The new magCIF format for describing magnetic structures

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magCIF history

Wieslawa Sikora's magnetic CIF project – late 90s

Early magCIF prototype introduced in ISODISTORT in 2010.

IUCr Commission on Magnetic Structures formed in 2011.

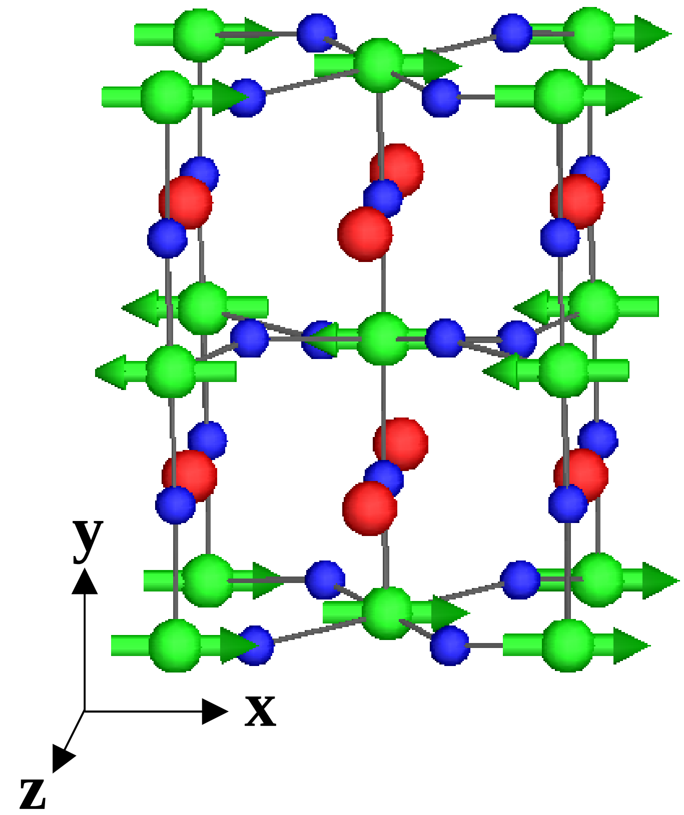
magCIF working group established in 2012.

Working group developed provisional tag set in May 2014.

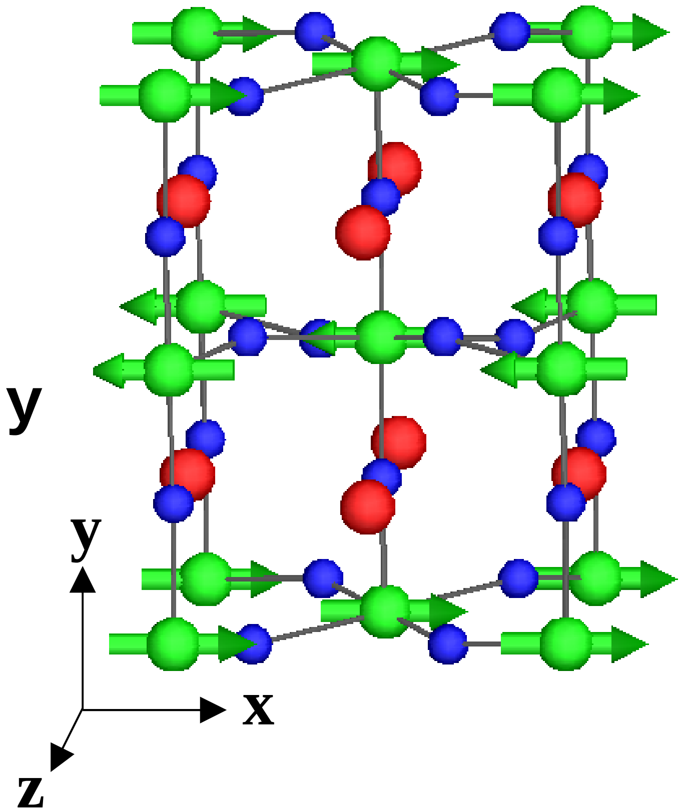
magCIF dictionary formally approved in Oct 2016.

