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International Tables for Crystallography
Volume A: *Space-Group Symmetry*

Edited by Th. Hahn

Fourth, Revised Edition 1995

Corrigenda and Addenda to the Third, Revised Edition (1992)

In the Fourth, Revised Edition (1995), new diagrams have been incorporated for the triclinic, monoclinic and orthorhombic space groups. These complete the space-group-diagram project.

The new graphical symbol ··—·· — for 'double' glide planes *e* oriented 'normal' and 'inclined' to the plane of projection has been incorporated in the following 17 space-group diagrams:

Orthorhombic	*Abm*2 (No. 39), *Aba*2 (41), *Fmm*2 (42), *Cmca* (64), *Cmma* (67), *Ccca* (68) (both origins), *Fmmm* (69)
Tetragonal	*I*4*mm* (107), *I*4*cm* (108), $I\bar{4}2m$ (121), *I*4/*mmm* (139), *I*4/*mcm* (140)
Cubic	$Fm\bar{3}$ (202), $Fm\bar{3}m$ (225), $Fm\bar{3}c$ (226), $I\bar{4}3m$ (217), $Im\bar{3}m$ (229).

Section 1, *Symbols and Terms*, has undergone substantial revision in the Fourth Edition to take into account changes recommended in three recent *Nomenclature Reports* published by the International Union of Crystallography and to include printed and graphical symbols for the new 'double' glide plane *e*. Purchasers of the previous editions of Volume A may obtain free copies of Section 1 from The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

New space-group symbols have been introduced for the following five space groups to take account of the glide plane *e*:

Space group No.	39	41	64	67	68
Present symbol	*Abm*2	*Aba*2	*Cmca*	*Cmma*	*Ccca*
New symbol	*Aem*2	*Aea*2	*Cmce*	*Cmme*	*Ccce*.

The new symbols have been added to the headlines of these space groups; they are also incorporated in the right-hand column of Table 12.5. These new symbols will be given as the 'main' symbols in the next edition of Volume A.

Page

xii Right column, line −8, change 'Im am' to 'I am'.

xiii Line 21, change 'are presently being prepared' to 'have appeared in 1993 and 1992'.

xiv Line 23, change 'section ... above.' to 'sections discuss lattice complexes and normalizers of space groups.'

3 Add to end of *Note* 'Symbols for Bravais lattices are contained in Tables 2.1.1, 9.2.1, and 9.2.2.'

4 Change heading '*Spaces, motions and groups*' to '*Spaces*'.
Insert heading '*Motions and matrices*' before entry 'W; M'.

5 Entry '*r*; or *x*', replace "Position vector described by an 'augmented' $(n + 1) \times 1$ column" with "Position vector or point (location of an atom), described by an $(n + 1) \times 1$ 'augmented' column".
Insert heading '*Groups*' before entry '$\mathfrak{G}$'.

6 *Notes on centred cells*
Note (i), replace 'Examples are contained in Table 5.1' by 'Examples of relevant transformation matrices are contained in Table 5.1'.
Note (ii), line 4, add 'an interesting example is provided by the triple rhombohedral *D* cell, described in Section 4.3.5'.
Note (iii), line 3, add 'especially Table 2.1.1, and de Wolff *et al.* (1985).'
Add '(iv) Symbols for crystal families and Bravais lattices in one, two, and three dimensions are listed in Table 2.1.1 and are explained in the *Nomenclature Report* by de Wolff *et al.* (1985).'

