International Tables for Crystallography (2016). Vol. A, Section 3.3.3.5, pp. 789–790.

Table 3.3.3.1 (continued)

No.	Schoen-flies symbol	Shubnikov symbol	Symbols of *International Tables*: 1935 Edition, Short	1935 Edition, Full	Present Edition, Short	Present Edition, Full	Comments†
215	T_d^1	$(a:(a:a)):\tilde{4}/3$	$P\bar{4}3m$	$P\bar{4}3m$	$P\bar{4}3m$	$P\bar{4}3m$	
216	T_d^2	$\left(\frac{a+c}{2}\Big/\frac{b+c}{2}\Big/\frac{a+b}{2}:a:(a:a)\right):\tilde{4}/3$	$F\bar{4}3m$	$F\bar{4}3m$	$F\bar{4}3m$	$F\bar{4}3m$	
217	T_d^3	$\left(\frac{a+b+c}{2}\Big/a:(a:a)\right):\tilde{4}/3$	$I\bar{4}3m$	$I\bar{4}3m$	$I\bar{4}3m$	$I\bar{4}3m$	
218	T_d^4	$(a:(a:a)):\tilde{4}//3$	$P\bar{4}3n$	$P\bar{4}3n$	$P\bar{4}3n$	$P\bar{4}3n$	
219	T_d^5	$\left(\frac{a+c}{2}\Big/\frac{b+c}{2}\Big/\frac{a+b}{2}:a:(a:a)\right):\tilde{4}//3$	$F\bar{4}3c$	$F\bar{4}3c$	$F\bar{4}3c$	$F\bar{4}3c$	
220	T_d^6	$\left(\frac{a+b+c}{2}\Big/a:(a:a)\right):\tilde{4}//3$	$I\bar{4}3d$	$I\bar{4}3d$	$I\bar{4}3d$	$I\bar{4}3d$	
221	O_h^1	$(a:(a:a)):4/\tilde{6}\cdot m$	$Pm3m$	$P4/m\ \bar{3}\ 2/m$	$Pm\bar{3}m$	$P4/m\ \bar{3}\ 2/m$	$Pm3m$ (*IT*, 1952)
222	O_h^2	$(a:(a:a)):4/\tilde{6}\cdot\widetilde{abc}$	$Pn3n$	$P4/n\ \bar{3}\ 2/n$	$Pn\bar{3}n$	$P4/n\ \bar{3}\ 2/n$	$Pn3n$ (*IT*, 1952)
223	O_h^3	$(a:(a:a)):4_2//\tilde{6}\cdot\widetilde{abc}$	$Pm3n$	$P4_2/m\ \bar{3}\ 2/n$	$Pm\bar{3}n$	$P4_2/m\ \bar{3}\ 2/n$	$Pm3n$ (*IT*, 1952)
224	O_h^4	$(a:(a:a)):4_2//\tilde{6}\cdot m$	$Pn3m$	$P4_2/n\ \bar{3}\ 2/m$	$Pn\bar{3}m$	$P4_2/n\ \bar{3}\ 2/m$	$Pn3m$ (*IT* ,1952)
225	O_h^5	$\left(\frac{a+c}{2}\Big/\frac{b+c}{2}\Big/\frac{a+b}{2}:a:(a:a)\right):4/\tilde{6}\cdot m$	$Fm3m$	$F4/m\ \bar{3}\ 2/m$	$Fm\bar{3}m$	$F4/m\ \bar{3}\ 2/m$	$Fm3m$ (*IT*, 1952)
226	O_h^6	$\left(\frac{a+c}{2}\Big/\frac{b+c}{2}\Big/\frac{a+b}{2}:a:(a:a)\right):4/\tilde{6}\cdot\tilde{c}$	$Fm3c$	$F4/m\ \bar{3}\ 2/c$	$Fm\bar{3}c$	$F4/m\ \bar{3}\ 2/c$	$Fm3c$ (*IT*, 1952)
227	O_h^7	$\left(\frac{a+c}{2}\Big/\frac{b+c}{2}\Big/\frac{a+b}{2}:a(a:a)\right):4_1//\tilde{6}\cdot m$	$Fd3m$	$F4_1/d\ \bar{3}\ 2/m$	$Fd\bar{3}m$	$F4_1/d\ \bar{3}\ 2/m$	$Fd3m$ (*IT*, 1952)
228	O_h^8	$\left(\frac{a+c}{2}\Big/\frac{b+c}{2}\Big/\frac{a+b}{2}:a:(a:a)\right):4_1//\tilde{6}\cdot\tilde{c}$	$Fd3c$	$F4_1/d\ \bar{3}\ 2/c$	$Fd\bar{3}c$	$F4_1/d\ \bar{3}\ 2/c$	$Fd3c$ (*IT*, 1952)
229	O_h^9	$\left(\frac{a+b+c}{2}\Big/a:(a:a)\right):4/\tilde{6}\cdot m$	$Im3m$	$I4/m\ \bar{3}\ 2/m$	$Im\bar{3}m$	$I4/m\ \bar{3}\ 2/m$	$Im3m$ (*IT*, 1952)
230	O_h^{10}	$\left(\frac{a+b+c}{2}\Big/a:(a:a)\right):4_1//\tilde{6}\cdot\frac{1}{2}\widetilde{abc}$	$Ia3d$	$I4_1/a\ \bar{3}\ 2/d$	$Ia\bar{3}d$	$I4_1/a\ \bar{3}\ 2/d$	$Ia3d$ (*IT*, 1952)

