**Extension of Hall-symbols of crystallographic space groups to magnetic space groups**

Javier González-Platas1, Nebil A. Katcho2 and Juan Rodríguez-Carvajal2

1Departamento de Física Fundamental, Universidad de La Laguna, Tenerife, Spain

2Institut Laue-Langevin, Diffraction Group, Grenoble, France

**Abstract**

The Hall-symbols for describing unambiguously the generators of space groups have been extended to describe whatever setting of the 1651 types of magnetic space groups (Shubnikov groups).

**Introduction**

The international symbols for crystallographic space groups (CSG) are based in the Hermann-Mauguin symbols containing information about the Bravais lattice of the translation subgroup and the nature and orientation of the symmetry elements. However, as pointed out by S.R. Hall (Hall, 1981), there is no explicit information about the position of the origin determining partially the translational part of the symmetry operators. This has, consequently, an important drawback: the impossibility of generating the full set of symmetry operators from the symmetry elements appearing in the symbol, in the general case, coinciding with the lists of the *International Tables for Crystallography* (ITC). The computer programs, not using a database, doing that task have always some special code to handle special cases in order to generate strictly the same set of operators. The proposal by S.R. Hall (Hall, 1981) solves this problem in an elegant way allowing, at the same time, the possibility of describing reasonable arbitrary settings of CSG. The word “reasonable” is used here to emphasize the fact that the symmetry operators (with rotational part described always by an integer matrix) may be very complicated if a unit cell setting, for instance, is selected in which a three-fold axis in along an arbitrary [uvw] direction. However, even in these cases, the Hall symbol can be written by using the standard symbols described below followed by a setting change included at the end of the symbol.

In this document, we propose to modify slightly the original Hall-symbols in order to extend them for describing magnetic space groups (MSG). For that, we had to change the original symbol ’ to ^  (see below). The reason is that the prime symbol ’is reserved for the time reversal operator to be consistent with the currently used symbols Belov-Neronova-Smirnova (BNS) and Opechowski-Guccione (OG) notations for MSG.

**New Hall symbols**

This section summarises the notation introduced in (Hall, 1981), and the modifications we propose.

The Hall-symbols try to describe a CSG or a MSG using a short set of generators. Each generator corresponds to a Seitz operator acting on atom positions or on magnetic moments. The action of the operator S={R, θ|**t**} on the atom position **r** having a magnetic moment **m** is given by:

**r**’= R **r** + **t**  (1)

The corresponding magnetic moment is obtained as:

**m**’= θ det(R) R **m** (2)

The integer θ is equal to -1 is the operator is “primed” (combined with time reversal) and equal to 1 in the “non-primed” case. The Hall-symbol is the combination of a series of Seitz operators with a lattice symbol and the presence or not of a centre of symmetry at the origin. Each operator is constituted by a particular notation for the operator S that describes unambiguously the matrix R, the value of θ and the translation vector **t**. The operators S may by represented as a Seitz matrix or in the Jones faithful notation. For instance, a Seitz matrix representing a primed two-fold screw rotation along the b-axis is given by:



Notice that we have no way to explicitly writing the time reversal operator within the matrix; only the knowledge of the presence of time reversal is used in applying effectively the equations (1) and (2). The same operator in Jones faithful notation can be written as: , which is more compact. We will use this last representation hereafter.

The newly proposed Hall-symbols have the general form (S. R. Hall and R. W. Grosse-Kunstleve, 2010):

 (3)

The symbol **L** is the lattice symbol (**L**= P, A, B, C, I, R, H, F, X) that may be preceded by a minus sign for indicating that a centre of symmetry exists at the origin. The X symbol is used for non-conventional lattice centrings, in such a case the explicit generators of the lattice must be provided within the *p* provided operators. The symbol *N* is 1, 2, 3, 4 or 6 for proper rotations and  (in text-only characters -1, -2, -3, -4 or -6) for improper rotations (the symbol -2 may be replaced by *m* for mirror plane). The symbol *θ*  is “ ’” when the operator is associated with time reversal or it is absent otherwise. The symbol *A* indicates the direction of the rotation axis. The possible values are x, y, z, ^, ” and \*, for rotation axis along **a**, **b**, **c**, **a**-**b** (or alternatively **b** - **c** or **c** - **a**), **a**+**b** (or alternatively **b** + **c** or **c** + **a**) and **a**+**b**+**c**, respectively. The **t** translation symbols are 1, 2, 3, 4, 5, 6, *a*, *b*, *c*, *n*, *u*, *v*, *w*, *d* and they are described in Table A1.4.2.3 in S. R. Hall and R. W. Grosse-Kunstleve, 2010. These translations apply additively [e.g. *ad* signifies a (3/4, 1/4, 1/4) translation].