magCIF: cell parameters

```
_cell_length_a     5.57313
_cell_length_b     7.88160
_cell_length_c     5.57313
_cell_angle_alpha 90.00000
_cell_angle_beta  90.00000
_cell_angle_gamma 90.00000
```



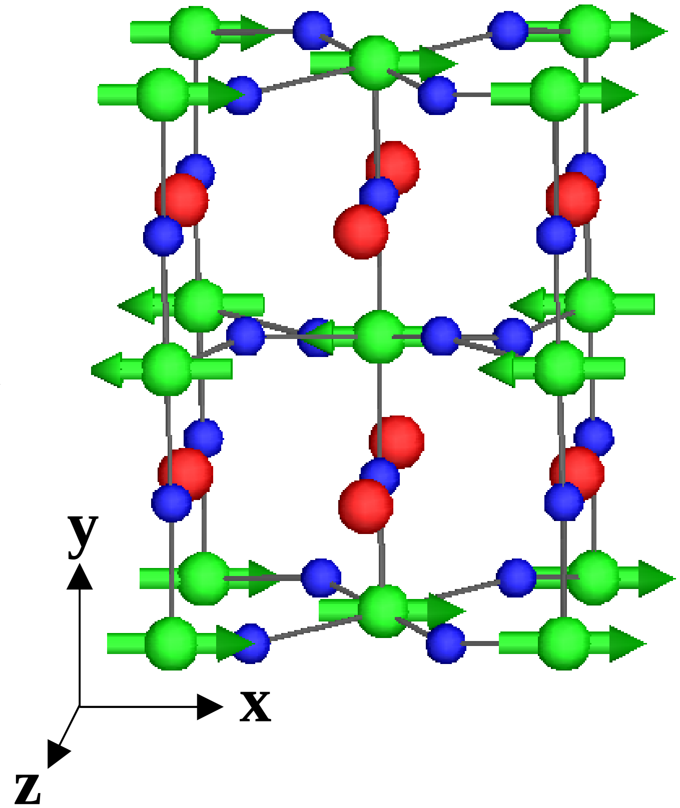
magCIF: non-magnetic parameters




```
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
La_1 La    4 c  0.50000  0.25000  0.00000  1.00000
Mn_1 Mn    4 a  0.00000  0.00000  0.00000  1.00000
O_1  O     8 d  0.75000  0.00000  0.75000  1.00000
O_2  O     4 c  0.00000  0.25000  0.00000  1.00000
```

magCIF: magnetic moments

```
loop_
_atom_site_moment.label
_atom_site_moment.crystalaxis_x
_atom_site_moment.crystalaxis_y
_atom_site_moment.crystalaxis_z
Mn_1  3.87000  0.00000  0.00000
```

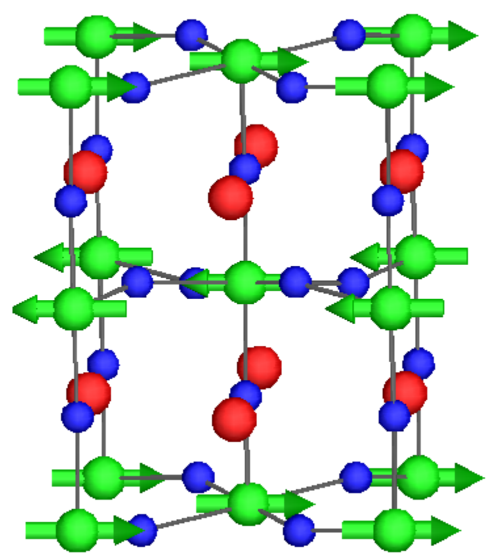


Convey only the magnetic moments of symmetry-unique atoms; the magnetic symmetry operations provide the other moments.

