



# Extension of Hall symbols of crystallographic space groups to magnetic space groups

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The Hall symbols for describing unambiguously the generators of space groups have been extended to describe any setting of the 1651 types of magnetic space groups (Shubnikov groups). A computer program called *MHall* has been developed for parsing the Hall symbols, generating the full list of symmetry operators and identifying the transformation to the standard setting.

## 1. Introduction

The international symbols for crystallographic space groups (CSGs) are based on the Hermann–Mauguin (HM) 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 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 *International Tables for Crystallography*. When computer programs do that task without using a database they always have some special code to handle special cases in order to generate strictly the same set of operators. The proposal by Hall (1981) solves this problem in an elegant way, allowing, at the same time, the possibility of describing reasonable arbitrary settings of CSGs. The word ‘reasonable’ is used here to emphasize the fact that the symmetry operators (with the rotational part described by an integer matrix) may be very complicated (with the rotational part normally described by a rational matrix) if a unit-cell setting, for instance, is selected in which a threefold axis is along an arbitrary  $[uvw]$  direction. However, even in these cases, the Hall symbol, as treated by Hall & Grosse-Kunstleve (2010) (hereafter referred to as HG-K), can be written using the standard symbols described below followed by a setting change included at the end of the symbol.

In this paper, we propose to modify slightly the original Hall symbols in order to extend them to describe magnetic space groups (MSGs). For that, we had to change the original symbol ‘ to ^’. The reason is that the prime symbol ‘ is reserved for the time reversal operator to be consistent with the currently used symbols in Belov–Neronova–Smirnova (BNS) and Opechowski–Guccione (OG) notations for MSGs. Here we will not discuss the derivation of MSGs or their relation with families of CSGs, which may be found in the literature

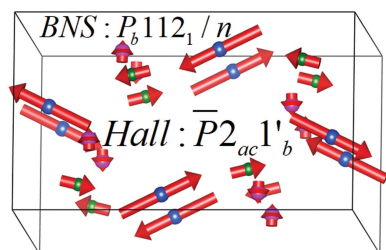


Table 1

Lattice symbols **L** (similar to Table A1.4.2.2 of HG-K).

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 a semicolon (;). In the general case,  $X$ , we have used the notation  $1\mathbf{t} \equiv x + t_1, y + t_2, z + t_3, 1$  where  $\mathbf{t} = (t_1, t_2, t_3)$ , with  $t_i$  rational numbers.

|                                                                             |                                                                                             |
|-----------------------------------------------------------------------------|---------------------------------------------------------------------------------------------|
| $P: x, y, z, 1$                                                             | $-P: -x, -y, -z, 1$                                                                         |
| $A: x, y + 1/2, z + 1/2, 1$                                                 | $-A: -x, -y, -z, 1; x, y + 1/2, z + 1/2, 1$                                                 |
| $B: x + 1/2, y, z + 1/2, 1$                                                 | $-B: -x, -y, -z, 1; x + 1/2, y, z + 1/2, 1$                                                 |
| $C: x + 1/2, y + 1/2, z, 1$                                                 | $-C: -x, -y, -z, 1; x + 1/2, y + 1/2, z, 1$                                                 |
| $I: x + 1/2, y + 1/2, z + 1/2, 1$                                           | $-I: -x, -y, -z, 1; x + 1/2, y + 1/2, z + 1/2, 1$                                           |
| $R: x + 2/3, y + 1/3, z + 1/3, 1; x + 1/3, y + 2/3, z + 2/3, 1$             | $-R: -x, -y, -z, 1; x + 2/3, y + 1/3, z + 1/3, 1; x + 1/3, y + 2/3, z + 2/3, 1$             |
| $H: x + 2/3, y + 1/3, z, 1; x + 1/3, y + 2/3, z, 1$                         | $-H: -x, -y, -z, 1; x + 2/3, y + 1/3, z, 1; x + 1/3, y + 2/3, z, 1$                         |
| $F: x + 1/2, y + 1/2, z, 1; x, y + 1/2, z + 1/2, 1; x + 1/2, y, z + 1/2, 1$ | $-F: -x, -y, -z, 1; x + 1/2, y + 1/2, z, 1; x, y + 1/2, z + 1/2, 1; x + 1/2, y, z + 1/2, 1$ |
| $X: 1\mathbf{t}_1; 1\mathbf{t}_2; \dots 1\mathbf{t}_p$                      | $-X: -x, -y, -z, 1; 1\mathbf{t}_1; 1\mathbf{t}_2; \dots 1\mathbf{t}_p$                      |

[see, for instance, Litvin (2013)]; we shall concentrate on the new proposed nomenclature aspects.