6 Section 1.3, entry for *m*, replace 'Reflection through a plane' with 'Reflection through the plane', 'Reflection through a line' with 'Reflection through the line' and 'Reflection through a point' with 'Reflection through the point'.
Section 1.3, entry for *a*, *b*, or *c*, replace 'Glide reflection through a plane' with 'Glide reflection through the plane'
Section 1.3, after entry for *c*, add following entries for $e^{\#}$:

Symmetry element and its orientation	Defining symmetry operation with glide or screw vector
'Double' glide plane (in centred cells only)	*Two* glide reflections through the plane, with perpendicular glide vectors
⊥ [001]	$\frac{1}{2}\mathbf{a}$ *and* $\frac{1}{2}\mathbf{b}$
⊥ [100]	$\frac{1}{2}\mathbf{b}$ *and* $\frac{1}{2}\mathbf{c}$
⊥ [010]	$\frac{1}{2}\mathbf{a}$ *and* $\frac{1}{2}\mathbf{c}$
⊥ [1$\bar{1}$0]; ⊥ [110]	$\frac{1}{2}(\mathbf{a} + \mathbf{b})$ *and* $\frac{1}{2}\mathbf{c}$; $\frac{1}{2}(\mathbf{a} - \mathbf{b})$ *and* $\frac{1}{2}\mathbf{c}$
⊥ [01$\bar{1}$]; ⊥ [011]	$\frac{1}{2}(\mathbf{b} + \mathbf{c})$ *and* $\frac{1}{2}\mathbf{a}$; $\frac{1}{2}(\mathbf{b} - \mathbf{c})$ *and* $\frac{1}{2}\mathbf{a}$
⊥ [$\bar{1}$01]; ⊥ [101]	$\frac{1}{2}(\mathbf{a} + \mathbf{c})$ *and* $\frac{1}{2}\mathbf{b}$; $\frac{1}{2}(\mathbf{a} - \mathbf{c})$ *and* $\frac{1}{2}\mathbf{b}$.

Section 1.3, entry for *n*, replace 'Glide reflection through a plane' with 'Glide reflection through the plane'.
Section 1.3, entry for *d*, replace 'Glide reflection through a plane' with 'Glide reflection through the plane'.
Section 1.3, entry for *g*, replace 'Glide reflection through a line' with 'Glide reflection through the line'.
Section 1.3, entry for 2,3,4,6, replace 'around an axis' with 'around the axis' and 'around a point' with 'around the point'.
Section 1.3, entry for $\bar{1}$, replace 'Inversion through a point' with 'Inversion through the point'.
Section 1.3, entry for $\bar{2} = m$,$\bar{3}$,$\bar{4}$,$\bar{6}$, add to 'Rotoinversion axis, $\bar{n}$' 'and inversion point on the axis[¶]'; replace 'around an axis followed by inversion through a point' by 'around the axis followed by inversion through the point'.
Section 1.3, last entry, replace 'around an axis' by 'around the axis'.
Section 1.3, add footnote:
$^{\#}$ For further explanations of the 'double' glide plane *e*, see Note (ix) below.
Section 1.3, footnote ‡, replace '$\frac{1}{4}(\mathbf{a} + \mathbf{b} + \mathbf{c})$ and $\frac{1}{4}(\mathbf{a} + \mathbf{b} - \mathbf{c})$' with '$\frac{1}{4}(\mathbf{a} + \mathbf{b})$ and $\frac{1}{4}(\mathbf{a} - \mathbf{b})$'.

7 *Notes on symmetry elements and symmetry operations*;
Renumber Note (iv) as Note (v) and insert new Note (iv):
"(iv) Whereas the term 'symmetry operation' is well-defined (*cf.* Section 8.1.2), the word 'symmetry element'

is used by crystallographers in a variety of often rather loose meanings. In 1989, the International Union of Crystallography published a *Nomenclature Report* which first defines a 'geometric element' as a geometric item that allows the fixed points of a symmetry operation (after removing of any intrinsic glide or screw translation) to be located and oriented in a coordinate system. A 'symmetry element' then is defined as a concept with a double meaning, namely the combination of a geometric element with the set of symmetry operations having this geometric element in common ('element set'). For further details and tables see de Wolff *et al.* (1989)."

Note (iv) [now labelled Note (v)], replace "The resulting vector represents a glide vector of a new glide reflection' by "Each resulting vector is a glide vector of a new glide reflection but with the same plane as the geometric element. Any of these glide operations can be used as a 'defining operation'."

Example (2), line 4, add "for this 'double' glide plane *e* see Note (ix) below."

