Acta Crystallographica Section A
Foundations of Crystallography
ISSN 0108-7673

Received 13 March 2006
Accepted 3 November 2006

Transformational space-group symbols

Kazimierz Stróż

Institute of Materials Science, University of Silesia, Bankowa 12, 40-007 Poland. Correspondence e-mail: kstroz@us.edu.pl

Ambiguities present in space-group construction from the Hermann–Mauguin (H–M) symbols enforce the use of other space-group designations or H–M symbol modifications. Therefore, a transformational space-group symbol (TSG) composed of the well defined standard space-group identifier, an axis-system transformation and origin shift is proposed as a symbol of any space-group description. The first description given in *International Tables for Crystallography* [(1983), Vol. A, *Space-Group Symmetry*, edited by Th. Hahn. Dordrecht: Reidel (ITA83)] or the second one for space groups with two origins is suggested here as a reference description. For standard descriptions based on the ITA generators and compiled list of the TSG symbols, all conventional space-group settings listed in ITA83 can be reconstructed.

1. Introduction

The space groups are usually referred to the crystallographic coordinate system and the crystallographic origin. They are designated as the Hermann–Mauguin (H–M) symbols and presented in *International Tables for Crystallography* (1983), Vol. A (abbreviated hereafter as ITA83).

There are two procedures in common use that transform the H–M space-group symbol into generators which are then used to produce all symmetry operations. The well documented procedure developed by Burzlaff and Hountas was implemented in several programs like *SYM* (Burzlaff & Hountas, 1982), *SPGR4D* (Fu & Fan, 1997) or *LAZY PULVERIX* (Yvon *et al.*, 1977). Another algorithm was presented by Larson (1969) and implemented in *DBWS* (Young) and *GSAS* (Larson & von Dreele, 1995) programs for Rietveld refinement. However, unlike the translation parts in the symmetry operation matrices, the H–M symbols are not sensitive to origin selection.

The limitations and also some ambiguities of the H–M symbols resulted in using other symbols in order to create a unique description of a space group. In such approaches, the origin is explicitly given in the coded generators [Zachariasen, 1967; Hall, 1981; Shmueli, 1984; Hall & Grosse-Kunstleve in *International Tables for Crystallography*, 2006, Vol. B (hereafter ITB), pp. 112–114]. For conventional space-group description, additional information about the origin choice or the hexagonal/rhombohedral axes resolves the ambiguities of the H–M symbol. Such unique symbols are equivalent to the generators selected by Wondratschek and used for construction of space-group descriptions in ITA83. Application of these specially selected generators instead of deriving them from the H–M symbols is justified by a very effective space-group-generation process known as the composition series method (Ledermann, 1976).

Here the idea of referring the space-group description and its construction in any coordinate system to the default description is discussed. This idea was tested (Stróż, 1997) in the fourth edition of ITA83 (printed in 1995), abbreviated as ITA83ed4. A number of subtle improvements resulting from this test were introduced in the fifth edition of ITA83 (printed in 2002, pp. xv, xix, xx) by Hahn, Aroyo & Konstantinov. Since then all different descriptions of the same group (settings, origin choices, cell choices) including rhombohedral space groups are generated from the same operations transformed to the new coordinate system (Hahn & Looijenga-Vos, ITA83ed5, p. 27).

The idea of extending the H–M symbols by the origin shift specification is not new (Burzlaff & Zimmermann, 1980; Kopsky, 2001). A translation added to the Hall symbol is only used to obtain translation parts of the generators which can be coded.

Linking the space-group symbol with the axis transformation is necessary to designate a non-conventional space-group description. Such an idea was also incorporated into the Hall symbols (Grosse-Kunstleve, 1999; ITB, pp. 112–114). It can be noticed that in the Hall symbol the transformation is related to the actual generators used in the symbol. Thus, non-conventional space-group descriptions can be designated by several well constructed Hall symbols.

2. Transformational space-group symbol

Let us assume that one conventional space-group description with its conventional crystallographic axis system, conventional origin and H–M symbol, called 'standard description' with 'standard symbol' (Hahn & Looijenga-Vos, p. 22, Bertaut, p. 60 in ITA83ed5) serves as the reference for all other descriptions. This means that only one setting can play a special role as the standard space-group description and becomes a reference for other descriptions. In the monoclinic system it corresponds to the *unique axis b*, *cell choice* 1. For the *R-centred* cell, it is a description in the *hexagonal axes*. For space groups with two origin choices, the centre of symmetry is chosen by default. The above conventions resolve the ambiguities in the interpretation of H–M symbols from the reduced set, hence the 'standard symbol' uniquely defines the symmetry operations.