The aim of the Hall symbols is to have an unambiguous descriptor of a CSG or MSG and not to substitute the HM, BNS or OG (or whatever new proposal is adopted) symbols used for a standard setting. Once we have a correspondence with the standard setting of a CSG or MSG, an appropriate computer program can parse the symbols and generate the full set of symmetry operators. We have to keep in mind that two different Hall symbols may represent the same space-group type in a particular setting. This is obvious by the fact that we can use different generators to obtain the same full representative operators of the group type.

## 2. New proposed Hall symbols

This section summarizes the notation described by HG-K and the modifications we propose. The Hall symbols try to describe a CSG or 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  $\mathbf{S} = \{R, \theta|\mathbf{t}\}$  (where  $R$  is a proper or improper rotation matrix,  $\mathbf{t}$  is a translation vector and  $\theta$  is an integer representing the time reversal operation) on the atom position  $\mathbf{r}$  having a magnetic moment  $\mathbf{m}$  is given by

$$\mathbf{r}_T = \{R, \theta|\mathbf{t}\} \mathbf{r} = R\mathbf{r} + \mathbf{t}. \quad (1)$$

The corresponding magnetic moment (axial vector) is obtained as

$$\mathbf{m}_T = \{R, \theta|\mathbf{t}\} \mathbf{m} = \theta \det(R) R\mathbf{m}, \quad (2)$$

where  $\mathbf{r}_T$  and  $\mathbf{m}_T$  are the transformed position and moment, respectively. The integer  $\theta$  is equal to  $-1$  if the operator is 'primed' (combined with time reversal operator  $1'$ ) and equal to  $1$  in the 'non-primed' case;  $\det(R)$  stands for the determinant of matrix  $R$ . 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  $\mathbf{S}$  that describes unambiguously the matrix  $R$ , the value of  $\theta$  and the translation vector  $\mathbf{t}$ . The operator  $\mathbf{S}$  may be represented as a Seitz matrix or in the extended form (see below) of Jones

faithful notation. For instance, a Seitz matrix representing a primed twofold screw rotation along the  $b$  axis is given by

$$2_1' = \{2'_{010}|0, \frac{1}{2}, 0\} = \begin{pmatrix} R & \mathbf{t} \\ 0 & 1 \end{pmatrix}^\theta = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1/2 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}'.$$

Notice that we have no way to write explicitly the time reversal operator within the matrix; only the knowledge of the presence of time reversal is used in applying effectively equations (1) and (2). The same operator in Jones faithful notation (extended with  $1$  or  $-1$  in the last position representing  $\theta$ ) can be written as  $-x, y + 1/2, -z, -1$ , which is more compact than the full matrix. We will use this last representation instead of matrices hereafter.

The newly proposed Hall symbols have the general form (compare with equation A1.4.2.4 of HG-K)

$$\mathbf{L}[N_t^{A\theta}]_1[N_t^{A\theta}]_2 \dots [N_t^{A\theta}]_p \mathbf{V}. \quad (3)$$

The symbol **L** is the lattice symbol,  $\mathbf{L} = P, A, B, C, I, R, H, F, X$ . The symbol may include a preceding minus sign to indicate that a centre of symmetry exists at the origin. The  $X$  symbol is used for non-conventional lattice centring, and in such a case the explicit generators of the lattice must be provided within the  $p$  provided operators. The operators related to the **L** symbols are described in Table 1.