The "crystal axis" coordinate system presents the projections of the moment onto the three lattice directions: $m_x = \vec{m} \cdot (\vec{a}/a)$. This works in non-orthogonal coordinate systems.

magCIF: magnetic space group (MSG)

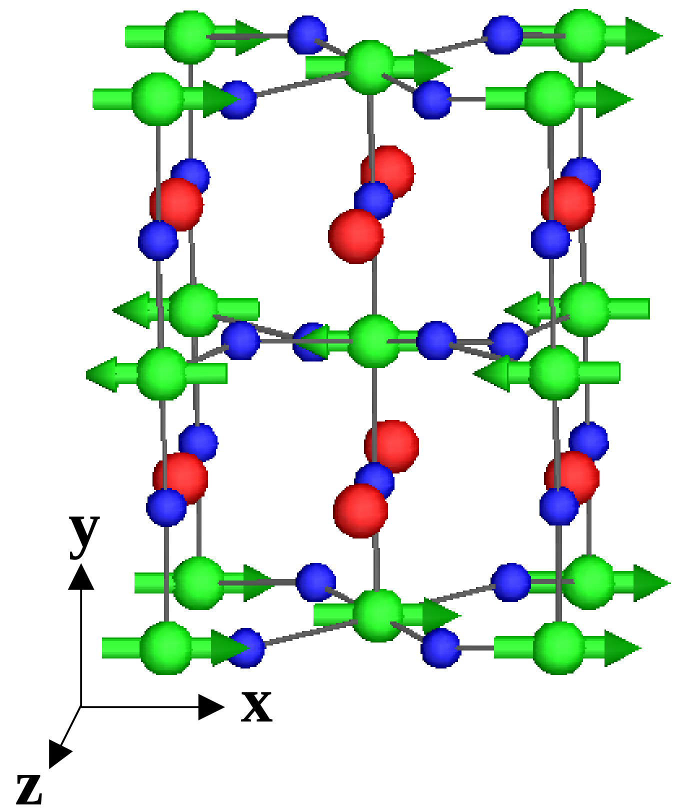
```
_space_group_magn.number_BNS     62.448
_space_group_magn.number_OG      62.8.509
_space_group_magn.name_BNS       Pn'ma'
_space_group_magn.name_OG        Pn'ma'
_space_group_magn.point_group    m'm'm
```



magCIF: MSG symmetry elements

62.448 *Pn'ma'*

```
loop_
_space_group_symop_magn_operation.id
_space_group_symop_magn_operation.xyz
1 x,y,z,+1
2 -x,y+1/2,-z,+1
3 -x,-y,-z,+1
4 x,-y+1/2,z,+1
5 x+1/2,-y+1/2,-z+1/2,-1
6 -x+1/2,-y,z+1/2,-1
7 -x+1/2,y+1/2,z+1/2,-1
8 x+1/2,y,-z+1/2,-1
```



n‘(7) *m*(4) *a*‘(8)

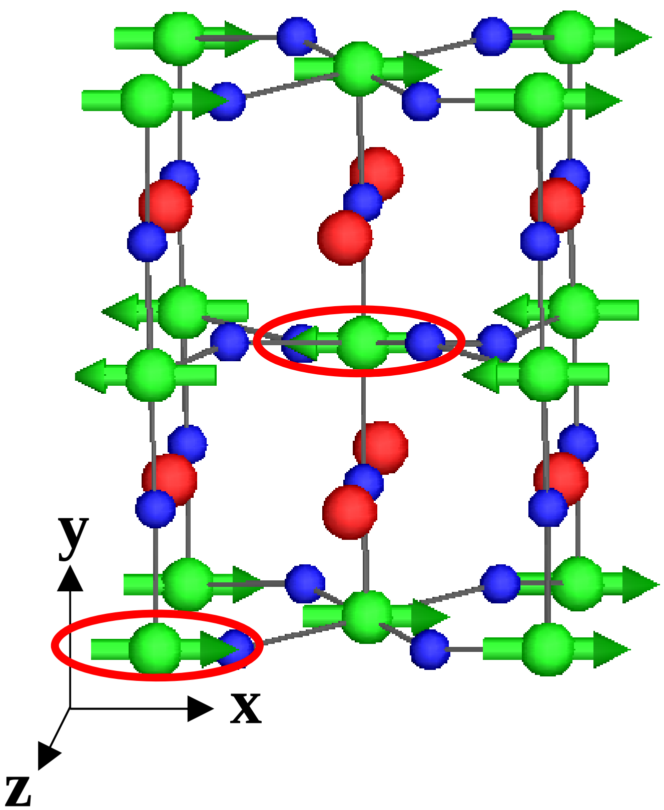
MSG symmetry elements

62.448 *Pn'ma'*

n′ ⊥ *a*

-x+1/2,y+1/2,z+1/2,-1

-mx,my,mz



$$R = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \text{ and } v = \begin{pmatrix} 1/2 \\ 1/2 \\ 1/2 \end{pmatrix}$$

