

Seitz symbols for symmetry operations of
subperiodic groupsDaniel B. Litvin^{a*} and Vojtech Kopský^b^aDepartment of Physics, Eberly College of Science, The Pennsylvania State University, PennState Berks, PO Box 7009, Reading, PA 19610-6009, USA, and ^bBajkalska 1170/28, 100 00 Prague 10, Czech Republic.

Correspondence e-mail: u3c@psu.edu

Recently adopted International Union of Crystallography conventions for the notation of Seitz symbols of symmetry operations require a revision of the Seitz notation used in *International Tables for Crystallography* Vol. E, *Subperiodic Groups*. This paper gives the subperiodic group symmetry operations blocks of Vol. E with the Seitz symbol for each included symmetry operation in the recently adopted conventions for Seitz notation.

© 2014 International Union of Crystallography

1. Introduction

The Commission on Crystallographic Nomenclature of the International Union of Crystallography (IUCr) has recently adopted (Glazer *et al.*, 2014) standard IUCr conventions for Seitz symbolism, *i.e.* for the Seitz notation of symmetry operations. For the three-dimensional space groups, layer groups and rod groups, this standard IUCr Seitz notation for symmetry operations can be found on the Bilbao Crystallographic Server (<http://www.cryst.ehu.es>). This Seitz symbolism will be added to the online version of Vol. A of *International Tables for Crystallography* (referred to as ITA) (Hahn, 2002).

The Seitz symbolism presently used in both the online and printed versions of Vol. E of *International Tables for Crystallography* (referred to as ITE; Kopský & Litvin, 2010) for the symmetry operations of the subperiodic groups, *i.e.* the frieze, rod and layer groups, differs from this standard IUCr Seitz notation and consequently is in need of revision. [The Seitz notation of symmetry operations used for one-, two- and three-dimensional space groups (Litvin & Kopský, 2011), and for one-, two- and three-dimensional magnetic and subperiodic groups (Litvin, 2013) is the same as in the present versions of ITE and consequently also differs from the recently adopted standard IUCr Seitz notation.] In ITE, Seitz symbols appear in the blocks of symmetry operations of each subperiodic group. To facilitate and encourage the use of the recently adopted standard IUCr Seitz notation in the context of subperiodic groups, we provide here a revised listing of the symmetry operation blocks of all subperiodic groups using the standard IUCr Seitz notation.

2. Symmetry operations for subperiodic groups

Seitz notation of a symmetry operation $\{R|v\}$ (Seitz, 1935) consists of a symbol v denoting the translational part of the operation and R the rotational part. The rotational part R consists of symbols that specify the type and order of the rotational part of the symmetry operation, and the orientation with respect to the basis of the coordinate system. The symbols for the rotational part R of symmetry operations defined in three-dimensional space, *i.e.* for layer-group and rod-group symmetry operations along with three-dimensional space-group symmetry operations, consistent with the IUCr conventions for Seitz

Table 1

Rotational parts R of the Seitz symbols $\{R|v\}$ for frieze-group symmetry operations.

For symmetry operations of type 1 and 2 no orientation is given as they are, respectively, the identity and a rotation about a point in two-dimensional space. The orientation of a type m reflection, a reflection with respect to a line, is given by the coordinates of that line; the subindex on the corresponding Seitz symbol denotes the direction perpendicular to that line.

No.	Coordinate doublet	Type	Orientation	Seitz symbol
1	x, y	1		1
2	\bar{x}, \bar{y}	2		2
3	\bar{x}, y	m	0, y	m_{10}
4	x, \bar{y}	m	$x, 0$	m_{01}

Table 2

The symmetry operations block of rod group $\mu 6cc$ (No. 69) with the Seitz notation of the symmetry operations given in the recently adopted conventions of Seitz symbolism.

Symmetry operations		
(1) 1 {1 0}	(2) 3 ⁺ 0, 0, z {3 ₀₀₁ ⁺ 0}	(3) 3 ⁻ 0, 0, z {3 ₀₀₁ ⁻ 0}
(4) 2 0, 0, z {2 ₀₀₁ 0}	(5) 6 ⁻ 0, 0, z {6 ₀₀₁ ⁻ 0}	(6) 6 ⁺ 0, 0, z {6 ₀₀₁ ⁺ 0}
(7) $c x, \bar{x}, z$ { m_{110} 0, 0, 1/2}	(8) $c x, 2x, z$ { m_{100} 0, 0, 1/2}	(9) $c 2x, x, z$ { m_{010} 0, 0, 1/2}
(10) $c x, x, z$ { $m_{1\bar{1}0}$ 0, 0, 1/2}	(11) $c x, 0, z$ { m_{120} 0, 0, 1/2}	(12) $c 0, y, z$ { m_{210} 0, 0, 1/2}

symbolism have been tabulated by Glazer *et al.* (2014). For the symmetry operations of frieze groups, symmetry operations defined in two-dimensional space, the specification of the rotational part symbols R , consistent with IUCr conventions, is given in Table 1. As an example of a symmetry operations block of a subperiodic group, we give, in Table 2, the symmetry operations block of the rod group $\mu 6cc$ (No. 69).¹

¹ The complete listing of all subperiodic group blocks of symmetry operations is available from the IUCr electronic archive (Reference: SC5079).

References

- Glazer, A. M., Aroyo, M. I. & Authier, A. (2014). *Acta Cryst.* **A70**, 300–302.
- Hahn, Th. (2002). Editor. *International Tables for Crystallography*, Vol. A, *Space-Group Symmetry*, 5th revised ed. Dordrecht: Kluwer Academic Publishers.
- Kopský, V. & Litvin, D. B. (2010). Editors. *International Tables for Crystallography*, Vol. E, *Subperiodic Groups*, 2nd ed. Chichester: Wiley.
- Litvin, D. B. (2013). *Magnetic Group Tables*. IUCr e-book. Freely available from <http://www.iucr.org/publ/978-0-9553602-2-0>.
- Litvin, D. B. & Kopský, V. (2011). *Acta Cryst.* **A67**, 415–418.
- Seitz, F. (1935). *Z. Kristallogr.* **91**, 336–366.