The symbol  $N$  is  $1, 2, 3, 4$  or  $6$  for proper rotations and  $\bar{1}, \bar{2}, \bar{3}, \bar{4}$  or  $\bar{6}$  (or in text-only characters  $-1, -2, -3, -4$  or  $-6$ ) for improper rotations (the symbol  $-2$  corresponds to mirror or glide planes depending on the associated translation). The symbol  $\theta$  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 of  $A$  are  $x, y, z, ^\wedge, ^\vee$  and  $*$  for a rotation axis along  $\mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{a} - \mathbf{b}$  (or alternatively  $\mathbf{b} - \mathbf{c}$  or  $\mathbf{c} - \mathbf{a}$ ),  $\mathbf{a} + \mathbf{b}$  (or alternatively  $\mathbf{b} + \mathbf{c}$  or  $\mathbf{c} + \mathbf{a}$ ) and  $\mathbf{a} + \mathbf{b} + \mathbf{c}$ , respectively. The  $\mathbf{t}$  translation symbols are  $1, 2, 3, 4, 5, 6, a, b, c, n, u, v, w, d$ . They are described in Table A1.4.2.3 of HG-K. This table is reproduced here as Table 2. Even if not explicit in Table 2, the symbols of screw axes  $4_2$  and  $6_3$  (with translation of  $1/2$  along the axis  $A$ ) are legal Hall symbols and may be written as  $4_c$  and  $6_c$  if they are oriented along the  $c$  axis; we recommend the use of this last form. These translations

**Table 2**

Translation symbols **t** (same as Table A1.4.2.3 of HG-K).

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 symbols together means the addition of the translation vectors corresponding to the given symbols.

| Translation symbol | Translation vector | Subscript symbol    | Fractional translation |
|--------------------|--------------------|---------------------|------------------------|
| <i>a</i>           | 1/2, 0, 0          | 1 in 3 <sub>1</sub> | 1/3                    |
| <i>b</i>           | 0, 1/2, 0          | 2 in 3 <sub>2</sub> | 2/3                    |
| <i>c</i>           | 0, 0, 1/2          | 1 in 4 <sub>1</sub> | 1/4                    |
| <i>n</i>           | 1/2, 1/2, 1/2      | 3 in 4 <sub>3</sub> | 3/4                    |
| <i>u</i>           | 1/4, 0, 0          | 1 in 6 <sub>1</sub> | 1/6                    |
| <i>v</i>           | 0, 1/4, 0          | 2 in 6 <sub>2</sub> | 1/3                    |
| <i>w</i>           | 0, 0, 1/4          | 4 in 6 <sub>4</sub> | 2/3                    |
| <i>d</i>           | 1/4, 1/4, 1/4      | 5 in 6 <sub>5</sub> | 5/6                    |

apply additively [e.g. *ad* signifies a (3/4, 1/4, 1/4) translation]. Notice that we can use, for anti-translations, a lattice symbol instead of two translation symbols. For instance, the following symbols are equivalent:  $1'_{bc} = 1'_A$ ,  $1'_{ac} = 1'_B$ ,  $1'_{ab} = 1'_C$ ,  $1'_n = 1'_I$ .

Examples of valid symbols for the  $[N_i^{A\theta}]$  generators are  $4'_a$ ,  $-2'_n$ ,  $3'_1$ ,  $1'_{avw}$ ,  $1'_{ad}$ , representing, respectively, the operators [in Seitz notation; see Glazer *et al.* (2014)]  $\{4'_{100} | \frac{1}{2}, 0, 0\}$ ,  $\{m_{001} | \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\}$ ,  $\{3'_{111} | \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\}$ ,  $\{1' | \frac{1}{2}, \frac{1}{4}, \frac{1}{4}\}$ ,  $\{1 | \frac{3}{4}, \frac{1}{4}, \frac{1}{4}\}$ .

The change of basis operator **V** is optional and may be used as described by HG-K. However, we propose an alternative change of notation that is more clearly related to its purpose: a change of reference frame, involving the basis vectors and origin, to which the symmetry operators refer.

## 3. Default axes from the positional order of operators

The superscripts indicating the directions of rotation axes may be suppressed by adopting the following rules (see Section A1.4.2.3.1 of HG-K) for the symbol given in expression (3):

- The first rotation (or roto-inversion) axis direction is always along **c**.
- The second rotation (if  $|N|$  is 2) axis direction is along **a** if preceded by an  $|N|$  of 2 or 4, or along **a** – **b** if preceded by an  $|N|$  of 3 or 6. We use the symbol  $|N|$  to describe any of the two symbols  $N$  or  $-N$ .
- The third rotation (if  $|N|$  is 3) has an axis direction of **a** + **b** + **c**.

This implies that in the majority of cases the symbol  $\wedge$  is not needed. If we ignore these rules, the superscript of the provided operators should be explicitly written. The rotational parts of  $[N_i^{A\theta}]$  operators ( $[N^A]$ ) are given explicitly in Tables 3, 4 and 5.

