagonal), r (rhombohedral).

references