$$|R| = -1 \quad \text{and} \quad \theta = -1$$

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = R \cdot \begin{pmatrix} x \\ y \\ z \end{pmatrix} + v = \begin{pmatrix} -x + 1/2 \\ y + 1/2 \\ z + 1/2 \end{pmatrix}$$

$$\begin{pmatrix} m_x{}' \\ m_y{}' \\ m_z{}' \end{pmatrix} = \theta |R| R \cdot \begin{pmatrix} m_x \\ m_y \\ m_z \end{pmatrix} = \begin{pmatrix} -m_x \\ m_y \\ m_z \end{pmatrix}$$

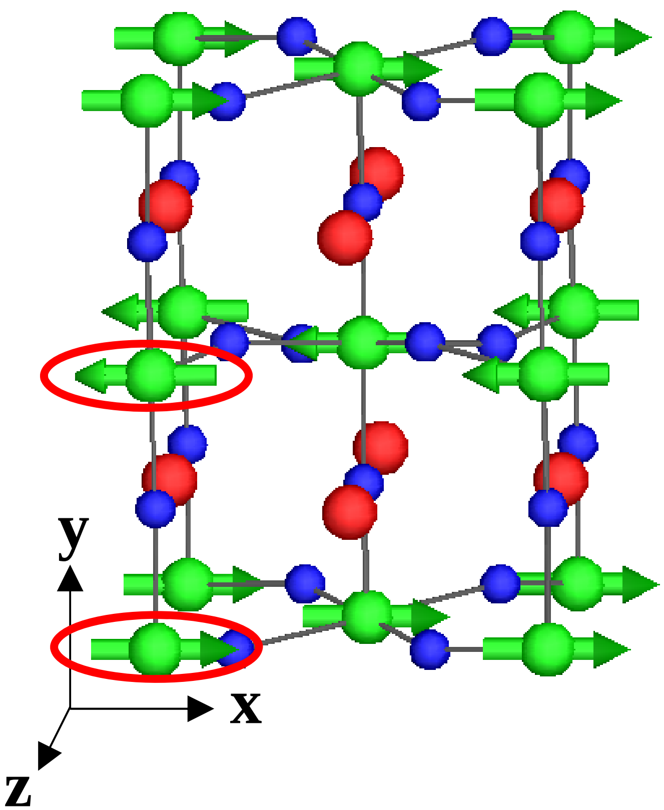
MSG symmetry elements

62.448 *Pn'ma'*

m* ⊥ *b

x,-y+1/2,z,+1

-mx,my,-mz



$$R = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \text{ and } v = \begin{pmatrix} 0 \\ 1/2 \\ 0 \end{pmatrix}$$

$$|R| = -1 \quad \text{and} \quad \theta = +1$$

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = R \cdot \begin{pmatrix} x \\ y \\ z \end{pmatrix} + v = \begin{pmatrix} x \\ -y + 1/2 \\ z \end{pmatrix}$$

$$\begin{pmatrix} m_x' \\ m_y' \\ m_z' \end{pmatrix} = \theta |R| R \cdot \begin{pmatrix} m_x \\ m_y \\ m_z \end{pmatrix} = \begin{pmatrix} -m_x \\ m_y \\ -m_z \end{pmatrix}$$

