The new magCIF format for communicating magnetic structures

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The role of magnetic symmetry in describing/determining 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.

Use of magCIF slowly expanded through 2013.

CMS working group developed provisional tag set in 2014.

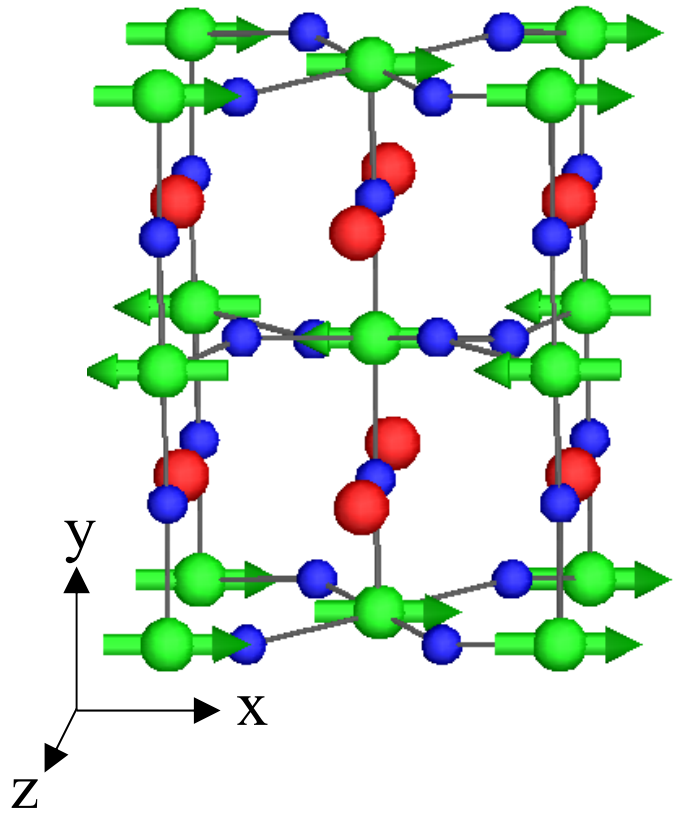
Formal magCIF dictionary should be completed in 2014.

magCIF

- **Supercell**: moments and magnetic space group
- **Wave**: incommens *k*-vectors, complex amplitudes, and magnetic superspace group.
- **Irrep-mode**: *k*-vectors, irreps, and mode amplitudes.

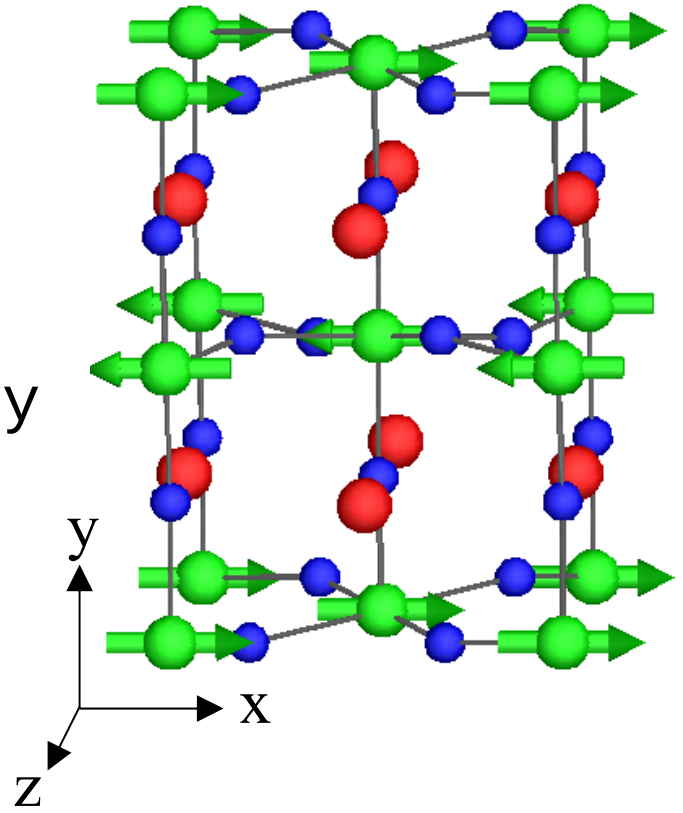
magCIF: cell parameters

```
_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
```



In a BNS setting, this is the actual magnetic repeating unit.
In an OG setting, this is half the actual magnetic repeating unit.

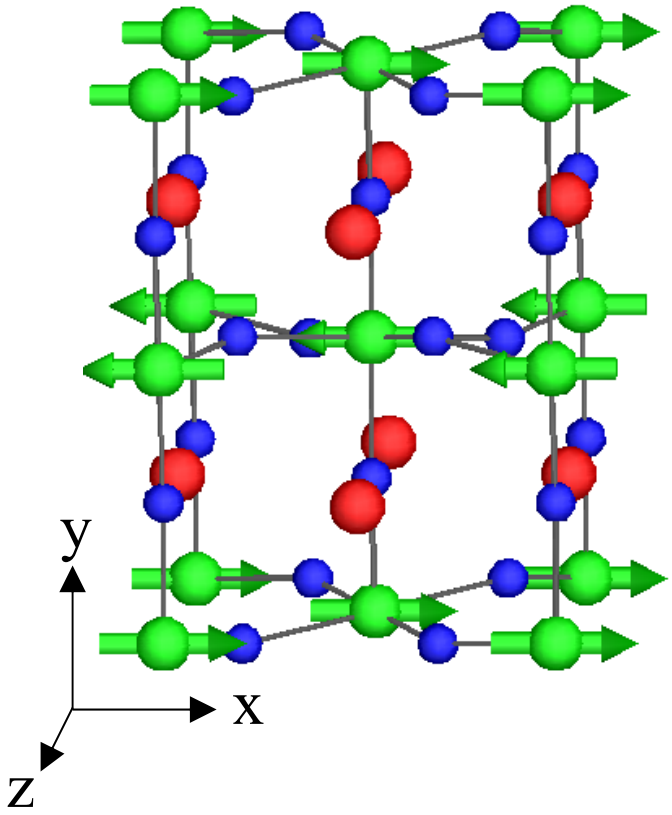
magCIF: non-magnetic parameters




```
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
```