† Abbreviations used in the column *Comments*: *IT*, 1952: *International Tables for X-ray Crystallography,* Vol. I (1952); Sh–K; Shubnikov & Koptsik (1972). Note that this table contains only one notation for the *b*-unique setting and one notation for the *c*-unique setting in the monoclinic case, always referring to cell choice 1 of the space-group tables.

3.3.3.5. Systematic absences

Hermann (1928*a*) emphasized that the short symbols permit the derivation of systematic absences of X-ray reflections caused by the glide/screw parts of the symmetry operations. If $\boldsymbol{h} = (hkl)$ describes the X-ray reflection and $(\boldsymbol{W}, \boldsymbol{w})$ is the matrix representation of a symmetry operation, the matrix can be expanded as follows:

$$(\boldsymbol{W}, \boldsymbol{w}) = (\boldsymbol{W}, \boldsymbol{w}_g + \boldsymbol{w}_l) = (\boldsymbol{W}, \begin{pmatrix} w_{g,1} \\ w_{g,2} \\ w_{g,3} \end{pmatrix} + \boldsymbol{w}_l).$$

The absence of a reflection is governed by the relation (i) $\boldsymbol{h}\cdot\boldsymbol{W} = \boldsymbol{h}$ and the scalar product (ii) $\boldsymbol{h}\cdot\boldsymbol{w}_g = hw_{g,1} + kw_{g,2} + lw_{g,3}$. A reflection $\boldsymbol{h}$ is absent if condition (i) holds and the scalar product (ii) is not an integer. The calculation must be made for all generators and indicators of the short symbol. Systematic absences, introduced by the further symmetry operations generated, are obtained by the combination of the extinction rules derived for the generators and indicators.

Example: Space group $D_4^{10} = I4_122$ (98)

The generators of the space group are the integral translations and the centring translation $x+\frac{1}{2}, y+\frac{1}{2}, z+\frac{1}{2}$, the rotation 2 in direction [100]: $x, \bar{y}, \bar{z}$ and the rotation 2 in direction $[1\bar{1}0]$: $\bar{y}, \bar{x}, \bar{z}-\frac{1}{4}$. The combination of the two generators gives the operation corresponding to the indicator, namely $\bar{y}, x, z+\frac{1}{4}$, which represents a fourfold screw rotation in the direction [001].

The integral translations imply no restriction because the scalar product is always an integer. For the centring, condition (i) with $\boldsymbol{W} = \boldsymbol{I}$ holds for all reflections (integral condition), but the scalar product (ii) is an integer only for $h+k+l = 2n$. Thus, reflections hkl with $h+k+l \neq 2n$ are absent. The screw rotation 4 has the screw part $\boldsymbol{w}_g = \begin{pmatrix} 0 \\ 0 \\ \frac{1}{4} \end{pmatrix}$. Only $00l$ reflections obey condition (i) (serial extinction). An integral value for the scalar product (ii) requires $l = 4n$. The twofold axes in the directions [100] and $[1\bar{1}0]$ do not imply further absences because $\boldsymbol{w}_g = \boldsymbol{o}$.

Detailed discussion of the theoretical background of conditions for possible general reflections and their derivation is given in Chapter 1.6.

3.3.3.6. Generalized symmetry

The international symbols can be suitably modified to describe generalized symmetry, *e.g.* colour groups, which occur when the symmetry operations are combined with changes of physical properties. For the description of antisymmetry (or 'black–white' symmetry), the symbols of the Bravais lattices are supplemented by additional letters for centrings accompanied by a change in colour. For symmetry operations that are not translations, a prime is added to the usual symbol if a change of colour takes place. A complete description of the symbols and a detailed list of references are given by Koptsik (1966). The Shubnikov symbols have not been extended to colour symmetry.

An introduction to the structure, properties and symbols of magnetic subperiodic and magnetic space groups is given in Chapter 3.6.

3.3.4. Changes introduced in space-group symbols since 1935

Before the appearance of the first edition of *International Tables* in 1935, different notations for space groups were in use. A summary and comparative tables may be found in the introduction to that edition. The international notation was proposed by Hermann (1928*a*,*b*) and Mauguin (1931), who used the concept of lattice symmetry directions (see Section 3.3.1) and gave preference to reflections or glide reflections as generators. Considerable changes to the original Hermann–Mauguin short symbols were made in *IT* (1952).