After *Example* (3), add 'If among the infinitely many glide operations of the element set of a plane there exists *one* operation with glide vector zero, then this symmetry element is a mirror plane.'

Renumber Note (v) as Note (vi).

After *Example*, add 'Again, if *one* of the screw vectors is zero, the symmetry element is a rotation axis.'

Renumber Note (vi) as Note (viii).

Insert new Note (ix):

"(ix) In the third *Nomenclature Report* of the IUCr (de Wolff *et al.*, 1992), two new printed symbols for glide planes were proposed: *e* for 'double' glide planes and *k* for 'transverse' glide planes.

For the *e* glide planes new graphical symbols were introduced (*cf.* Section 1.4 (*a*), (*b*), (*c*) and Note iv); they are applied to the diagrams of the relevant space groups: Seven orthorhombic *A*-, *C*- and *F*-space groups, five tetragonal *I*-space groups, and five cubic *F*- and *I*-space groups. The *e* glide plane occurs only in centred cells and is defined by *two* perpendicular glide vectors related by a centring translation; thus, in *Cmma* (67) two glide operations *a and b* occur, their glide vectors being related by the centring vector $\frac{1}{2}(\mathbf{a} + \mathbf{b})$; the symbol *e* removes the ambiguity between *a* and *b*.

For five space groups, the Hermann–Mauguin symbol has to be modified:

Space group No.	39	41	64	67	68
Present symbol	*Abm*2	*Aba*2	*Cmca*	*Cmma*	*Ccca*
New symbol	*Aem*2	*Aea*2	*Cmce*	*Cmme*	*Ccce*

The new symbol is indicated in the headline of these space groups

For the *k* glide planes, no new graphical symbol and no modification of a space-group symbol are proposed."

7 Section 1.4(*a*), 4th line, "'Axial' glide plane", change entry in glide vector column to '$\frac{1}{2}$ lattice vector along line in projection plane'

Section 1.4(*a*), 5th line, 'Glide line (two dimensions)', change entry in glide vector column to '$\frac{1}{2}$ lattice vector along line in plane'.

Section 1.4(*a*), below 6th line, insert entries given in Table *A* below.

Section 1.4(*a*), 7th line, "'Diagonal' glide plane", change entry in glide vector column to '*One* glide vector with *two* components: $\frac{1}{2}$ along line parallel to projection plane, $\frac{1}{2}$ normal to projection plane'.

Section 1.4(*a*), 8th line, add footnote key § to "'Diamond' glide plane".

Section 1.4(*a*), insert footnotes:

For further explanations of the 'double' glide plane *e* see Note (iv) below and Section 1.3.

§ See footnote ‡ to Section 1.3 (p. 5).

8 Section 1.4(*b*), 2nd line, "'Axial' glide plane", change entry in glide vector column to '$\frac{1}{2}$ lattice vector in the direction of the arrow'.

Section 1.4(*b*), replace all entries in 3rd line with entries given in Table *B* below.

Section 1.4(*b*), 5th line, add footnote key § to "'Diamond' glide plane".

Section 1.4(*b*), add footnotes:

For further explanations of the 'double' glide plane *e* see Note (iv) below and Section 1.3.

§ See footnote ‡ to Section 1.3 (p. 5).

8 Section 1.4(*c*), 3rd line, "'Axial' glide plane", glide vector entries, change to '$\frac{1}{2}$ lattice vector along [100]' and '$\frac{1}{2}$ lattice vector along [010]'.

Section 1.4(*c*), below 5th line, insert entries given in Table *C* below.

Section 1.4(*c*), 6th line, add footnote key § to "'Diamond' glide plane".

Section 1.4(*c*), add footnotes:

For further explanations of the 'double' glide plane *e* see Note (iv) below and Section 1.3.

§ See footnote ‡ to Section 1.3 (p. 5).

9 Section 1.4(*d*), table heading, change '(subelements in parentheses)' to '(partial elements in parentheses)'.

10 Section 1.4(*e*), table heading, change '(subelements in parentheses)' to '(partial elements in parentheses)'.

Change '*Notes on graphical symbols of symmetry elements*' to '*Notes on graphical symbols of symmetry planes*'.