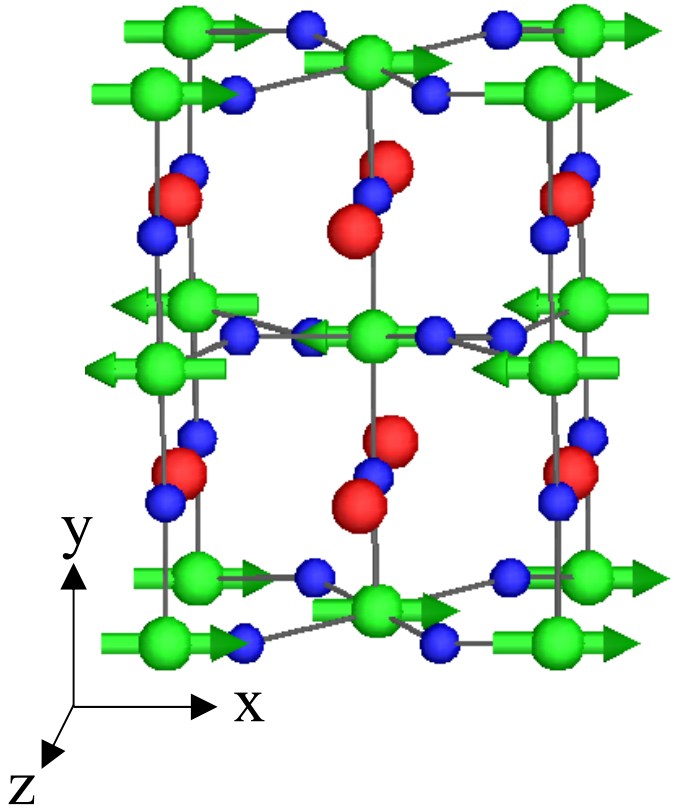
magCIF: magnetic space group (MSG)

```
_space_group.magn_number_BNS "62.448“
_space_group.magn_name_BNS "Pn'ma'“
_space_group.magn_point_group "m'm'm"
```



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
```

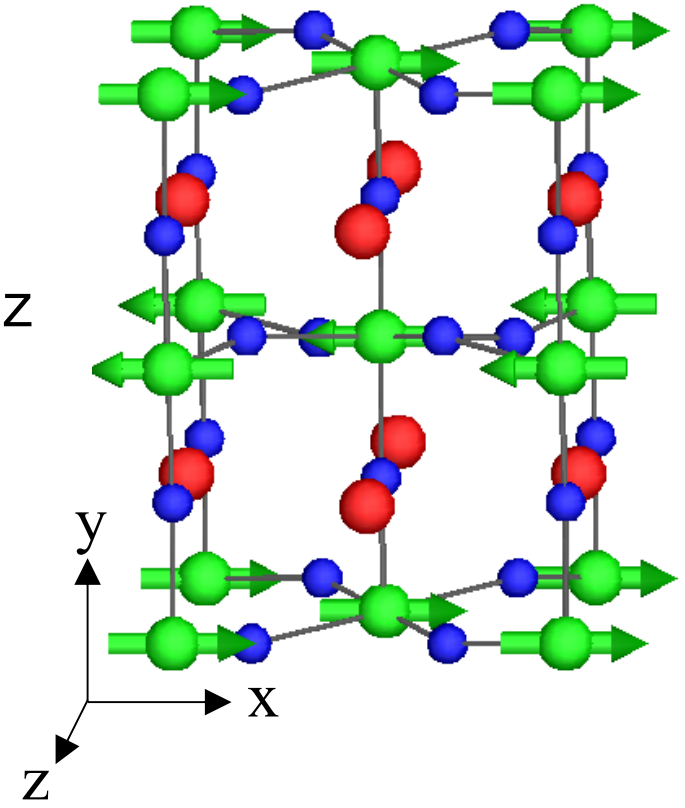


The “crystal axis” coordinate system presents the projections of the moment onto the three lattice directions: $m_x = \vec{\boldsymbol{m}} \cdot (\vec{\boldsymbol{a}}/a)$. This works in non-orthogonal coordinate systems.

magCIF: MSG symmetry elements

62.448 *Pn'ma'*

```
loop_
_space_group_symop.magn_id
_space_group_symop.magn_operation_xyz
_space_group_symop.magn_operation_mxmymz
1 x,y,z,+1 mx,my,mz
2 -x,y+1/2,-z,+1 -mx,my,-mz
3 -x,-y,-z,+1 mx,my,mz
4 x,-y+1/2,z,+1 -mx,my,-mz
5 x+1/2,-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+1/2,z+1/2,-1 -mx,my,mz
8 x+1/2,y,-z+1/2,-1 mx,my,-mz
```



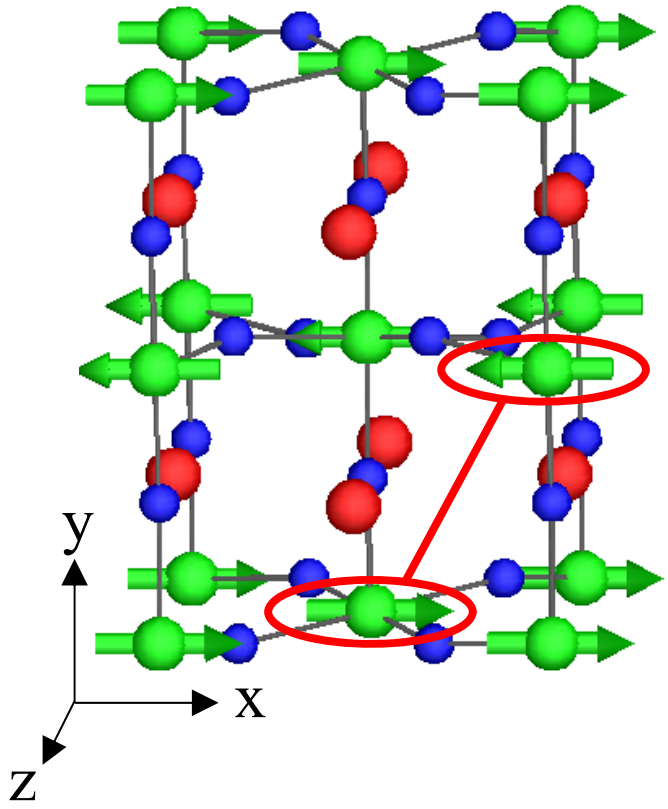
$n'(7)\ \ m(4)\ \ a'(8)$

magCIF: MSG symmetry elements

62.448 $Pn'ma'$

$n' \perp a$