Another additional convention is that anti-translations ( $1'_I$ ) should appear after the rotational operators and non-conventional lattice translations ( $1'_X$ ). We also adopt the convention that the computer-entry symbols should be case sensitive. This allows one to distinguish the translations '*a*' and '*A*' for instance. In case we obtain the same operators with different symbols, the recommendation is to use the shortest notation. The symbol '*I*' of Table 1 is identical to the trans-

**Table 3**

Operators  $[N^A]$  (similar to Table A1.4.2.4 of HG-K).

Jones faithful operators for proper rotations along the three principal unit-cell directions are given below. For improper rotations ( $-2$ ,  $-3$ ,  $-4$  and  $-6$ ) the symbols are identical except that all signs are reversed. The identity 1 ( $x, y, z$ ) and inversion centre  $-1$  ( $-x, -y, -z$ ) are omitted because they do not depend on the axis. The same holds for time reversal.

|               |                 | Rotation order $N$ and Jones faithful symbol |                |            |               |
|---------------|-----------------|----------------------------------------------|----------------|------------|---------------|
| Rotation axis | <i>A</i> symbol | 2                                            | 3              | 4          | 6             |
| <b>a</b>      | <i>x</i>        | $x, -y, -z$                                  | $x, -z, y - z$ | $x, -z, y$ | $x, y - z, y$ |
| <b>b</b>      | <i>y</i>        | $-x, y, -z$                                  | $z - x, y, -x$ | $z, y, -x$ | $z, y, z - x$ |
| <b>c</b>      | <i>z</i>        | $-x, -y, z$                                  | $-y, x - y, z$ | $-y, x, z$ | $x - y, x, z$ |

**Table 4**

Operators  $[N^A]$  (similar to Table A1.4.2.5 of HG-K).

Jones faithful operators for proper twofold rotations along the diagonal unit-cell directions.

| Preceding rotation | Rotation symbol | Axis                | Jones faithful symbol |
|--------------------|-----------------|---------------------|-----------------------|
| $N^x$              | $2^\wedge$      | <b>b</b> – <b>c</b> | $-x, -z, -y$          |
|                    | $2''$           | <b>b</b> + <b>c</b> | $-x, z, y$            |
| $N^y$              | $2^\wedge$      | <b>a</b> – <b>c</b> | $-z, -y, -x$          |
|                    | $2''$           | <b>a</b> + <b>c</b> | $z, -y, x$            |
| $N^z$              | $2^\wedge$      | <b>a</b> – <b>b</b> | $-y, -x, -z$          |
|                    | $2''$           | <b>a</b> + <b>b</b> | $y, x, -z$            |

**Table 5**

Operator  $3^*$  (similar to Table A1.4.2.6 of HG-K).

The operator for a proper threefold rotation along the body diagonal unit-cell direction.

| Rotation symbol | Axis                           | Jones faithful symbol |
|-----------------|--------------------------------|-----------------------|
| $3^*$           | <b>a</b> + <b>b</b> + <b>c</b> | $z, x, y$             |

lation symbol  $n$ ; however the first symbol is used only with  $N = 1$  (pure translations or anti-translations).

## 4. New change of basis operator **V**

HG-K extend the original shift of origin symbol to a complete change of basis; however, they use a vector form in which a symbol close to the Jones faithful representation of symmetry operators is used to represent this time a change of basis. Symmetry operators are implicitly referred to a reference frame  $\{O, \mathbf{a}, \mathbf{b}, \mathbf{c}\}$ , where  $O$  represents a point in 3D space and **a**, **b**, **c** are the basis vectors. In previous forms of the Hall symbol (see HG-K), the operator **V** is represented in vectorial form  $\mathbf{V} = (v_1, v_2, v_3)$  with  $v_i = r_{i1}X + r_{i2}Y + r_{i3}Z + t_i$ , where  $r_{ij}$  and  $t_i$  are rational numbers. The operator can be written as a Seitz matrix as given by HG-K:

$$\mathbf{V} = \begin{pmatrix} r_{11} & r_{12} & r_{13} & t_1 \\ r_{21} & r_{22} & r_{23} & t_2 \\ r_{31} & r_{32} & r_{33} & t_3 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \quad (4)$$

In the case of a simple change of origin,  $r_{ij} = 0$  if  $i \neq j$  and  $r_{ii} = 1$ , we conserve the same notation as proposed by Hall (1981) and HG-K, where the Hall symbol finishes with an integer vector

in parentheses of the form  $(n_1, n_2, n_3)$ , meaning  $t_1 = n_1/12$ ,  $t_2 = n_2/12$  and  $t_3 = n_3/12$ .