The change of basis operator **V** may be used as described in (S. R. Hall and R. W. Grosse-Kunstleve, 2010), however we propose an alternative change of notation that is more clearly related to its purpose.

**Table of Lattice symbols L**(similar to table A1.4.2.2. in S. R. Hall and R. W. Grosse-Kunstleve, 2010)

The lattice symbol **L** implies the following generators in Jones’ faithful notation. The identity is always implied even if not provided, the time reversal operator is provided as the last item, the different generators are separated by “;”. In the general case X we have used the notation 1**t** ≡ *x*+*t*1, *y*+*t*2, *z*+*t*3, 1, where **t**=(*t*1, *t*2, *t*3), with *t*i rational numbers.

P: *x*, *y*, *z*, 1 -P: -*x*, -*y*, -*z*, 1

A: *x*, *y*+1/2, *z*+1/2, 1 -A: -*x*, -*y*, -*z*, 1; *x*, *y*+1/2, *z*+1/2, 1

B: *x*+1/2, *y*, *z*+1/2, 1 -B: -*x*, -*y*, -*z*, 1; *x*+1/2, *y*, *z*+1/2, 1

C: *x*+1/2, *y*+1/2, *z*, 1 -C: -*x*, -*y*, -*z*, 1; *x*+1/2, *y*+1/2, *z*, 1

I: *x*+1/2, *y*+1/2, *z*+1/2, 1 -I: -*x*, -*y*, -*z*, 1; *x*+1/2, *y*+1/2, *z*+1/2, 1

R: *x*+2/3, *y*+1/3, *z*+1/3, 1; *x*+1/3, *y*+2/3, *z*+2/3, 1 -R: -*x*, -*y*, -*z*, 1; *x*+2/3, *y*+1/3, *z*+1/3, 1; *x*+1/3, *y*+2/3, *z*+2/3, 1

H: *x*+2/3, *y*+1/3, *z*, 1; *x*+1/3, *y*+2/3, *z*, 1 -H: -*x*, -*y*, -*z*, 1; *x*+2/3, *y*+1/3, *z*, 1; *x*+1/3, *y*+2/3, *z*, 1

F: *x*+1/2, *y*+1/2, *z*, 1; *x*, *y*+1/2, *z*+1/2, 1; *x*+1/2, *y*, *z*+1/2, 1 -F: -*x*, -*y*, -*z*, 1; *x*+1/2, *y*+1/2, *z*, 1; *x*, *y*+1/2, *z*+1/2, 1; *x*+1/2, *y*, *z*+1/2, 1

X: 1**t**1 ; 1**t**2; …1**t**p -X: -*x*, -*y*, -*z*, 1; 1**t**1 ; 1**t**2; …1**t**p

**Table of translation symbols t** (same as table A1.4.2.3. in S. R. Hall and R. W. Grosse-Kunstleve, 2010)

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. Putting several letters together means the addition of the translation vectors corresponding to given letters.

Translation Translation Subscript Fractional

Symbol Vector Symbol Translation

*a* 1/2, 0, 0 1 in 31 1/3

*b* 0, 1/2, 0 2 in 32 2/3

*c* 0, 0, 1/2 1 in 41 1/4

*n* 1/2, 1/2, 1/2 3 in 43 3/4

*u* 1/4, 0, 0 1 in 61 1/6

*v* 0, 1/4, 0 2 in 62 1/3

*w* 0, 0, 1/4 4 in 64 2/3

*d* 1/4, 1/4, 1/4 5 in 65 5/6

**References**

Hall, S.R. *Acta Cryst.* (1981). **A37**, 517-525

S. R. Hall and R. W. Grosse-Kunstleve in *International Tables for Crystallography* (2010). Vol. B, Appendix 1.4.2, pp. 122–134.