```
-x+1/2,y+1/2,z+1/2,-1
-mx,my,mz
```



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

$$|P| = -1$$

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = P \cdot \begin{pmatrix} x \\ y \\ z \end{pmatrix} + t = \begin{pmatrix} -x + 1/2 \\ y + 1/2 \\ z + 1/2 \end{pmatrix}$$

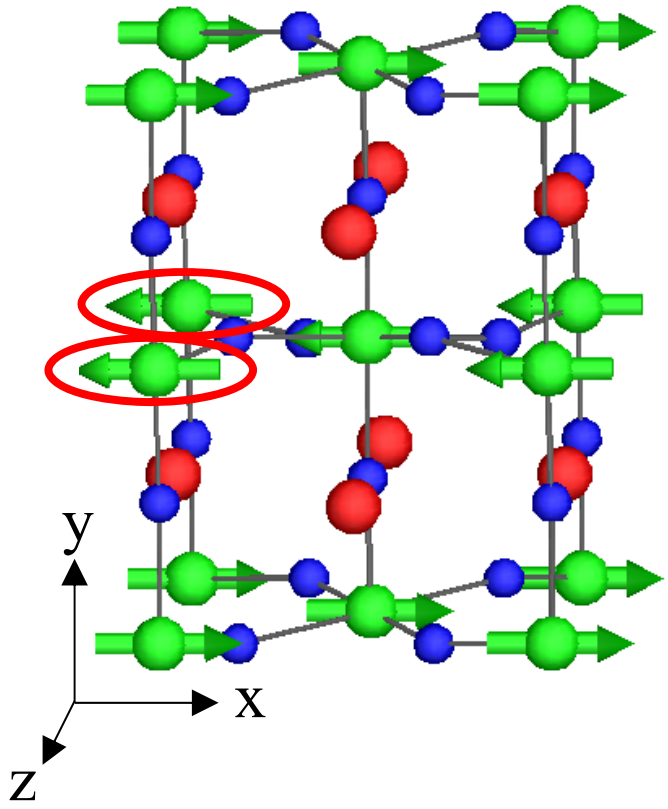
$$\begin{pmatrix} m_x' \\ m_y' \\ m_z' \end{pmatrix} = (-1)|P|P \cdot \begin{pmatrix} m_x \\ m_y \\ m_z \end{pmatrix} = \begin{pmatrix} -m_x \\ m_y \\ m_z \end{pmatrix}$$

magCIF: MSG symmetry elements

62.448 *Pn'ma'*

m ⊥ ***b***