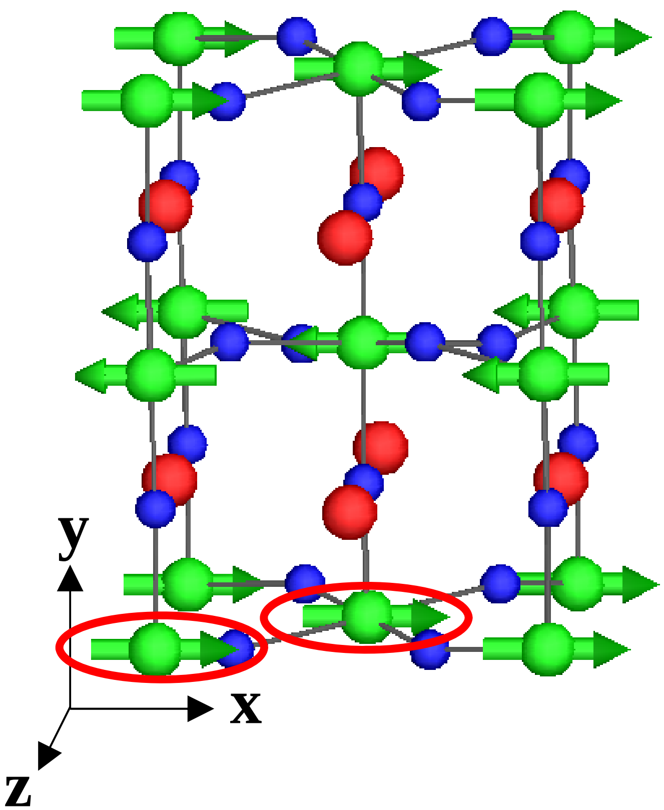
MSG symmetry elements

62.448 *Pn'ma'*

$a' \perp c$

x+1/2,y,-z+1/2,-1

mx,my,-mz



$$R = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \text{ and } v = \begin{pmatrix} 1/2 \\ 0 \\ 1/2 \end{pmatrix}$$

$$|R| = -1 \quad \text{and} \quad \theta = -1$$

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = R \cdot \begin{pmatrix} x \\ y \\ z \end{pmatrix} + v = \begin{pmatrix} x + 1/2 \\ y \\ -z + 1/2 \end{pmatrix}$$

$$\begin{pmatrix} {m_x}' \\ {m_y}' \\ {m_z}' \end{pmatrix} = \theta |R| R \cdot \begin{pmatrix} m_x \\ m_y \\ m_z \end{pmatrix} = \begin{pmatrix} m_x \\ m_y \\ -m_z \end{pmatrix}$$

Without centering loop

20.37 C_A222_1

```
loop_
_space_group_symop_magn_operation.id
_space_group_symop_magn_operation.xyz
_space_group_symop_magn_operation.mxmymz
1 x,y,z,+1 mx,my,mz
2 x,-y,-z,+1 mx,-my,-mz
3 -x,y,-z+1/2,+1 -mx,my,-mz
4 -x,-y,z+1/2,+1 -mx,-my,mz
5 x,y+1/2,z+1/2,-1 -mx,-my,-mz
6 x+1/2,-y,-z+1/2,-1 -mx,my,mz
7 -x+1/2,y,-z,-1 mx,-my,mz
8 -x+1/2,-y,z,-1 mx,my,-mz
9 x+1/2,y+1/2,z,+1 mx,my,mz
10 x+1/2,-y+1/2,-z,+1 mx,-my,-mz
11 -x+1/2,y+1/2,-z+1/2,+1 -mx,my,-mz
12 -x+1/2,-y+1/2,z+1/2,+1 -mx,-my,mz
13 x+1/2,y,z+1/2,-1 -mx,-my,-mz
14 x,-y+1/2,-z+1/2,-1 -mx,my,mz
15 -x,y+1/2,-z,-1 mx,-my,mz
16 -x,-y+1/2,z,-1 mx,my,-mz
```