The most important change refers to the symmetry directions. In the original Hermann–Mauguin symbols [*IT* (1935)], the distribution of symmetry elements is prescribed by the point-group symbol in the traditional setting, for example $\bar{4}2m$ (not $\bar{4}m2$) but $\bar{6}m2$ (not $\bar{6}2m$). This procedure sometimes implies the use of a larger unit cell than would be necessary. In *IT* (1952) and in the present series, however, the lattice symmetry directions always refer to the conventional cell (*cf.* Chapter 3.1) of the Bravais lattice. The results of this change are (*a*) different symbols for centring types and (*b*) different sequences of the symbols referring to the point group. These differences occur only in some space groups that have a tetragonal or hexagonal lattice.

Thus, the two different space groups D^1_{2d} and D^5_{2d} were symbolized by $P\bar{4}2m$ and $C\bar{4}2m$ in *IT* (1935) because in both cases the twofold axis had to be connected with the secondary set of symmetry directions. The new international symbols are $P\bar{4}2m$ and $P\bar{4}m2$; since in the point group $4/m\ 2/m\ 2/m$ of the Bravais lattice the secondary and tertiary set cannot be distinguished, the twofold axis in the subgroups $\bar{4}2m$ and $\bar{4}m2$ may occur in either the secondary or the tertiary set. Accordingly, the *C*-centred cell of $D^5_{2d} - C\bar{4}2m$, used in *IT* (1935), was transformed to a primitive one with the twofold axis along the tertiary set, resulting in the symbol $P\bar{4}m2$.

The same considerations hold for $\bar{6}m2$ and $\bar{6}2m$ and for space groups with a hexagonal lattice belonging to the point groups 32, $3m$ and $\bar{3}m$, which can be oriented in two ways with respect to the lattice.

For example, the point group $3m$ has two sets of symmetry directions. If the basis vector **a** is normal to the mirror plane *m*, two hexagonal cells with different centrings are possible:

(i) the hexagonal primitive cell, always described by *C* in *IT* (1935), leads to $C3m = C^1_{3v}$;

(ii) the hexagonal *H*-centred cell, with centring points in $\frac{2}{3}, \frac{1}{3}, 0$ and $\frac{1}{3}, \frac{2}{3}, 0$, leads to $H3m = C^2_{3v}$ (*cf.* Chapter 3.1).

The latter can be transformed to a primitive cell in which the mirror plane is normal to the representative of the tertiary set of the hexagonal lattice. In *IT* (1952) and the present editions, the primitive hexagonal cell is described by *P*. Thus, the above space groups receive the symbols $P3m1 = C^1_{3v}$ and $P31m = C^2_{3v}$.

Further changes are:

(i) In *IT* (1952), symbols for space groups related to the point groups 422, 622 and 432 contain the twofold axis of the tertiary set. The advantage is that these groups can be generated by operations of the secondary and tertiary set. The symbol of the indicator is provided with the appropriate index to identify the screw part, thus fixing the intersection parameter.

(ii) Some standard settings are changed in the monoclinic system. In *IT* (1935), only one setting (*b* unique, one cell choice) was tabulated for the monoclinic space groups. In *IT* (1952), two choices were offered, *b* and *c* unique, each with one cell choice. In the present edition, the two choices (*b* and *c* unique) are retained but for each one three different cells are available. The standard short symbol, however, is that of *IT* (1935) (*b*-unique setting).

(iii) In the short symbols of centrosymmetric space groups in the cubic system, $\bar{3}$ is written instead of 3, *e.g.* $Pm\bar{3}$ instead of $Pm3$ [as in *IT* (1935) and *IT* (1952)].

(iv) Beginning with the fourth edition of this volume (1995), the following five orthorhombic space-group symbols have been modified by introducing the new glide-plane symbol *e*, according to a Nomenclature Report of the IUCr (de Wolff *et al.*, 1992).

Space group No.	39	41	64	67	68
Former 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. Further details are given in Section 2.1.2.

Difficulties arising from these changes are avoided by selecting the lexicographically first one of the two possible glide parts for the generating operation.

Example: $Aea2 \sim Aba2 = C^{17}_{2v}$ (41)

The generators are

A centring:	$x, y + \frac{1}{2}, z + \frac{1}{2}$	$(1) + (0, \frac{1}{2}, \frac{1}{2})$
glide reflection b_{100}:	$\bar{x}, y + \frac{1}{2}, z$	(4)
or glide reflection c_{100}:	$\bar{x}, y, z + \frac{1}{2}$	$(4) + (0, \frac{1}{2}, \frac{1}{2})$
The first possibility is selected.		
glide reflection a_{010}:	$x + \frac{1}{2}, \bar{y}, z$	(3).

A shift of origin by $(-\frac{1}{4}, -\frac{1}{2}, 0)$ is necessary.

The 1935 symbols and all the changes adopted in the present edition of *International Tables* can be seen in Table 3.3.3.1. Differences in the symbols between *IT* (1952) and the present edition may be found in the last column of this table; *cf.* also Section 2.1.3.4.

references