Notes on graphical symbols, replace Note (i) by

"(i) The *graphical* symbols and their explanations (columns 2 and 3) are independent of the projection direction and the labelling of the basis vectors. They are, therefore, applicable to any projection diagram of a space group. The *printed* symbols of *glide planes* (column 4), however, may change with a change of the basis vectors, as shown by the following example.

In the rhombohedral space groups $R3c$ and $R\bar{3}c$, the dotted line refers to a *c* glide when described with 'hexagonal axes' and projected along [001]; for a description with 'rhombohedral axes' and projection along [111], the same dotted glide plane would be called *n*. The dash-dotted *n* glide in the hexagonal description becomes an *a*, *b*, or *c* glide in the rhombohedral description; *cf.* Section 1.3."

Add Note (iv):

"(iv) In 1992 the International Union of Crystallography introduced the concept of the 'double' glide plane *e* and the graphical symbol · · — · · — for the *e* glide planes oriented 'normal' and 'inclined' to the plane of projection (de Wolff *et al.*, 1992); for details of *e* glide planes see Section 1.3. Note that the graphical symbol ⌐⌐ for double glide planes oriented 'parallel' to the projection plane has already been used in *IT*(1935) and *IT*(1952)."

10 Add following reference list:

WOLFF, P. M. DE, BELOV, N. V., BERTAUT, E. F., BUERGER, M. J., DONNAY, J. D. H., FISCHER, W., HAHN, TH., KOPTSIK, V. A., MACKAY, A. L., WONDTRATSCHEK, H., WILSON, A. J. C. & ABRAHAMS, S. C. (1985). *Nomenclature for crystal families, Bravais-lattice types and arithmetic classes. Report of the International Union of Crystallography Ad-hoc Committee on the Nomenclature of Symmetry. Acta Cryst.* A**41**, 278–280.

WOLFF, P. M. DE, BILLIET, Y., DONNAY, J. D. H., FISCHER, W., GALIULIN, R. B., GLAZER, A. M., SENECHAL, M., SHOEMAKER, D. P., WONDRATSCHEK, H., HAHN, TH., WILSON, A. J. C. & ABRAHAMS, S. C. (1989). *Definition of symmetry elements in space groups and point groups. Report of the International Union of Crystallography Ad-hoc Committee on the Nomenclature of Symmetry. Acta Cryst.* A**45**, 494–499.

WOLFF, P. M. DE, BILLIET, Y., DONNAY, J. D. H., FISCHER, W., GALIULIN, R. B., GLAZER, A. M., HAHN, TH., SENECHAL, M., SHOEMAKER, D. P., WONDRATSCHEK, H., WILSON, A. J. C. & ABRAHAMS, S. C. (1992). *Symbols for symmetry elements and symmetry operations. Final Report of the International Union of Crystallography Ad-hoc Committee on the Nomenclature of Symmetry. Acta Cryst.* A**48**, 727–732.

12 Left column, line 30, after 'Section 8.2.2', add 'below and Chapter 1.4 of Vol. C'.

13 Table 2.1.1, last line, rightmost column, change '*cl*' to '*cl*'.
Footnote †, change 'Laue classes' to 'Laue groups' and 'point groups' to 'Laue groups'.

14 Line 7, delete comma after α.

15 Left column, line 37, add "For five orthorhombic space groups, a 'new space-group symbol' is given; *cf.* Section 1.3."

17 Right column, line 9, change 'If the other two axes' to 'If other axes'.
Right column, line 13, change 'the rhombohedral axes' to 'the three rhombohedral axes'.

18 Left column, line 5, delete comma.
Right column, line 15, change 'basis vectors' to 'outlines'.

19 Right column, line 26, change '1 has two different symbols while 11' to '2 have two different symbols while 10'.

20 Table 2.6.1, entry for 2 distinct projections, change '(1 space group)' to '(2 space groups)'; add '*I* $2_1/b$ $2_1/c$ $2_1/a$ (73)' to 2/*m* 2/*m* 2/*m* column.
Table 2.6.1, entry for 1 distinct projection, change '(11 space groups)' to '(10 space groups)'; delete '*I* $2_1/b$ $2_1/c$ $2_1/a$ (73)' from 2/*m* 2/*m* 2/*m* column.