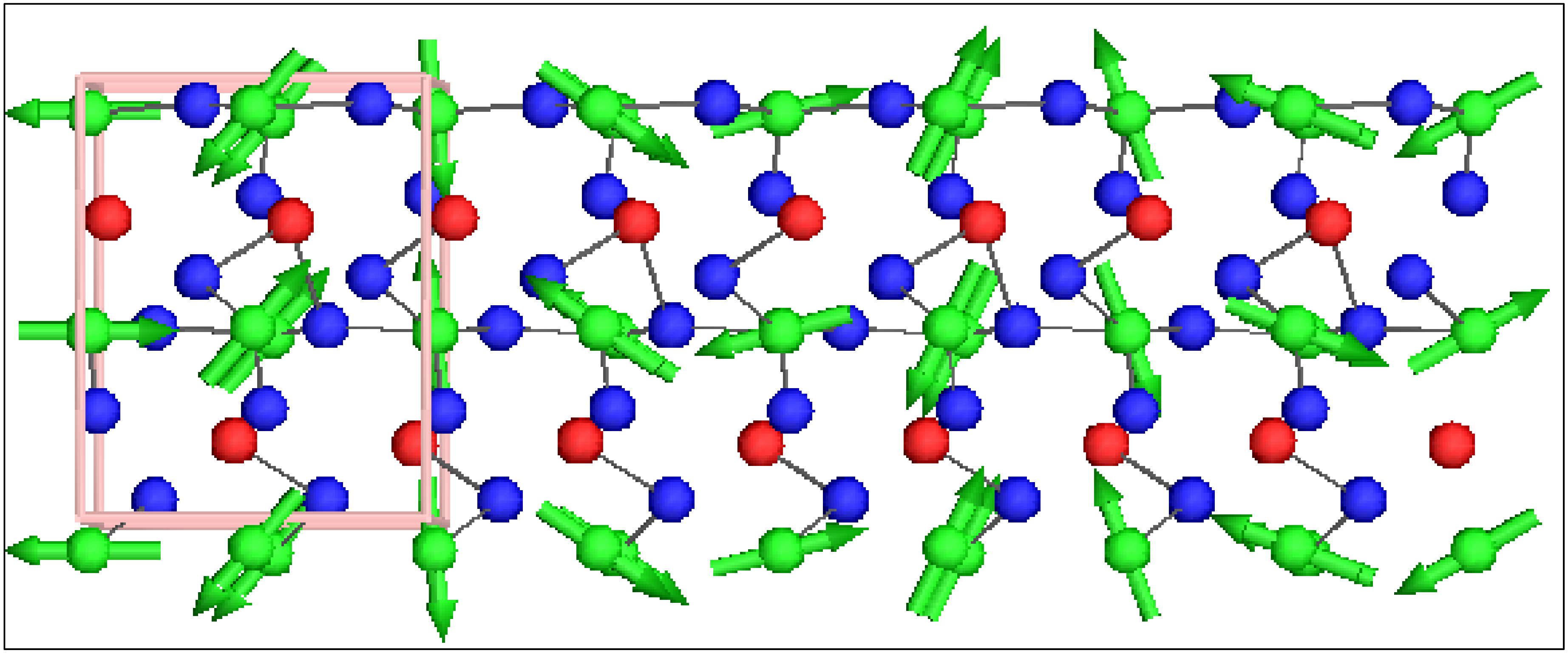
With centering loop

$20.37\ C_A222_1$

```
loop_
_space_group_symop_magn_operation.id
_space_group_symop_magn_operation.xyz
_space_group_symop_magn_operation.mxmymz
1 x,y,z,        +1  mx,my,mz
2 x,-y,-z,      +1  mx,-my,-mz
3 -x,y,-z+1/2,  +1 -mx,my,-mz
4 -x,-y,z+1/2,  +1 -mx,-my,mz

loop_
_space_group_symop_magn_centering.id
_space_group_symop_magn_centering.xyz
_space_group_symop_magn_centering.mxmymz
1 x,y,z,            +1  mx,my,mz
2 x,y+1/2,z+1/2,    -1 -mx,-my,-mz
3 x+1/2,y+1/2,z,    +1  mx,my,mz
4 x+1/2,y,z+1/2,    -1 -mx,-my,-mz
```

Incommensurate Multiferroic $TbMnO_3$

Kenzelmann et al., Phys. Rev. Lett. 95, 087206 (2005).



