**Supplementary Material - 1**

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.

**Supplementary Material – 2**

**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

**Examples without entering the input in the command line**

*First example*: MSG P\_C4\_2/m using a strange setting (Hall symbol -P 4n' 1u') followed by a change of basis putting back the operators in the standard setting.

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MHall: Testing Hall symbols

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=> Enter the magnetic Hall symbol or a list of generators in Jones'faithful notation:

-P 4n' 1u' : -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

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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' 1u' : -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

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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.

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MHall: Testing Hall symbols

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=> 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

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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

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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