27 Left column, line 24, add 'for diffraction by radiation'.

38 Left column, line −7, change '$m \equiv 1$' to '$m \equiv \bar{1}$'.

45 Table 3.2 (*cont.*), ORTHORHOMBIC, right column, below '***Ibca*** (73)', add '*Icab* (73)'.

58 Table 4.3.1 (*cont.*), delete footnote key ⁺ on '73' and delete footnote ⁺.

61 Table 4.3.1 (*cont.*), right block, space group No. 127, change '2/*n*' to '2/*m*'.

80 Figs. 5.10 and 5.11, add (*a*) below left halves of figures, (*b*) below right halves of figures.

90 Table 5.1 (*cont.*), right column, change 'space group' to 'space groups' in all entries.

236 Below 'No. 39', add 'New space-group symbol *Aem*2; *cf.* Section 1.3'.

240 Below 'No. 41', add 'New space-group symbol *Aea*2; *cf.* Section 1.3'.
Space-group diagram has not been updated; graphical *e*-glide symbol does not appear. This will be corrected in the next Edition.

292 Below 'No. 64', add 'New space-group symbol *Cmce*; *cf.* Section 1.3'.

300 Below 'No. 67', add 'New space-group symbol *Cmme*; *cf.* Section 1.3'.

302 Below 'No. 68', add 'New space-group symbol *Ccce*; *cf.* Section 1.3'.

304 Below 'No. 68', add 'New space-group symbol *Ccce*; *cf.* Section 1.3'.

318 Top left diagram, symbol at left; bottom left diagram, top symbol; top right diagram, top symbol; change '$I\,\frac{2_1}{b}\,\frac{2_1}{c}\,\frac{2_1}{a}$' to '$I\,\frac{2_1}{c}\,\frac{2_1}{a}\,\frac{2_1}{b}$'.

681 Entries (41) for $\left(0,\frac{1}{2},\frac{1}{2}\right)^+$ set, (41) and (47) for $\left(\frac{1}{2},0,\frac{1}{2}\right)^+$ set, and (47) for $\left(\frac{1}{2},\frac{1}{2},0\right)^+$ set, change '4^-' to '$\bar{4}^{-?}$'.

685 Entries (41) for $\left(0,\frac{1}{2},\frac{1}{2}\right)^+$ set, (41) and (47) for $\left(\frac{1}{2},0,\frac{1}{2}\right)^+$ set, and (47) for $\left(\frac{1}{2},\frac{1}{2},0\right)^+$ set, change '4^-' to '$\bar{4}^{-?}$'.

689 Entries (41) for $(0,0,0)^+$ set, (47) for $\left(0,\frac{1}{2},\frac{1}{2}\right)^+$ set, (47) for $\left(\frac{1}{2},0,\frac{1}{2}\right)^+$ set, and (41) and (47) for $\left(\frac{1}{2},\frac{1}{2},0\right)^+$ set, change '4^-' to '$\bar{4}^-$'.

693 Entries (41) for $(0,0,0)^+$ set, (47) for $\left(0,\frac{1}{2},\frac{1}{2}\right)^+$ set, (47) for $\left(\frac{1}{2},0,\frac{1}{2}\right)^+$ set, and (41) and (47) for $\left(\frac{1}{2},\frac{1}{2},0\right)^+$ set, change '4^-' to '$\bar{4}^-$'.