Incommensurate cycloidal magnetic modulation

Magnetic superspace-group: $Pna2_1 1'(a00)000s$

magCIF: incommensurate case

Magnetic superspace group (MSSG) operators

```
_space_group_magn.ssg_name_BNS   P2_1cn1'(0,0,g)000s
_space_group_magn.ssg_number_BNS 33.1.9.5.m145.?
_space_group_magn.point_group    2mm1'

loop_
_space_group_symop_magn_ssg_operation.id
_space_group_symop_magn_ssg_operation.algebraic
1 x1,x2,x3,x4,+1
2 x1+1/2,-x2,-x3,-x4,+1
3 x1+1/2,x2+1/2,-x3+1/2,-x4,+1
4 x1,-x2+1/2,x3+1/2,x4,+1

loop_
_space_group_symop_magn_ssg_centering.id
_space_group_symop_magn_ssg_centering.xyz
1 x1,x2,x3,x4,+1
2 x1,x2,x3,x4+1/2,-1
```

magCIF: incommensurate case

Basic unit cell of MSSG

```
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Tb   Tb   4 a  0.75000  -0.01640  0.91900  1.00000
Mn   Mn   4 a  0.00000   0.50000  0.00000  1.00000
O1   O    4 a  0.75000   0.10830  0.53060  1.00000
O2_1 O    4 a  0.94770   0.70850  0.67330  1.00000
O2_2 O    4 a  0.55230   0.79150  0.17330  1.00000
```

magCIF: incommensurate case

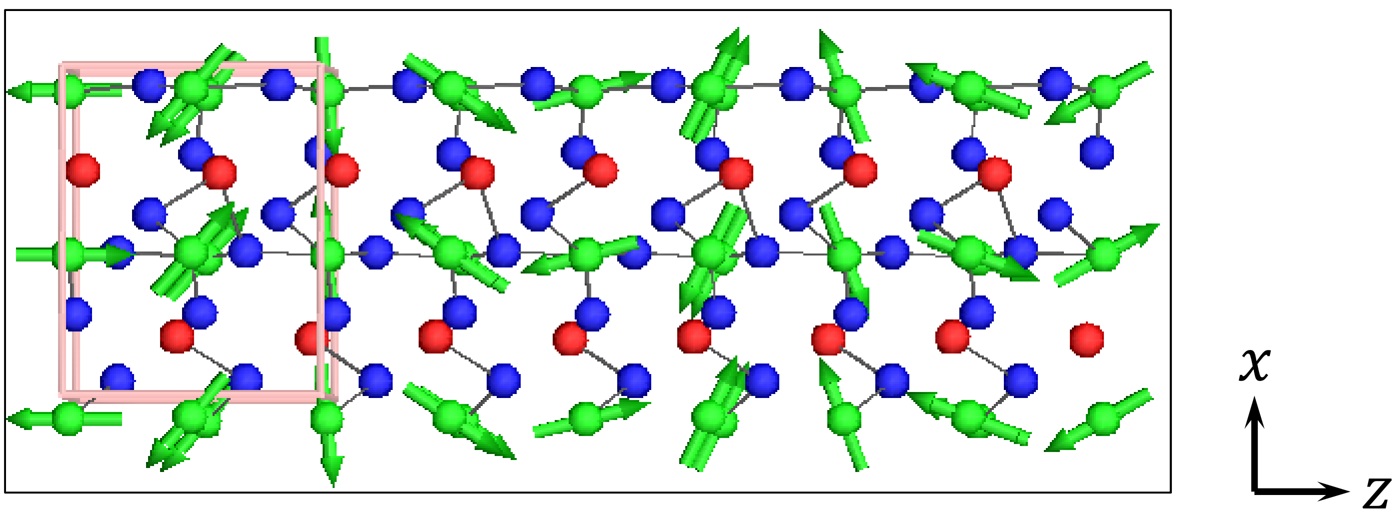
Magnetic superspace group: propagation vectors

```
_cell_modulation_dimension 1

loop_
_cell_wave_vector_seq_id
_cell_wave_vector_x
_cell_wave_vector_y
_cell_wave_vector_z
  1   0.00000   0.00000  -0.27000

loop_
_atom_site_Fourier_wave_vector_seq_id
_atom_site_Fourier_wave_vector_x
_atom_site_Fourier_wave_vector_y
_atom_site_Fourier_wave_vector_z
_atom_site_Fourier_wave_vector_q1_coeff
1    0.00000   0.00000  -0.27000  1
```

magCIF: incommensurate case

Magnetic superspace group: wave amplitudes

```
loop_
_atom_site_moment.label
_atom_site_moment.crystalaxis_x
_atom_site_moment.crystalaxis_y
_atom_site_moment.crystalaxis_z
Mn    1 x    0.00000   -3.95980
Mn    1 y    0.00000    0.00000
Mn    1 z   -5.51543    0.00000
```



magCIF: BNS vs OG settings

magCIF fully supports both BNS and OG settings.