```
x,-y+1/2,z,+1
-mx,my,-mz
```



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

$$|P| = -1$$

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = P \cdot \begin{pmatrix} x \\ y \\ z \end{pmatrix} + t = \begin{pmatrix} x \\ -y + 1/2 \\ z \end{pmatrix}$$

$$\begin{pmatrix} m_x{}' \\ m_y{}' \\ m_z{}' \end{pmatrix} = (+1)|P|P \cdot \begin{pmatrix} m_x \\ m_y \\ m_z \end{pmatrix} = \begin{pmatrix} -m_x \\ m_y \\ -m_z \end{pmatrix}$$

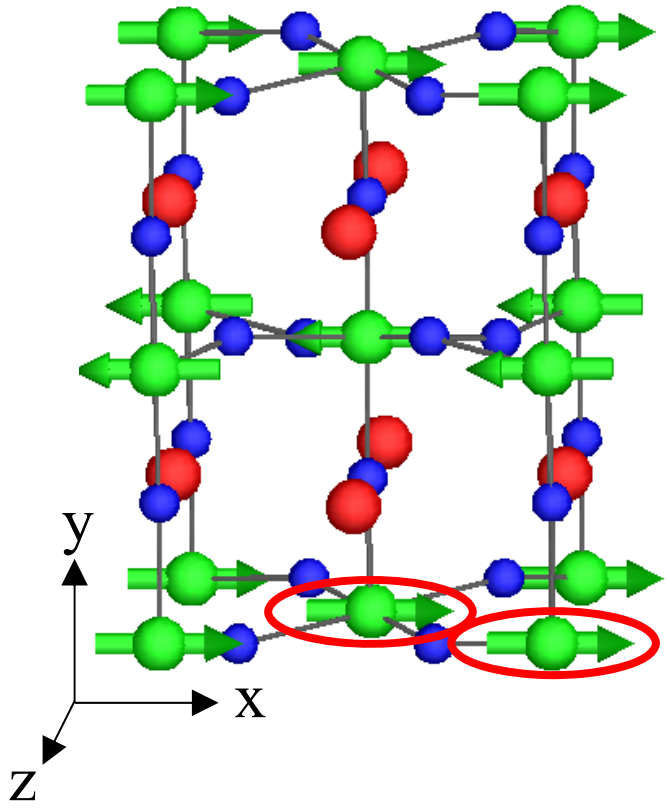
magCIF: MSG symmetry elements

62.448 *Pn'ma'*

$a' \perp c$

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

mx,my,-mz



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

$$|P| = -1$$

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = P \cdot \begin{pmatrix} x \\ y \\ z \end{pmatrix} + t = \begin{pmatrix} x + 1/2 \\ y \\ -z + 1/2 \end{pmatrix}$$

$$\begin{pmatrix} m_x' \\ m_y' \\ m_z' \end{pmatrix} = (-1)|P|P \cdot \begin{pmatrix} m_x \\ m_y \\ m_z \end{pmatrix} = \begin{pmatrix} m_x \\ m_y \\ -m_z \end{pmatrix}$$

Magnetic Wyckoff coordinates

BNS: 62.448 OG: 62.8.509 *Pn'ma'*

8d	$(x, y, z)(m_x, m_y, m_z)$	$(x+½, \bar{y}+½, \bar{z}+½)(\bar{m}_x, m_y, m_z)$
	$(\bar{x}, y+½, \bar{z})(\bar{m}_x, m_y, \bar{m}_z)$	$(\bar{x}+½, \bar{y}, z+½)(m_x, m_y, \bar{m}_z)$
	$(\bar{x}, \bar{y}, \bar{z})(m_x, m_y, m_z)$	$(\bar{x}+½, y+½, z+½)(\bar{m}_x, m_y, m_z)$
	$(x, \bar{y}+½, z)(\bar{m}_x, m_y, \bar{m}_z)$	$(x+½, y, \bar{z}+½)(m_x, m_y, \bar{m}_z)$
4c	$(x, ¼, z)(0, m_y, 0)$	$(x+½, ¼, \bar{z}+½)(0, m_y, 0)$
	$(\bar{x}, ¾, \bar{z})(0, m_y, 0)$	$(\bar{x}+½, ¾, z+½)(0, m_y, 0)$
4b	$(0,0,½)(m_x, m_y, m_z)$	$(½, ½, 0)(\bar{m}_x, m_y, m_z)$
	$(0, ½, ½)(\bar{m}_x, m_y, \bar{m}_z)$	$(½, 0,0)(m_x, m_y, \bar{m}_z)$
4a	$(0,0,0)(m_x, m_y, m_z)$	$(½, ½, ½)(\bar{m}_x, m_y, m_z)$
	$(0, ½, 0)(\bar{m}_x, m_y, \bar{m}_z)$	$(½, 0, ½)(m_x, m_y, \bar{m}_z)$

Magnetic space-group types 1-4

Examples based on *P*2/*m*

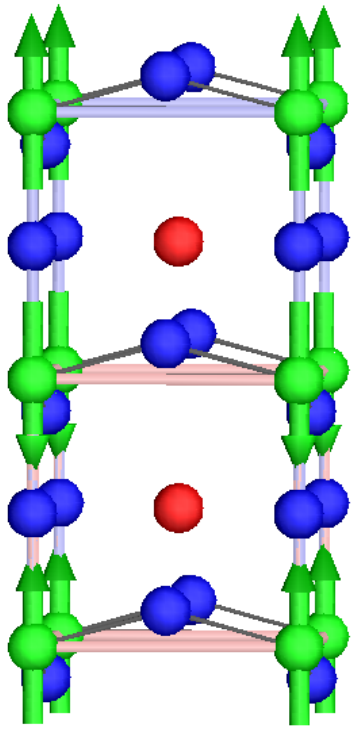
Type-1 MSG
Federov group
10.42 (10.1.49) $P2/m$
(x, y, z)
$(-x, y, -z)$
$(-x, -y, -z)$
$(x, -y, z)$

Type-2 MSG
gray group
10.43 (10.2.50) $P2/m1'$
(x, y, z)
$(-x, y, -z)$
$(-x, -y, -z)$
$(x, -y, z)$
$(x, y, z)'$
$(-x, y, -z)'$
$(-x, -y, -z)'$
$(x, -y, z)'$

Type-4 MSG
black/white lattice
BNS: 10.48 P_b2/m
OG: 10.7.55 $P_{2b}2/m$
(x, y, z)
$(-x, y, -z)$
$(-x, -y, -z)$
$(x, -y, z)$
$(x, y + 1/2, z)'$
$(-x, y + 1/2)'$
$(-x, -y + 1/2)'$
$(x, -y + 1/2, z)'$

Type-3 MSG
black/white PG
10.44 (10.3.51) $P2'/m$
(x, y, z)
$(-x, y, -z)'$
$(-x, -y, -z)'$
$(x, -y, z)$

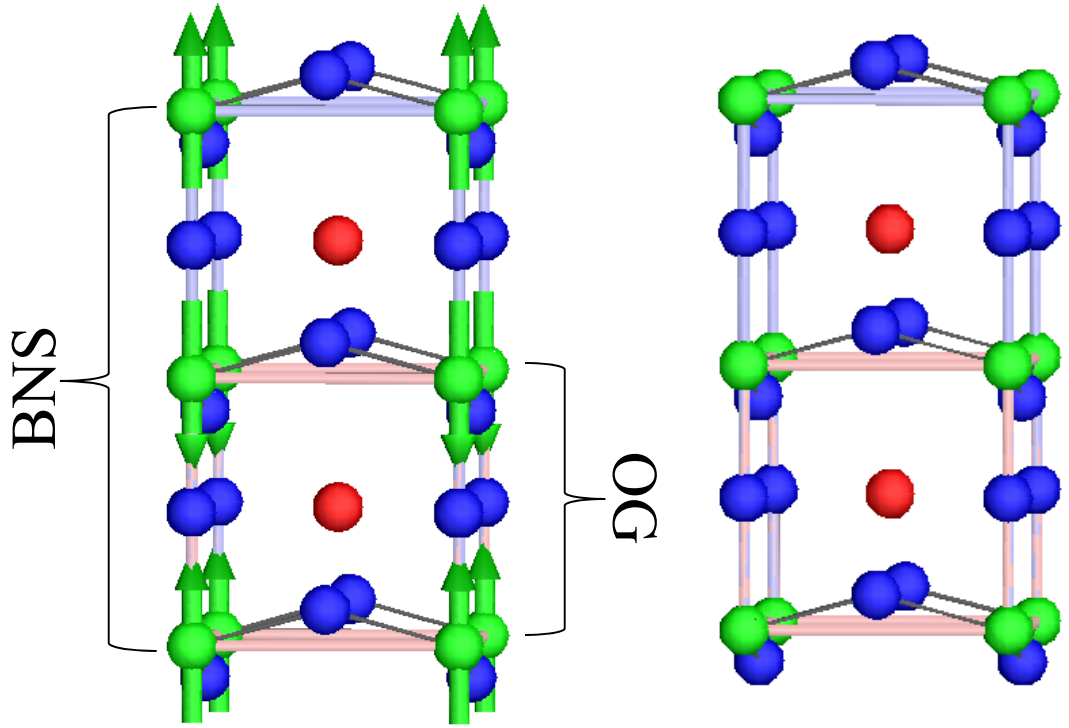
magCIF: BNS vs OG cell