697 Entry (41) for $(0,0,0)^+$ set, change '4^-' to '$\bar{4}^-$'.

739 Table 9.1.1, three dimensions, first line, change '2*m*' to '2/*m*'.

741 Table 9.2.1, change 'γ=90' to 'γ=90°', 'γ=120' to 'γ=120°'.

761 Table 10.2.2 (*cont.*), 4th column, 7th and 24th lines, change 'dispenoid' to 'disphenoid'.

773 Table 10.2.2 (*cont.*), 3rd column, last entry, change '2*m*..' to '2*mm*..'

783 Table 10.4.2 (*cont.*), 2nd column, last entry for Cylindrical system, change '$D_{\infty h}$' to '$D_{\infty h} \equiv D_{\infty d}$'.
Table 10.4.2 (*cont.*), footnote †, line 2, change 'Class $\infty m \equiv \infty$' to 'Class $\infty/m \equiv \overline{\infty}$'.

785 Table 10.4.3 (*cont.*), rotate left figure 90° anticlockwise.

786 Right column, lines 5 and 9, change '$\frac{2}{m}\overline{\infty}$' to '$2/m\overline{\infty}$' and '$\frac{2}{m}\bar{3}\bar{5}$' to '$2/m\bar{3}\bar{5}$'.
Line 16, change 'for dimensions' to 'for two dimensions'.

805 Table 12.5 (*cont.*), right column heading, delete † footnote key, change '798' to '804'.
Table 12.5 (*cont.*), space group No. 39, right column, add 'New symbol *Aem*2 (*cf.* Section 1.3)'.
Table 12.5 (*cont.*), space group No. 41, right column, add 'New symbol *Aea*2 (*cf.* Section 1.3)'.

806 Table 12.5 (*cont.*), right column heading, delete † footnote key, change '798' to '804'.
Table 12.5 (*cont.*), space group No. 64, right column, add 'New symbol *Cmce* (*cf.* Section 1.3)'.

806 Table 12.5 (*cont.*), space group No. 67, right column, add 'New symbol *Cmme* (*cf.* Section 1.3)'.
Table 12.5 (*cont.*), space group No. 68, right column, add 'New symbol *Ccce* (*cf.* Section 1.3)'.
807 Table 12.5 (*cont.*), right column heading, delete † footnote key, change '798' to '804'.
808 Table 12.5 (*cont.*), right column heading, delete † footnote key, change '798' to '804'.
809 Table 12.5 (*cont.*), right column heading, delete † footnote key, change '798' to '804'.
810 Table 12.5 (*cont.*), right column heading, delete † footnote key, change '798' to '804'.
874 Left column, change 'Laue class and symmetry' to 'Laue class, group, and symmetry'.

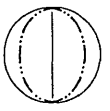
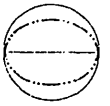
Table *A*; *Insert for Section* 1.4(*a*), *page* 7

Symmetry plane or symmetry line	Graphical symbol	Glide vector in units of lattice translation vectors parallel and normal to the projection plane	Printed symbol
'Double' glide plane# (in centred cells only)	· · — · · — · · — · ·	*Two* glide vectors: $\frac{1}{2}$ along plane parallel to projection plane, $\frac{1}{2}$ normal to projection plane	*e*

Table *B*; *Replacement for Section* 1.4(*b*), *page* 8

Symmetry plane	Graphical symbol	Glide vector in units of lattice translation vectors parallel to the projection plane	Printed symbol
'Double' glide plane# (in centred cells only)		*Two* glide vectors: $\frac{1}{2}$ in either of the directions of the two arrows	*e*

Table *C*; *Insert for Section* 1.4(*c*), *page* 8

Symmetry plane	Graphical symbol* for planes normal to		Glide vector in units of lattice translation vectors for [planes normal to		Printed symbol
	[011] and [01$\bar{1}$]	[101] and [10$\bar{1}$]	[011] and [01$\bar{1}$]	[101] and [10$\bar{1}$]	
'Double' glide plane# (in space groups $I\bar{4}3m$ (217) and $Im\bar{3}m$ (229) only)			*Two* glide vectors: $\frac{1}{2}$ along [100] *and* $\frac{1}{2}$ along [01$\bar{1}$] or $\frac{1}{2}$ along [011]	*Two* glide vectors: $\frac{1}{2}$ along [010] *and* $\frac{1}{2}$ along [10$\bar{1}$] or $\frac{1}{2}$ along [101]	*e*