Let us introduce the transformational space-group symbol (TSG) as the symbol with the explicitly given transformation referred to the well established space-group standard description.

Table 1
Transformational space-group symbols for different descriptions in ITA83.

The letters *b* and *c* symbolize the *unique axis*, the numbers 1, 2 or 3 characterize the *cell choice* and *r* symbolizes the *rhombohedral axes*. Transformation matrices *P* are taken from Table 5.1.3.1 in ITA83.

Standard H–M symbol	Setting	Exemplary TSG symbol
$P2$, $P2_1$, Pm, $P2/m$, $2_1/m$	*c*	*P*2 (3) (0,0,1; 1,0,0; 0,1,0)
$C2$, Pc, Cm, Cc, $C2/m$, $P2/c$, $P2_1/c$, $C2/c$	*c*, 1	*C* 2 (5) (0,0,1; 1,0,0; 0,1,0)
	c, 2	*C* 2 (5) (1,0,0; −1,0,−1; 0,1,0)
	c, 3	*C* 2 (5) (−1,0,−1; 0,0,1; 0,1,0)
	b, 2	*C* 2 (5) (−1,0,−1; 0,1,0; 1,0,0)
	b, 3	*C* 2 (5) (0,0,1; 0,1,0; −1,0,−1)
$R3$, $R\bar{3}$, $R32$, $R3m$, $R3c$, $R\bar{3}m$, $R\bar{3}c$	*r*	*R*3 (146) (2/3,1/3,1/3; −1/3,1/3,1/3; −1/3,−2/3,1/3)†

† Compatible only with descriptions in ITA83ed5. For earlier editions of ITA83, the R_2 transformation, *e.g.* *R*3*m* (146) (−1/3,−2/3,1/3; 2/3,1/3,1/3; −1/3,1/3,1/3), should be applied (Stróż, 1997).

Any transformation from the standard to the new coordinate system is symbolized as ($P_{11}, P_{21}, P_{31}; P_{12}, P_{22}, P_{32}; P_{13}, P_{23}, P_{33}$), *i.e.* a shortened form of the following equation:

$$(\mathbf{a}', \mathbf{b}', \mathbf{c}') = (\mathbf{a}, \mathbf{b}, \mathbf{c}) \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix}. \quad (1)$$

The origin shift specification (p_1, p_2, p_3) stands for

$$\mathbf{O}' = \mathbf{O} + p_1\mathbf{a} + p_2\mathbf{b} + p_3\mathbf{c}. \quad (2)$$

Generally, the TSG takes the form: H–M (S. G. No.) (P_{11}, P_{21}, P_{31}; P_{12}, P_{22}, P_{32}; P_{13}, P_{23}, P_{33}) (p_1, p_2, p_3). The identity transformation (1, 0, 0; 0, 1, 0; 0, 0, 1) and the zero origin shift (0, 0, 0) are omitted in the symbol. The number of the H–M symbols is limited to the 230 standard symbols, hence the computer algorithms for H–M interpretation can be simplified or even replaced by the predefined generators corresponding to the space-group number. Some examples of the TSG designation are given below:

*R*3*m* (160) – hexagonal axes (standard description);

*R*3*m* (160) (2/3, 1/3, 1/3; −1/3, 1/3, 1/3; −1/3, −2/3, 1/3) – rhombohedral axes (ITA83ed5);

*R*3*m* (160) (−1/3, −2/3, 1/3; 2/3, 1/3, 1/3; −1/3, 1/3, 1/3) – rhombohedral axes (ITA83ed4);

$Fm\bar{3}m$ (225) (2, 0, 0; 0, 2, 0; 0, 0, 2) – 2 × 2 × 2 supercell;

$Pn\bar{3}$ (201) (−1/4, −1/4, −1/4) – origin choice 1.

3. TSG symbols and conventional H–M symbols (in ITA83)

The TSG symbols of monoclinic space-group settings can be obtained by adding the transformation part contained in the exemplary symbol (Table 1, column 3) to the standard H–M symbol. For seven *rhombohedral* space groups, two transformation matrices can be used, one for the R_1 relation (ITA83ed5) and one for the R_2 relation (ITA83ed4) between *hexagonal axes* and *rhombohedral axes*. This is a result of the selection of one generator according to the sequence of coordinate triplets in *International Tables for X-ray Crystallography* (1952), instead of using the generator transformed from *hexagonal axes* (Hahn & Vos, ITA83ed4, p. 25).

For 24 centrosymmetric groups containing points of high site symmetry that do not coincide with the centre of symmetry, the origin shift in the TSG symbol can be taken from the origin statements in ITA83.

Table 2
Space-group description in the ITA83 style constructed from *Fdd*2 (43) (0,1/2,1/2; 1/2,0,1/2; 1/2,1/2,0) symbol.