The meaning of the change of basis operator  $\mathbf{V}$  is the following: the new basis vectors  $\mathbf{a}_T, \mathbf{b}_T, \mathbf{c}_T$  are obtained as

$$(\mathbf{a}_T \ \mathbf{b}_T \ \mathbf{c}_T) = (\mathbf{a} \ \mathbf{b} \ \mathbf{c}) \begin{pmatrix} r_{11} & r_{21} & r_{31} \\ r_{12} & r_{22} & r_{32} \\ r_{13} & r_{23} & r_{33} \end{pmatrix}. \quad (5)$$

Notice that the  $3 \times 3$  submatrix is transposed to that of  $\mathbf{V}$ . The new origin  $O_T$  has coordinates  $(t_1, t_2, t_3)$  with respect to the original  $\{O, \mathbf{a}, \mathbf{b}, \mathbf{c}\}$  basis.

The symmetry operators provided in the Hall symbol (generators) should be transformed, if the operator  $\mathbf{V}$  is provided, according to the equation

$$\mathbf{S}_n^T = \mathbf{V} \mathbf{S}_n \mathbf{V}^{-1}, \quad (6)$$

where the new operators  $\mathbf{S}_n^T$  are now implicitly referred to the basis  $\{O_T, \mathbf{a}_T, \mathbf{b}_T, \mathbf{c}_T\}$ .

We maintain the original convention for change of origin but, in order to be compatible with this form, we propose to use a colon (:) as separator between the first part of the symbol and  $\mathbf{V}$  to tell the parsing program that we use the new symbolic form for the  $\mathbf{V}$  operator. Thus expression (3), in the general case of basis change, is written as

$$\mathbf{L} [N_1^{A\theta}]_1 [N_2^{A\theta}]_2 \dots [N_p^{A\theta}]_p : r_{11}a + r_{12}b + r_{13}c, r_{21}a + r_{22}b + r_{23}c, r_{31}a + r_{32}b + r_{33}c; t_1, t_2, t_3. \quad (7)$$

Notice the semicolon separating the 'rotational' part of the matrix (4) from the coordinates of the new origin  $(t_1, t_2, t_3)$ .

## 5. Detailed examples

The header 'ASCII' given in the examples below means that we use characters from the ASCII character set available to computers and coded with 1 byte (8 bits), so subscripts and superscripts are not used. Instead, the translation symbols are just juxtaposed to the rotational symbols. When using the text (ASCII) form of the Hall symbols we use one or more spaces between symbols as in:

$$\mathbf{L} \ [N_1^{A\theta}]_1 \ [N_2^{A\theta}]_2 \ \dots \ [N_p^{A\theta}]_p \ \mathbf{V}.$$

When writing the Hall symbol in text-only mode the operator  $[N_1^{A\theta}]$  should be written in the form  $N'A\mathbf{t}$ ,  $NA'\mathbf{t}$  or  $NA'\mathbf{t}$  with the axis symbol preceding the translation part. Notice that the prime symbol commutes with the axis and translation symbols. We recommend, however, using the form  $NA'\mathbf{t}$  for  $|N| \neq 1$  and the form  $N'A\mathbf{t}$  for  $|N| = 1$ . The symbols used throughout this paper comply with this prescription.

An example of a legal Hall symbol for an MSG is  $P6_c\bar{2}1'$ , which in ASCII form is represented as P 6c -2 1' c.

The above Hall symbol corresponds to the MSG  $P6_3cm$  (in BNS notation) in the standard setting. We can also use the symbol (see the comment above about Table 2) P 63 -2 1' c in which the traditional form of a screw axis  $6_3$  is explicitly given.

One can create a Hall symbol without knowing to which MSG standard type it corresponds. A computer program can identify the standard MSG type and calculate the change of basis to obtain the standard setting. For instance, a symbol like  $-P \ 4n' \ 1' u \ (\bar{P}4'_n1'_u)$  corresponds to the group  $P_{-C}4_2/m$  ( $P_C4_2/m$ ) in a particular setting. To obtain the standard setting one has to apply the following basis change:  $-a/4 - b/4, a/4 - b/4, c; -1/8, -1/8, 0$ .

