JOURNAL OF APPLIED CRYSTALLOGRAPHY

Volume 54 (2021)

Supporting information for article:

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

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S1. Hall symbols of the 1651 Magnetic Space Groups

List of the standard setting Hall symbols for the 1651 MSG and their correspondence with the conventional BNS and OG symbols. This list is in a separated text file called `Magnetic_Hall_Symbols.txt`. The provided symbols are ordered as in (Litvin, D.B., 2013, *Magnetic Space Group Types*, IUCr e-book). The new ordering, proposed by some member of the Commission for Magnetic Structures of the IUCr, is also provided. A list of the generators, in Jones faithful notation, is provided in the last column of the document.

S2. Procedure for installing and running the program MHALL

The program **MHALL** is distributed within the file `MHall.zip`. It contains the executable program `MHall.exe` for Windows (64 bits) and `MHall.x` for Linux. For working with the program, the following steps should be respected (this is for Windows, for Linux is similar):

1: Extract the files of `MHall.zip` in the directory of your choice

2: Open a Windows terminal (using cmd.exe) and go to the previous directory.

3: Type `MHall` in the terminal followed by the `<Enter>` key.

4: Introduce the Hall symbol of your choice (or a set of generators in Jones faithful notation separated by semicolons)

5: Type the `<Enter>` key

6: For exiting the program you should enter a void Hall symbol.

Notice that the database `magnetic_data.txt`, by Stokes & Campbell, is provided with the program. If you have already this database in another directory, you may define the environment variable `CRYSFML_DB` pointing to the directory where `magnetic_data.txt` is.

The program may be run also by entering the input information in the command line (do not forget to put the information within double quotes). For instance, we can run the program and redirect the standard output to the file `output.txt`:

```
MyPrompt> MHall "x,-y,z+1/4,-1;-x,-y,-z,1;x+1/2,y+1/2,z,1" > output.txt
MyPrompt> MHall "-F 2yw' -1'n" >> output.txt
```

This allows the preparation of a batch file for testing many examples at the fly. The standard output is sent to `output.txt`

S3. Examples of running the program MHALL

First example: MSG `P_C4_2/m` using a strange setting (Hall symbol `-P 4n' 1'u`) followed by a change of basis putting back the operators in the standard setting

```
 ----------------------------
  MHall: Testing Hall symbols
 ----------------------------
=> Enter the magnetic Hall symbol or a list of generators in Jones'faithful notation:
   -P 4n' 1'u : -a/4-b/4,a/4-b/4,c;-1/8,-1/8,0
=> Obtained generators: -y+1/2,x+1/2,z+1/2,-1;x+1/4,y,z,-1;-x,-y,-z,1
=> Followed by a change of basis: -a/4-b/4,a/4-b/4,c;-1/8,-1/8,0
=> Newly obtained generators: -y+1/2,x+1/2,z+1/2,-1;x+1/2,y+1/2,z,-1;-x,-y,-z,1
   General Space Group
   -------------------
                Op-Dimension:    4
             Space-Dimension:    3
                Multiplicity:   16
                     MagType:    4, Black-White:2
                      NumOps:    8
                     Centred:    2
    Num. Centring translation:    0
       Num. Anti-translations:    1
              Crystal system: Tetragonal
 Crystallographic Point group: 4/m
                  Laue class: 4/m
          Space Group number:   84
       Shubnikov Group number:  717
                 Hall symbol: -P 4n' 1'u : -a/4-b/4,a/4-b/4,c;-1/8,-1/8,0
  Shubnikov Group BNS-symbol: P_C4_2/m
  Shubnikov Group BNS-label : 84.57
  Shubnikov Group  OG-symbol: P_P4_2/m
        Magnetic Point Group: 4/m1'
 To Standard Shubnikov Group: a,b,c;0,0,0
             Generators List: -y+1/2,x+1/2,z+1/2,-1;x+1/2,y+1/2,z,-1;-x,-y,-z,1
                Centre_coord: [ 0 0 0 ]
           Anti-Centre_coord: [ 1/4 1/4 0 ]

           Anti-translations:
                             [ 1/2 1/2 0 ]

 Complete list of symmetry operators and symmetry symbols
 ========================================================
 SymmOp   1: x,y,z,1                              Symbol: 1
 SymmOp   2: -x,-y,z,1                            Symbol: 2 0,0,z
 SymmOp   3: -y,x,z+1/2,1                         Symbol: 4+ (0,0,1/2) 0,0,z
 SymmOp   4: y,-x,z+1/2,1                         Symbol: 4- (0,0,1/2) 0,0,z
 SymmOp   5: -y+1/2,x+1/2,z+1/2,-1                Symbol: 4+' (0,0,1/2) 0,1/2,z
 SymmOp   6: x+1/2,y+1/2,z,-1                     Symbol: t' (1/2,1/2,0)
 SymmOp   7: y+1/2,-x+1/2,z+1/2,-1                Symbol: 4-' (0,0,1/2) 1/2,0,z
 SymmOp   8: -x+1/2,-y+1/2,z,-1                   Symbol: 2' 1/4,1/4,z
```

```
 SymmOp   9: -x,-y,-z,1                          Symbol: -1 0,0,0
 SymmOp  10: x,y,-z,1                            Symbol: m x,y,0
 SymmOp  11: y,-x,-z+1/2,1                       Symbol: -4+ 0,0,z; 0,0,1/4
 SymmOp  12: -y,x,-z+1/2,1                       Symbol: -4- 0,0,z; 0,0,1/4
 SymmOp  13: y+1/2,-x+1/2,-z+1/2,-1              Symbol: -4+' 1/2,0,z; 1/2,0,1/4
 SymmOp  14: -x+1/2,-y+1/2,-z,-1                 Symbol: -1' 1/4,1/4,0
 SymmOp  15: -y+1/2,x+1/2,-z+1/2,-1              Symbol: -4-' 0,1/2,z; 0,1/2,1/4
 SymmOp  16: x+1/2,y+1/2,-z,-1                   Symbol: n' (1/2,1/2,0) x,y,0

 => Total CPU_TIME for this calculation:        0.406 seconds
```