```
_space_group.magn_number_BNS "116.296“
_space_group.magn_name_BNS "P_c-4c2“
_space_group.magn_point_group "-4m21'"

loop_
_space_group_transform_id
_space_group_transform_Pp_abc
_space_group_transform_description
1 a,b,c;0,0,0
      "to magnetic BNS, ISO P_c-4c2 setting“
2 a,b,1/2c;0,0,1/2
      "to magnetic OG, Litvin P_2c-4'm'2 setting"
```

BNS: $P_c\bar{4}c2$ OG: $P_{2c}\bar{4}'m'2$ Mod: $P\bar{4}c21'_c$

BNS vs OG cell of type-4 MSG



Magnetic order lowers the symmetry relative to non-magnetic parent.

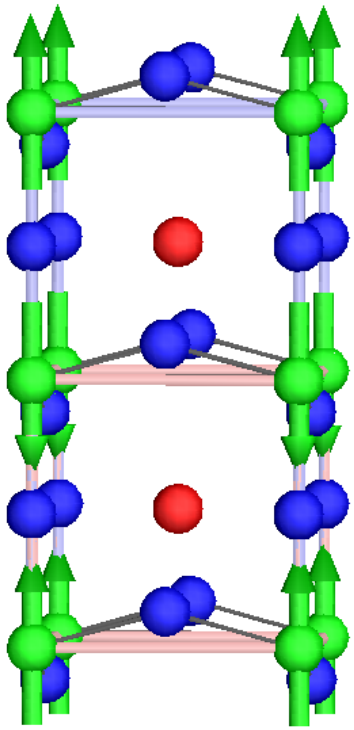
Non-magnetic degrees of freedom (e.g. displacements) also arise.

If we zero the moments, the resulting non-magnetic cell is OG cell.

magCIF: operators of type-4 MSG

116.296 $P_C\bar{4}c2$

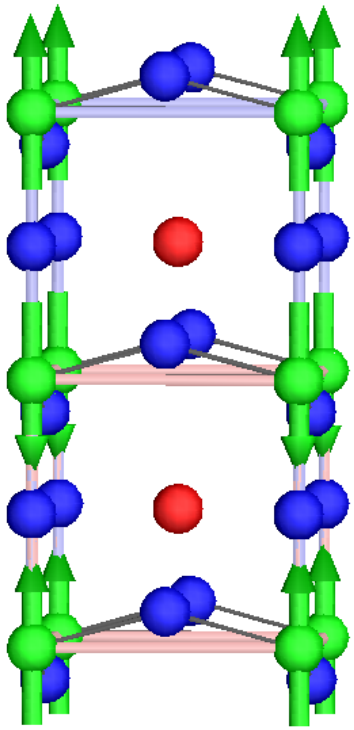
```
loop_
_space_group_symop.magn_id
_space_group_symop.magn_operation_xyz
_space_group_symop.magn_operation_mxmymz
1 x,y,z,+1 mx,my,mz
2 -x,-y,z,+1 -mx,-my,mz
3 -y,-x,-z+1/2,+1 -my,-mx,-mz
4 y,x,-z+1/2,+1 my,mx,-mz
5 -x,y,z+1/2,+1 mx,-my,-mz
6 x,-y,z+1/2,+1 -mx,my,-mz
7 y,-x,-z,+1 -my,mx,mz
8 -y,x,-z,+1 my,-mx,mz
9 x,y,z+1/2,-1 -mx,-my,-mz
10 -x,-y,z+1/2,-1 mx,my,-mz
11 -y,-x,-z,-1 my,mx,mz
12 y,x,-z,-1 -my,-mx,mz
13 -x,y,z,-1 -mx,my,mz
14 x,-y,z,-1 mx,-my,mz
15 y,-x,-z+1/2,-1 my,-mx,-mz
16 -y,x,-z+1/2,-1 -my,mx,-mz
```



magCIF: operators of type-4 MSG

116.296 $P_C\bar{4}c2$

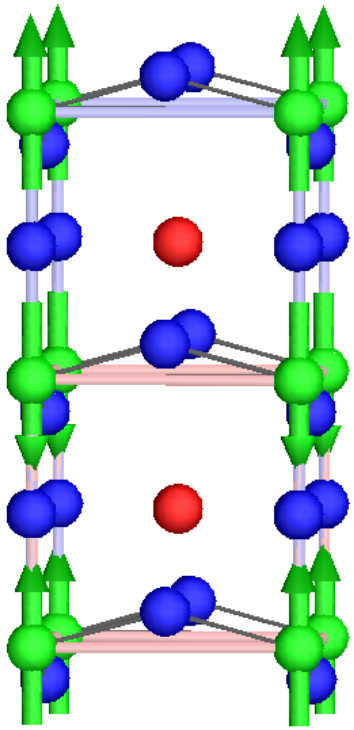
```
loop_
_space_group_symop.magn_id
_space_group_symop.magn_operation_xyz
_space_group_symop.magn_operation_mxmymz
1 x,y,z,+1 mx,my,mz
2 -x,-y,z,+1 -mx,-my,mz
3 -y,-x,-z+1/2,+1 -my,-mx,-mz
4 y,x,-z+1/2,+1 my,mx,-mz
5 -x,y,z+1/2,+1 mx,-my,-mz
6 x,-y,z+1/2,+1 -mx,my,-mz
7 y,-x,-z,+1 -my,mx,mz
8 -y,x,-z,+1 my,-mx,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,z+1/2,-1 -mx,-my,-mz
```



magCIF: operators of type-4 MSG

116.296 $P_C\bar{4}c2$

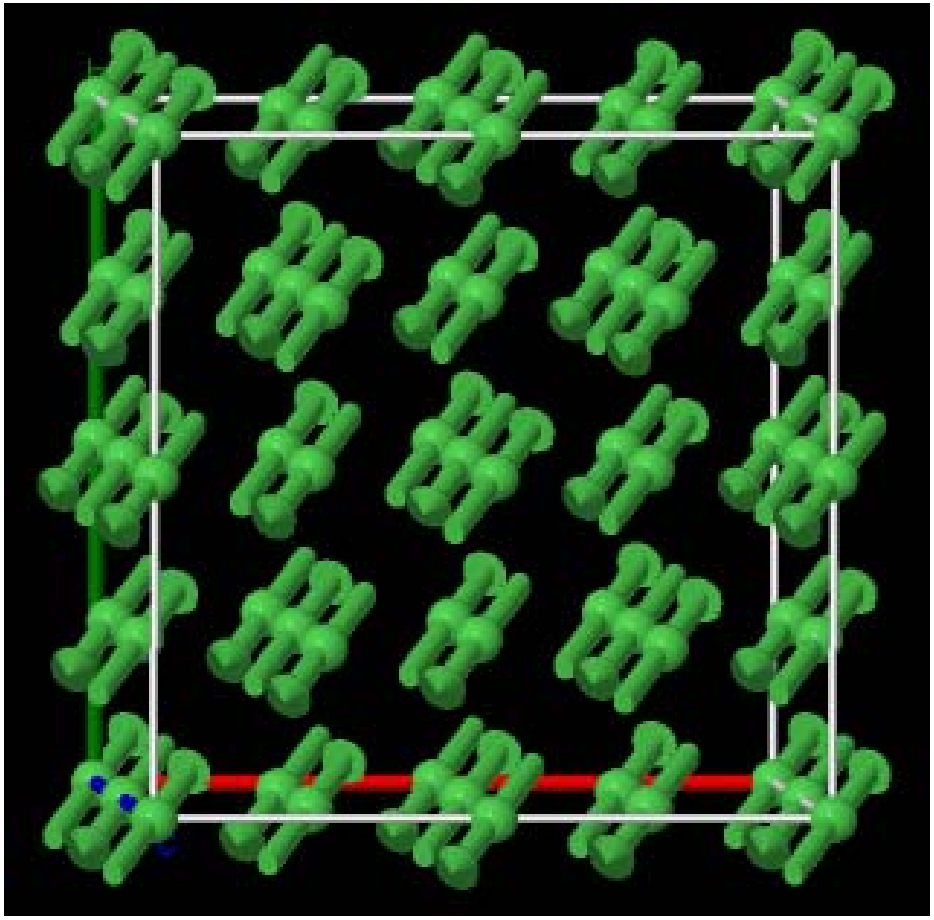
```
loop_
_space_group_symop.magn_id
_space_group_symop.magn_operation_xyz
_space_group_symop.magn_operation_mxmymz
1 x,y,z,+1 mx,my,mz
2 -x,-y,z,+1 -mx,-my,mz
3 -y,-x,-z+1/2,+1 -my,-mx,-mz
4 y,x,-z+1/2,+1 my,mx,-mz
5 -x,y,z+1/2,+1 mx,-my,-mz
6 x,-y,z+1/2,+1 -mx,my,-mz
7 y,-x,-z,+1 -my,mx,mz
8 -y,x,-z,+1 my,-mx,mz