Let us consider conventional settings of MSGs as examples. MSGs are usually divided into four types:

Type 1 MSGs, also called colourless groups, are those having  $\theta = 1$  for all operators. They are isomorphous to the 230 CSGs. The BNS and OG symbols coincide in this case with the HM symbols of CSGs. The Hall symbols are the same as those of the CSGs. Examples of the symbols can be found in Table A1.4.2.7 of HG-K.

Type 2 MSGs, also called paramagnetic groups, are those having two sets of operators. The first set is the same as those of Type 1 groups and in the second set the operators have  $\theta = -1$  combined with all operators of the first set. Their number is also 230 and the BNS and OG symbols are those of the corresponding CSG followed by the time reversal operator. The Hall symbols are obtained from the Hall symbols of Type 1 groups by putting the time reversal operator as the last generator.

### Examples

| BNS/OG Symbol | BNS/OG ASCII  | Compact ASCII  | Hall Symbol       | Hall ASCII    |
|---------------|---------------|----------------|-------------------|---------------|
| $P4_2, 21'$   | P 41 21 2 1'  | $P4\_12\_121'$ | $P4_{ab}2_{ac}1'$ | P 4abw 2nw 1' |
| $P4_2/mmc1'$  | P 42/m m c 1' | $P4\_2/mmc1'$  | $\bar{P}4_21'$    | -P 4c 2 1'    |

The full set of operators for the first group ( $P4_2, 21'$ ) can be obtained by the generators  $-y + 1/2, x + 1/2, z + 1/4, 1$  ( $4_{abw}$ );  $x + 1/2, -y + 1/2, -z + 3/4, 1$  ( $2_{nw}$ );  $x, y, z, -1$  ( $1'$ ).

The full set of operators for the second group ( $P4_2/mmc1'$ ) can be obtained by the generators  $-x, -y, -z, 1$  ( $-1$ );  $-y, x, z + 1/2, 1$  ( $4_c$ );  $x, -y, -z, 1$  ( $2$ );  $x, y, z, -1$  ( $1'$ ).

Type 3 MSGs, also called Type 1 black and white (BW1) groups, are those having the same lattice as that of the paramagnetic group, but half of the operators are associated with time reversal. Their number is 674 and the BNS and OG symbols are the same.

### Examples

| BNS/OG Symbol | BNS/OG ASCII | Compact ASCII | Hall Symbol             | Hall ASCII        |
|---------------|--------------|---------------|-------------------------|-------------------|
| $Pc'cn'$      | P c' c n'    | $Pc'cn'$      | $\bar{P}2'_{ab}2'_{ac}$ | -P 2ab' 2ac'      |
| $P6'_22'$     | P 62' 2 2'   | $P6\_2'22'$   | $P6'_22'_c(001)$        | P 62' 2c' (0 0 1) |

The full set of operators for the first group ( $Pc'cn'$ ) can be obtained by the generators  $-x + 1/2, -y + 1/2, z, -1$  ( $2_{ab}'$ );  $x + 1/2, -y, -z + 1/2, -1$  ( $2_{ac}'$ );  $-x, -y, -z, 1$  ( $-1$ ).

The full set of operators for the second group ( $P6'_22'$ ) can be obtained by the generators  $x - y, x, z + 1/3, -1$  ( $6_2'$ );  $-y, -x, -z + 2/3, -1$  ( $2_c'$ ).

Notice that the second operator without taking into account the change of origin would have the form  $-y, -x, -z + 1/2, -1$  according to rule (ii) and Table 4. The shift of the origin is then needed to describe the standard setting of the  $P6'_222'$  group.

Type 4 MSGs, also called Type 2 black and white (BW2) groups, are those containing anti-translations: lattice translations associated with time reversal. Of course, these anti-translations are not lattice vectors. Their number is 517 and the BNS and OG symbols are different. Here we have conserved the columns concerning the ASCII representations of the BNS and OG in compact form.