Second example: MSG `P4'` in a non-conventional setting (Hall symbol `X 4' 1u`) corresponding to the use a supercell `4a,4b,c` of the standard setting. Notice the high number of lattice centring vectors.

```
  ----------------------------
   MHall: Testing Hall symbols
  ----------------------------
 => Enter the magnetic Hall symbol or a list of generators in Jones' faithful notation: X 4'
1u
 => Obtained generators: -y,x,z,-1;x+1/4,y,z,1
    General Space Group
    -------------------
                  Op-Dimension:    4
               Space-Dimension:    3
                  Multiplicity:   64
                       MagType:    3, Black-White:1
                        NumOps:    4
                       Centred:    1
     Num. Centring translation:   15
        Num. Anti-translations:    0
                Crystal system: Tetragonal
  Crystallographic Point group: 4
                    Laue class: 4/m
            Space Group number:   75
        Shubnikov Group number:  663
                   Hall symbol: X 4' 1u
    Shubnikov Group BNS-symbol: P4'
    Shubnikov Group BNS-label : 75.3
    Shubnikov Group  OG-symbol: P4'
          Magnetic Point Group: 4'
   To Standard Shubnikov Group: -a/4,-b/4,c;0,0,0
               Generators List: -y,x,z,-1;x+1/4,y,z,1
                  Centre_coord: none!

         Centring translations:
                              [ 1/4 0 0 ]
                              [ 1/2 0 0 ]
                              [ 3/4 0 0 ]
                              [ 0 3/4 0 ]
```

```
                              [ 0 1/4 0 ]
                              [ 1/4 3/4 0 ]
                              [ 0 1/2 0 ]
                              [ 3/4 3/4 0 ]
                              [ 1/4 1/4 0 ]
                              [ 3/4 1/4 0 ]
                              [ 1/2 3/4 0 ]
                              [ 1/4 1/2 0 ]
                              [ 3/4 1/2 0 ]
                              [ 1/2 1/4 0 ]
                              [ 1/2 1/2 0 ]

Complete list of symmetry operators and symmetry symbols
========================================================
SymmOp   1: x,y,z,1                                Symbol: 1
SymmOp   2: -x,-y,z,1                              Symbol: 2 0,0,z
SymmOp   3: -y,x,z,-1                              Symbol: 4+' 0,0,z
SymmOp   4: y,-x,z,-1                              Symbol: 4-' 0,0,z
SymmOp   5: x+1/4,y,z,1                            Symbol: t (1/4,0,0)
SymmOp   6: -x+1/4,-y,z,1                          Symbol: 2 1/8,0,z
SymmOp   7: -y+1/4,x,z,-1                          Symbol: 4+' 1/8,1/8,z
SymmOp   8: y+1/4,-x,z,-1                          Symbol: 4-' 1/8,-1/8,z
SymmOp   9: x+1/2,y,z,1                            Symbol: t (1/2,0,0)
SymmOp  10: -x+1/2,-y,z,1                          Symbol: 2 1/4,0,z
SymmOp  11: -y+1/2,x,z,-1                          Symbol: 4+' 1/4,1/4,z
SymmOp  12: y+1/2,-x,z,-1                          Symbol: 4-' 1/4,-1/4,z
SymmOp  13: x+3/4,y,z,1                            Symbol: t (3/4,0,0)
SymmOp  14: -x+3/4,-y,z,1                          Symbol: 2 3/8,0,z
SymmOp  15: -y+3/4,x,z,-1                          Symbol: 4+' 3/8,3/8,z
SymmOp  16: y+3/4,-x,z,-1                          Symbol: 4-' 3/8,-3/8,z
SymmOp  17: x,y+3/4,z,1                            Symbol: t (0,3/4,0)