loop_
_space_group_symop.magn_kvec_id
_space_group_symop.magn_kvec_xyz
1 0,0,0
2 0,0,1/2
```



magCIF: separate centering loop

(NiO in non-standard setting)

```
loop_
_space_group_symop.magn_id
_space_group_symop.magn_operation_xyzR
_space_group_symop.magn_operation_mxmymz
1 x,y,z,+1 mx,my,mz
2 -y+3/4,-x+3/4,-z,+1 -my,-mx,-mz
3 -x+3/4,-y+1/4,-z,+1 mx,my,mz
4 y+1/2,x,z,+1 -my,-mx,-mz
5 x+3/4,y+3/4,z,-1 -mx,-my,-mz
6 -y,-x,-z,-1 my,mx,mz
7 -x+1/2,-y,-z,-1 -mx,-my,-mz
8 y+3/4,x+1/4,z,-1 my,mx,mz
9 x,y+1/4,z+3/4,+1 mx,my,mz
10 -y+3/4,-x,-z+3/4,+1 -my,-mx,-mz
11 -x+3/4,-y+1/2,-z+3/4,+1 mx,my,mz
12 y+1/2,x+1/4,z+3/4,+1 -my,-mx,-mz
13 x+3/4,y,z+3/4,-1 -mx,-my,-mz
14 -y,-x+1/4,-z+3/4,-1 my,mx,mz
15 -x+1/2,-y+1/4,-z+3/4,-1 -mx,-my,-mz
16 y+3/4,x+1/2,z+3/4,-1 my,mx,mz
17 x,y+1/2,z+1/2,+1 mx,my,mz
18 -y+3/4,-x+1/4,-z+1/2,+1 -my,-mx,-mz
19 -x+3/4,-y+3/4,-z+1/2,+1 mx,my,mz
20 y+1/2,x+1/2,z+1/2,+1 -my,-mx,-mz
21 x+3/4,y+1/4,z+1/2,-1 -mx,-my,-mz
22 -y,-x+1/2,-z+1/2,-1 my,mx,mz
23 -x+1/2,-y+1/2,-z+1/2,-1 -mx,-my,-mz
24 y+3/4,x+3/4,z+1/2,-1 my,mx,mz
25 x,y+3/4,z+1/4,+1 mx,my,mz
26 -y+3/4,-x+1/2,-z+1/4,+1 -my,-mx,-mz
27 -x+3/4,-y,-z+1/4,+1 mx,my,mz
28 y+1/2,x+3/4,z+1/4,+1 -my,-mx,-mz
29 x+3/4,y+1/2,z+1/4,-1 -mx,-my,-mz
30 -y,-x+3/4,-z+1/4,-1 my,mx,mz
31 -x+1/2,-y+3/4,-z+1/4,-1 -mx,-my,-mz
32 y+3/4,x,z+1/4,-1 my,mx,mz
```

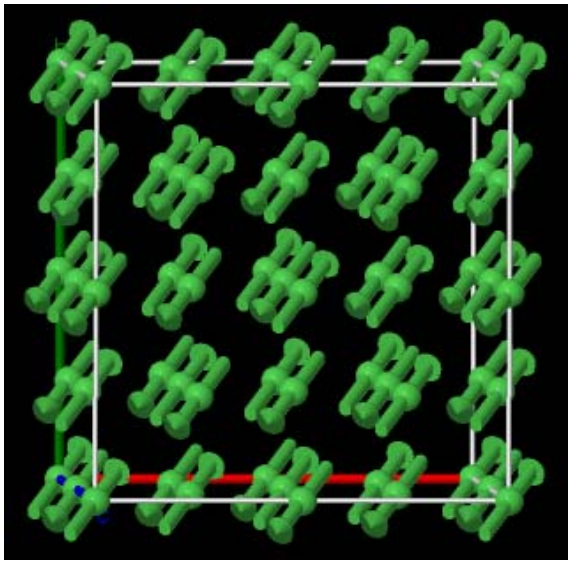