Centring vector	Order No.	Coordinate triplet	Operation symbol
(0,0,0)	(1)	x, y, z	1
(0,0,0)	(2)	$y, x, \bar{x} - y - z$	$2\ \bar{x}, \bar{x}, x$
(0,0,0)	(3)	$\bar{z} + \frac{1}{4}, x + y + z + \frac{1}{4}, \bar{x} + \frac{1}{4}$	$b\ \bar{x} + \frac{1}{4}, y, x$
(0,0,0)	(4)	$x + y + z + \frac{1}{4}, \bar{z} + \frac{1}{4}, \bar{y} + \frac{1}{4}$	$a\ x, y + \frac{1}{4}, \bar{y}$

4. TSG symbols and the generation of the ITA83-like space-group descriptions

The TSG symbols can be easily interpreted by the Burzlaff & Hountas or Larson algorithms but they are especially useful for obtaining the ITA83-like results. By applying the ITA generators used for the standard space-group description, the composition series method and the TSG symbols, one can reconstruct all space-group descriptions given in ITA83.

The numbering scheme of the symmetry operations introduced in ITA83 results from the order of generators. It is not changed by the axis system transformation and it remains valid for all descriptions of each space group.

For example, the operation number (2) (Table 2) in the group *Fdd*2 is related to the twofold axis. Its geometric element defines the special position *a* in any description of this group.

With the aid of the TSG symbols, a subtle distinction between different settings of some space groups is clearly visible. According to Kopsky, the space-group symbol $P2_12_12_1$ as described in *International Tables* is equivalent to the symbols $P2_12_12_1$ (19), $P2_12_12_1$(19) (0, 1, 0; 0, 0, 1; 1, 0, 0), $P2_12_12_1$ (19) (0, 0, 1; 1, 0, 0; 0, 1, 0). Other transformations contained in the symbols $P2_12_12_1$ (19) (0, 1, 0; 1, 0, 0; 0, 0, −1), $P2_12_12_1$ (19) (0, 0, −1; 0, 1, 0; 1, 0, 0), $P2_12_12_1$ (19) (1, 0, 0; 0, 0, −1; 0, 1, 0) are equivalent to the origin shift symbolized by $P2_12_12_1$ (19) (1/4, 1/4, 1/4). The above relations cannot be shown by means of the H–M symbols only. With the use of the Hall formalism, on the other hand, the problem would be unintelligible.

5. Conclusions

The TSG symbol plays a role similar to the Zachariasen/Shmueli or the Hall symbol, *i.e.* it names the specific space-group description. It is very informative and flexible. Its great merit is that computer algorithms can be simplified to interpret only 230 standard H–M symbols or to read only one set from 230 sets of generators.

The TSG symbol is longer than the Hall symbol for the conventional space-group descriptions and comparable for the non-conventional descriptions. In any case, the symbol is easy to construct and interpret.

References

Burzlaff, H. & Hountas, A. (1982). *J. Appl. Cryst.* **15**, 464–467.
Burzlaff, H. & Zimmermann, H. (1980). *Z. Kristallogr.* **153**, 151–179.
Fu, Z. Q. & Fan, H. F. (1997). *J. Appl. Cryst.* **30**, 73–78.
Grosse-Kunstleve, R. W. (1999). *Acta Cryst.* A**55**, 383–395.
Hall, S. R. (1981). *Acta Cryst.* A**37**, 517–525.
International Tables for Crystallography (1983). Vol. A, *Space-Group Symmetry*, edited by Th. Hahn. Dordrecht: Reidel.
International Tables for Crystallography (2006). Vol. B, *Reciprocal Space*, edited by U. Shmueli. Dordrecht: Kluwer.
International Tables for X-ray Crystallography (1952). Vol. I. Birmingham: Kynoch Press.

Kopsky, V. (2001). *Advances in Structure Analysis, Materials of ECM-18*, edited by R. Kužel & J. Hašek, pp. 334–353. Praha: CSCA.
Larson, A. C. (1969). *Acta Cryst.* A**25**, S1.
Larson, A. C. & von Dreele, R. B. (1995). *GSAS – General Structure Analysis System.* LANL, NM 87545, USA.
Ledermann, W. (1976). *Introduction to Group Theory.* London: Longman.
Shmueli, U. (1984). *Acta Cryst.* A**40**, 559–567.
Stróż, K. (1997). *J. Appl. Cryst.* **30**, 178–181.
Yvon, K., Jeitschko, W. & Parthé, E. (1977). *J. Appl. Cryst.* **10**, 73–74.
Zachariasen, W. H. (1967). *Theory of X-ray Diffraction in Crystals.* New York: Dover.