SymmOp  18: -x,-y+3/4,z,1                          Symbol: 2 0,3/8,z
SymmOp  19: -y,x+3/4,z,-1                          Symbol: 4+' -3/8,3/8,z
SymmOp  20: y,-x+3/4,z,-1                          Symbol: 4-' 3/8,3/8,z
SymmOp  21: x,y+1/4,z,1                            Symbol: t (0,1/4,0)
SymmOp  22: -x,-y+1/4,z,1                          Symbol: 2 0,1/8,z
SymmOp  23: -y,x+1/4,z,-1                          Symbol: 4+' -1/8,1/8,z
SymmOp  24: y,-x+1/4,z,-1                          Symbol: 4-' 1/8,1/8,z
SymmOp  25: x+1/4,y+3/4,z,1                        Symbol: t (1/4,3/4,0)
SymmOp  26: -x+1/4,-y+3/4,z,1                      Symbol: 2 1/8,3/8,z
SymmOp  27: -y+1/4,x+3/4,z,-1                      Symbol: 4+' -1/4,1/2,z
SymmOp  28: y+1/4,-x+3/4,z,-1                      Symbol: 4-' 1/2,1/4,z
SymmOp  29: x,y+1/2,z,1                            Symbol: t (0,1/2,0)
SymmOp  30: -x,-y+1/2,z,1                          Symbol: 2 0,1/4,z
SymmOp  31: -y,x+1/2,z,-1                          Symbol: 4+' -1/4,1/4,z
SymmOp  32: y,-x+1/2,z,-1                          Symbol: 4-' 1/4,1/4,z
SymmOp  33: x+3/4,y+3/4,z,1                        Symbol: t (3/4,3/4,0)
SymmOp  34: -x+3/4,-y+3/4,z,1                      Symbol: 2 3/8,3/8,z
SymmOp  35: -y+3/4,x+3/4,z,-1                      Symbol: 4+' 0,3/4,z
SymmOp  36: y+3/4,-x+3/4,z,-1                      Symbol: 4-' 3/4,0,z
SymmOp  37: x+1/4,y+1/4,z,1                        Symbol: t (1/4,1/4,0)
```

```
 SymmOp  38: -x+1/4,-y+1/4,z,1                 Symbol: 2 1/8,1/8,z
 SymmOp  39: -y+1/4,x+1/4,z,-1                 Symbol: 4+' 0,1/4,z
 SymmOp  40: y+1/4,-x+1/4,z,-1                 Symbol: 4-' 1/4,0,z
 SymmOp  41: x+3/4,y+1/4,z,1                   Symbol: t (3/4,1/4,0)
 SymmOp  42: -x+3/4,-y+1/4,z,1                 Symbol: 2 3/8,1/8,z
 SymmOp  43: -y+3/4,x+1/4,z,-1                 Symbol: 4+' 1/4,1/2,z
 SymmOp  44: y+3/4,-x+1/4,z,-1                 Symbol: 4-' 1/2,-1/4,z
 SymmOp  45: x+1/2,y+3/4,z,1                   Symbol: t (1/2,3/4,0)
 SymmOp  46: -x+1/2,-y+3/4,z,1                 Symbol: 2 1/4,3/8,z
 SymmOp  47: -y+1/2,x+3/4,z,-1                 Symbol: 4+' -1/8,5/8,z
 SymmOp  48: y+1/2,-x+3/4,z,-1                 Symbol: 4-' 5/8,1/8,z
 SymmOp  49: x+1/4,y+1/2,z,1                   Symbol: t (1/4,1/2,0)
 SymmOp  50: -x+1/4,-y+1/2,z,1                 Symbol: 2 1/8,1/4,z
 SymmOp  51: -y+1/4,x+1/2,z,-1                 Symbol: 4+' -1/8,3/8,z
 SymmOp  52: y+1/4,-x+1/2,z,-1                 Symbol: 4-' 3/8,1/8,z
 SymmOp  53: x+3/4,y+1/2,z,1                   Symbol: t (3/4,1/2,0)
 SymmOp  54: -x+3/4,-y+1/2,z,1                 Symbol: 2 3/8,1/4,z
 SymmOp  55: -y+3/4,x+1/2,z,-1                 Symbol: 4+' 1/8,5/8,z
 SymmOp  56: y+3/4,-x+1/2,z,-1                 Symbol: 4-' 5/8,-1/8,z
 SymmOp  57: x+1/2,y+1/4,z,1                   Symbol: t (1/2,1/4,0)
 SymmOp  58: -x+1/2,-y+1/4,z,1                 Symbol: 2 1/4,1/8,z
 SymmOp  59: -y+1/2,x+1/4,z,-1                 Symbol: 4+' 1/8,3/8,z
 SymmOp  60: y+1/2,-x+1/4,z,-1                 Symbol: 4-' 3/8,-1/8,z
 SymmOp  61: x+1/2,y+1/2,z,1                   Symbol: t (1/2,1/2,0)
 SymmOp  62: -x+1/2,-y+1/2,z,1                 Symbol: 2 1/4,1/4,z
 SymmOp  63: -y+1/2,x+1/2,z,-1                 Symbol: 4+' 0,1/2,z
 SymmOp  64: y+1/2,-x+1/2,z,-1                 Symbol: 4-' 1/2,0,z

=> Total CPU_TIME for this calculation:        0.391 seconds
```