```
97 x+3/4,y,z+1/4,+1 mx,my,mz
98 -y+1/2,-x+3/4,-z+1/4,+1 -my,-mx,-mz
99 -x+1/2,-y+1/4,-z+1/4,+1 mx,my,mz
100 y+1/4,x,z+1/4,+1 -my,-mx,-mz
101 x+1/2,y+3/4,z+1/4,-1 -mx,-my,-mz
102 -y+3/4,-x,-z+1/4,-1 my,mx,mz
103 -x+1/4,-y,-z+1/4,-1 -mx,-my,-mz
104 y+1/2,x+1/4,z+1/4,-1 my,mx,mz
105 x+3/4,y+1/4,z,+1 mx,my,mz
106 -y+1/2,-x,-z,+1 -my,-mx,-mz
107 -x+1/2,-y+1/2,-z,+1 mx,my,mz
108 y+1/4,x+1/4,z,+1 -my,-mx,-mz
109 x+1/2,y,z,-1 -mx,-my,-mz
110 -y+3/4,-x+1/4,-z,-1 my,mx,mz
111 -x+1/4,-y+1/4,-z,-1 -mx,-my,-mz
112 y+1/2,x+1/2,z,-1 my,mx,mz
113 x+3/4,y+1/2,z+3/4,+1 mx,my,mz
114 -y+1/2,-x+1/4,-z+3/4,+1 -my,-mx,-mz
115 -x+1/2,-y+3/4,-z+3/4,+1 mx,my,mz
116 y+1/4,x+1/2,z+3/4,+1 -my,-mx,-mz
117 x+1/2,y+1/4,z+3/4,-1 -mx,-my,-mz
118 -y+3/4,-x+1/2,-z+3/4,-1 my,mx,mz
119 -x+1/4,-y+1/2,-z+3/4,-1 -mx,-my,-mz
120 y+1/2,x+3/4,z+3/4,-1 my,mx,mz
121 x+3/4,y+3/4,z+1/2,+1 mx,my,mz
122 -y+1/2,-x+1/2,-z+1/2,+1 -my,-mx,-mz
123 -x+1/2,-y,-z+1/2,+1 mx,my,mz
124 y+1/4,x+3/4,z+1/2,+1 -my,-mx,-mz
125 x+1/2,y+1/2,z+1/2,-1 -mx,-my,-mz
126 -y+3/4,-x+3/4,-z+1/2,-1 my,mx,mz
127 -x+1/4,-y+3/4,-z+1/2,-1 -mx,-my,-mz
128 y+1/2,x,z+1/2,-1 my,mx,mz
```

magCIF: separate centering loop

(NiO in non-standard setting)

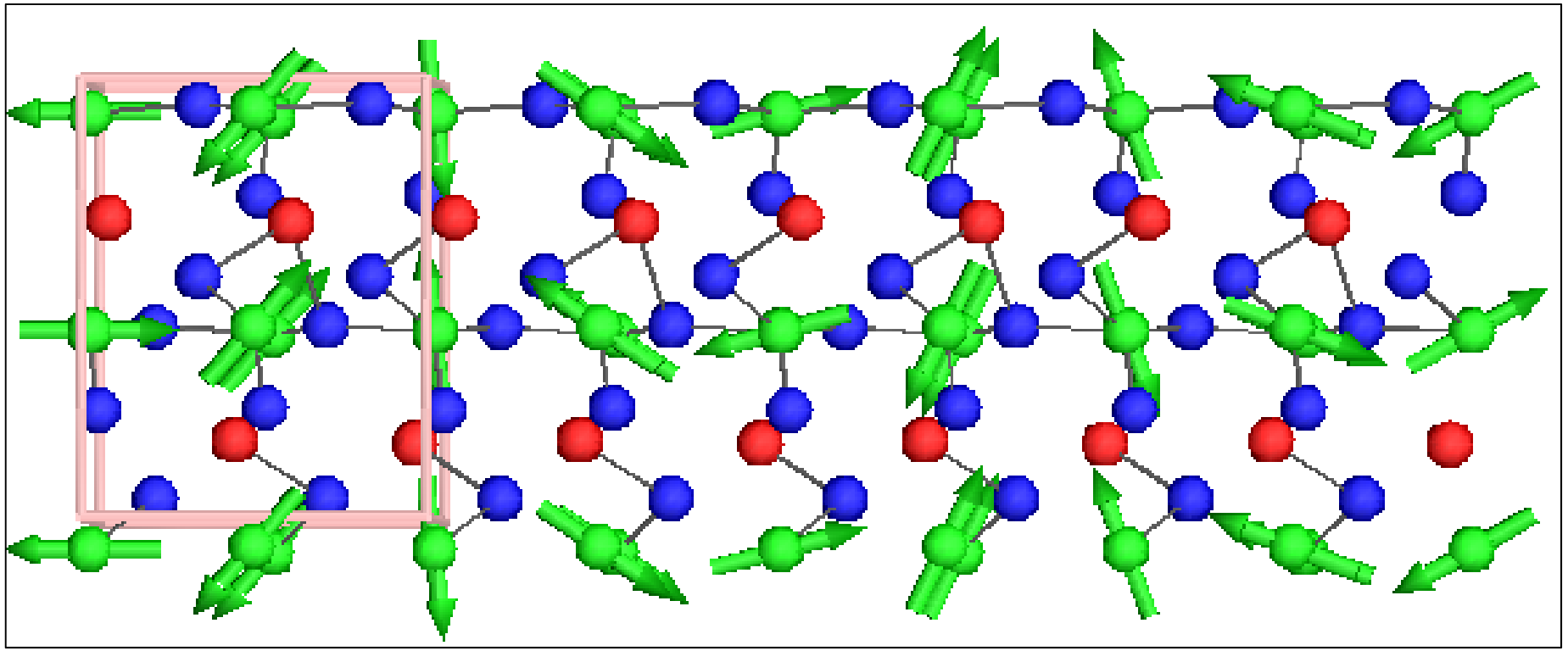
```
loop_
_space_group_symop.magn_id
_space_group_symop.magn_operation_xyzR
_space_group_symop.magn_operation_mxmymz
1 x,y,z,+1 mx,my,mz
2 -y+3/4,-x+3/4,-z,+1 -my,-mx,-mz
3 -x+3/4,-y+1/4,-z,+1 mx,my,mz
4 y+1/2,x,z,+1 -my,-mx,-mz
```