Examples

| BNS Symbol     | OG Symbol      | BNS ASCII    | OG ASCII     | Hall Symbol                | Hall ASCII             |
|----------------|----------------|--------------|--------------|----------------------------|------------------------|
| $F_s dd2$      | $P_1 mn2$      | $F\_Sdd2$    | $P\_Inn2$    | $F2\bar{2}_d1'_n$          | $F\ 2\ -2d\ 1'n$       |
| $P_c bcn$      | $C_p m'cm$     | $P\_Cbcn$    | $C\_Pm'cm$   | $\bar{P}2_n2_{ab}1'_c$     | $-P\ 2n\ 2ab\ 1'c$     |
| $P_c 6_3cm$    | $P_c 6'm'm$    | $P\_c6\_3cm$ | $P\_2c6'm'm$ | $P6_c\bar{2}1'_c$          | $P\ 6c\ -2\ 1'c$       |
| $F_s d\bar{3}$ | $P_f n\bar{3}$ | $F\_Sd-3$    | $P\_Fn-3$    | $\bar{F}2_{uv}2_{vw}31'_n$ | $-F\ 2uv\ 2vw\ 3\ 1'n$ |

The full set of operators for the first group ( $F_s dd2$ ) can be obtained by the generators  $-x, -y, z, 1 (2)$ ;  $-x + 1/4, y + 1/4, z + 1/4, 1 (\bar{2}_d)$ ;  $x + 1/2, y + 1/2, z + 1/2, -1 (1'_n)$  and the  $F$ -centring translations  $x, y + 1/2, z + 1/2, 1$ ;  $x + 1/2, y, z + 1/2, 1$  and  $x + 1/2, y + 1/2, z, 1$ .

The full set of operators for the second group ( $P_c bcn$ ) can be obtained by the generators  $-x + 1/2, -y + 1/2, z + 1/2, 1 (2_n)$ ;  $x + 1/2, -y + 1/2, -z, 1 (2_{ab})$ ;  $-x, -y, -z, 1 (\bar{1})$ ;  $x + 1/2, y + 1/2, z, -1 (1'_c)$ .

The full set of operators for the third group ( $P_c 6_3cm$ ) can be obtained by the generators  $-x - y, x, z + 1/2, 1 (6_c)$ ;  $y, x, z, 1 (\bar{2})$ ;  $x, y, z + 1/2, -1 (1'_c)$ .

The full set of operators for the fourth group ( $F_s d\bar{3}$ ) can be obtained by the generators  $-x + 1/4, -y + 1/4, z, 1 (2_{zuv})$ ,  $x, -y + 1/4, -z + 1/4, 1 (2_{xuv})$ ;  $z, x, y, 1 [3 \text{ along } \mathbf{a} + \mathbf{b} + \mathbf{c}, \text{ the star symbol in } 3^* \text{ is not needed according to rule (iii) and Table 5}]$ , the centre of symmetry  $-x, -y, -z, 1$  and the  $F$ -centring translations.

We provide a supporting information text document in which all the standard MSG are listed together with the Hall symbols and the explicit generators used in Jones faithful form. The newly proposed international symbols (to be discussed by the Commission for Magnetic Structures of the IUCr) for the standard settings are also in the list.

## 6. A console program for calculating symmetry operators from Hall symbols

We have developed a console program (*MHall*) that is able to interpret Hall symbols as described in this paper. (The Windows console version of the program *MHall* can be obtained as a standalone executable from <https://code.ill.fr/scientific-software/crysfml/-/blob/master/BinariesDistributions/Windows/MHall.zip>.) The program is based on the new version of the *CrysFML* library (González-Platas *et al.*, 2021) handling general space groups (crystallographic, magnetic and

superspace groups). The source code of the library as well as the program are written in the Fortran2008 standard. The program asks for a Hall symbol (or a set of generators in Jones faithful notation) as input and produces the full list of operators as well as the corresponding geometric symmetry element symbols (international notation) and the transformation to the standard setting as defined by Stokes *et al.* (2013). The geometric symmetry element symbols are only provided for settings that are not too complicated. Two examples of running the program from a Windows console are provided in the supporting information, as well as details of the installation of the program. The program will be available within the forthcoming update of the *FullProf* suite (Rodríguez-Carvajal *et al.*, 2020).

## 7. Conclusions

The extension of the Hall symbols to MSGs has been straightforward to implement from the already existing definitions with a minimal change in one axis symbol. The use of the list of standard Hall symbols for the 1651 MSGs allows the generation, in a faster and compact way, of the full list of symmetry operators of these groups. A further extension of Hall symbols is projected for general superspace groups (crystallographic and magnetic) by just adding the modulation vectors followed by the phase symbols, commonly used in the current symbols, indicating the translation component for each generator in the additional dimensions.

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