For type-1, type-2, and type-3 magnetic space groups, the two setting are essentially identical. For type-4 magnetic space groups, the BNS cell (the true repeating unit) is twice the size of the OG cell. When the unit cell doubles relative to the parent, the OG cell matches the parent cell, which can be convenient.

The magCIF implementation of BNS and OG settings is always different. With BNS, explicitly give the time-reversal component for translation generators. With OG, give only the propagation vector $\boldsymbol{k}_p$ and let the reader calculate the time-reversal component of any translation.

$$e^{2\pi i \boldsymbol{k}_p \cdot \boldsymbol{T}} = \pm 1 \quad (-1 \text{ is time reversed, } +1 \text{ is normal})$$

magCIF: reference settings

When two presentations of the same magnetic space group or magnetic superspace group employ different settings, it's not a trivial exercise to determine that they are equivalent or to find the transformation from one to the other. When publishing a magnetic structure, *always* list your symmetry operators, and *always* give a transformation to a reference settings.

```
_space_group_magn.transform_BNS_Pp_abc '-a-c,-b,c;0,0,0'
_space_group_magn.transform_OG_Pp_abc  '-a-c,-b,1/2c;0,0,0'

loop_
_space_group_magn_ssg_transforms.id
_space_group_magn_ssg_transforms.Pp_superspace
_space_group_magn_ssg_transforms.source
1  'a1,-a3,a2,a4;0,0,0,0'  'ISO(3+d)D'
2  'a1,-a3,a2,a4;0,0,0,0'  'ISOMAG-ISO(3+d)D'
```

magCIF: reference settings

$(\boldsymbol{a}_r, \boldsymbol{b}_r, \boldsymbol{c}_r)$ and $\boldsymbol{o}_r$ are the basis and origin of the reference setting.
$(\boldsymbol{a}_c, \boldsymbol{b}_c, \boldsymbol{c}_c)$ and $\boldsymbol{o}_c$ are the basis and origin of the reference setting.

Interpretation of `'-a-c,-b,c;1/4,0,1/2'`:

$(\boldsymbol{a}_r, \boldsymbol{b}_r, \boldsymbol{c}_r) = (-\boldsymbol{a}_c - \boldsymbol{c}_c, -\boldsymbol{b}_c, \boldsymbol{c}_c)$ and $\boldsymbol{o}_r = \boldsymbol{o}_c + \left(\frac{1}{4}, 0, \frac{1}{2}\right)$

magCIF: parent symmetry and setting

```
_parent_space_group.name_H-M_alt   ‘Fd-3m‘
_parent_space_group.IT_number   227
_parent_space_group.transform_Pp_abc
                                  'a,b,c;1/8,1/8,1/8‘
_parent_space_group.child_transform_Pp_abc
                                  'a/2+b/2,a/2-b/2,c;0,0,0‘

loop_
_parent_propagation_vector.id
_parent_propagation_vector.kxkykz
k1 [0.5 0.50 0.00]
```

magCIF implementation progress (2016)

JANA [C, I]
Now: magCIF (r&w), magsuperCIF (r&w)

FULLPROF [C, I]
Now: magCIF (r&w)
Future: magsuperCIF (r&w)

VESTA [C]
Now: magCIF (r)
Future: magCIF(w)

JMOL [C, I]
Now: magCIF (r), magsuperCIF (r)

Bilbao Crystallographic Server [C,I]
Now: magCIF (r,w), magsuperCIF (w)

ISOCIF [C]
Now: magCIF (r&w)
Future: magsuperCIF (r&w)

ISODISTORT [C, I]
Now: magCIF (r&w), magsuperCIF (w)

TOPAS Academic [C]
Future: magCIF (r&w)

GSAS-2 [C]
Now: magnetic capabilities planned
Future: magCIF (r&w)

C = commensurate, I = incommensurate, r = read, w = write

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