```
loop_
_space_group_symop.magn_centering_id
_space_group_symop.magn_centering_xyzR
_space_group_symop.magn_centering_mxmym
z
1  x,y,z,+1 mx,my,mz
2  x+3/4,y+3/4,z,-1 -mx,-my,-mz
3  x,y+1/4,z+3/4,+1 mx,my,mz
4  x+3/4,y,z+3/4,-1 -mx,-my,-mz
5  x,y+1/2,z+1/2,+1 mx,my,mz
6  x+3/4,y+1/4,z+1/2,-1 -mx,-my,-mz
7  x,y+3/4,z+1/4,+1 mx,my,mz
8  x+3/4,y+1/2,z+1/4,-1 -mx,-my,-mz
9  x+1/4,y,z+3/4,+1 mx,my,mz
10 x,y+3/4,z+3/4,-1 -mx,-my,-mz
11 x+1/4,y+1/4,z+1/2,+1 mx,my,mz
12 x,y,z+1/2,-1 -mx,-my,-mz
13 x+1/4,y+1/2,z+1/4,+1 mx,my,mz
14 x,y+1/4,z+1/4,-1 -mx,-my,-mz
15 x+1/4,y+3/4,z,+1 mx,my,mz
16 x,y+1/2,z,-1 -mx,-my,-mz
17 x+1/2,y,z+1/2,+1 mx,my,mz
18 x+1/4,y+3/4,z+1/2,-1 -mx,-my,-mz
19 x+1/2,y+1/4,z+1/4,+1 mx,my,mz
20 x+1/4,y,z+1/4,-1 -mx,-my,-mz
21 x+1/2,y+1/2,z,+1 mx,my,mz
22 x+1/4,y+1/4,z,-1 -mx,-my,-mz
23 x+1/2,y+3/4,z+3/4,+1 mx,my,mz
24 x+1/4,y+1/2,z+3/4,-1 -mx,-my,-mz
25 x+3/4,y,z+1/4,+1 mx,my,mz
26 x+1/2,y+3/4,z+1/4,-1 -mx,-my,-mz
27 x+3/4,y+1/4,z,+1 mx,my,mz
28 x+1/2,y,z,-1 -mx,-my,-mz
29 x+3/4,y+1/2,z+3/4,+1 mx,my,mz
30 x+1/2,y+1/4,z+3/4,-1 -mx,-my,-mz
31 x+3/4,y+3/4,z+1/2,+1 mx,my,mz
32 x+1/2,y+1/2,z+1/2,-1 -mx,-my,-mz
```

Multiferroic $TbMnO_3$

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



Two simple ways to combine the modulations:

In phase: (a,0;0,b) 14.1 $P2_1/c1'$(a0g)00s, origin=(0,0,0,1/4)

Out of phase: (a,0;b,0) 33.5 $Pna2_11'$(a00)000s, origin=(0,0,0,0)

magCIF: incommensurate case

Magnetic superspace group (MSSG)

```
_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_ssg_transform_id
_space_group_ssg_transform_Pp_a1a2a3
_space_group_ssg_transform_description
1 a3,a2,-a1,a4;0,0,0,0
      "to magnetic BNS ISO Pna2_11' setting"
2 a3,a2,-a1,a4;0,0,0,0
      "to magnetic OG Litvin Pna2_11' setting"
3 a1,a2,a3,a4;0,0,0,0
      "to nonmagnetic SSG ISO P2_1cn(0,0,g)000 setting"
```

magCIF: incommensurate case

Magnetic superspace group (MSSG) operators

```
loop_
_space_group_symop.magn_ssg_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

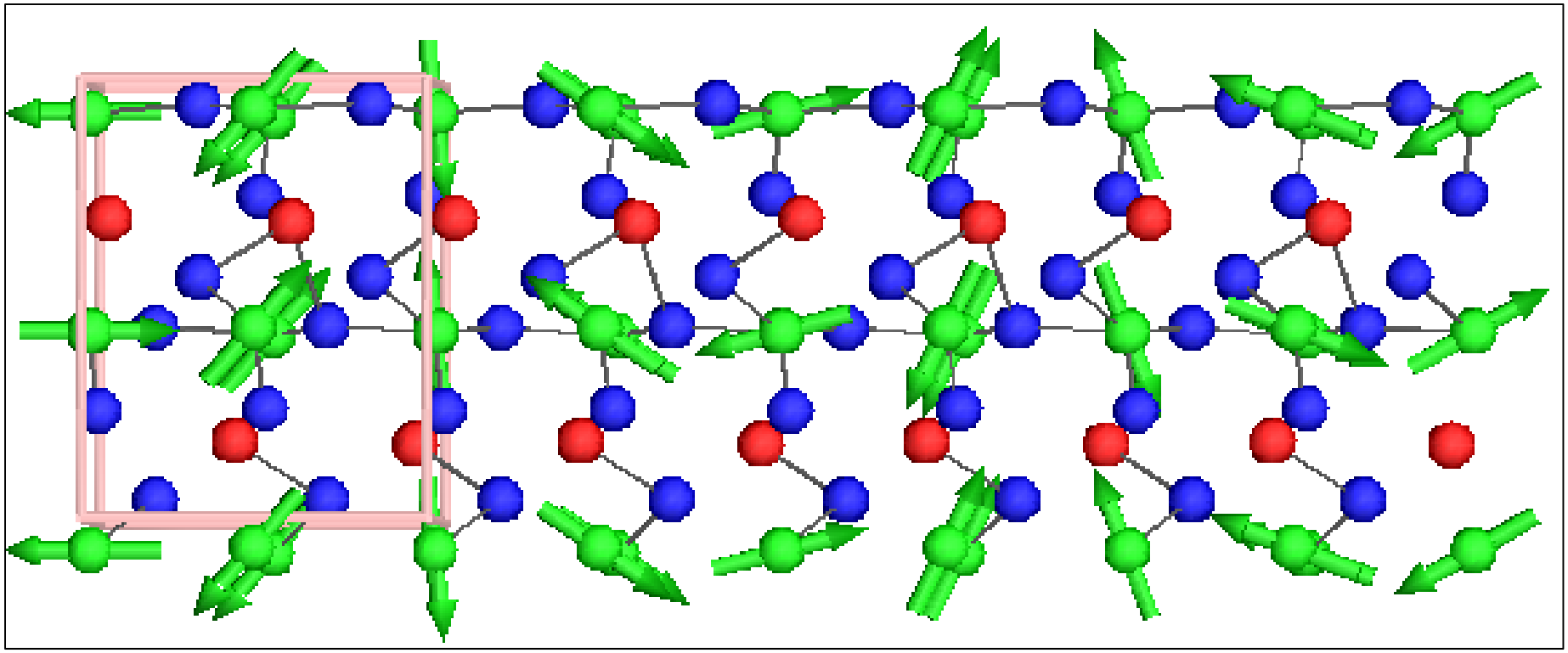
Magnetic superspace group: propagation vectors

```
_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
_jana_atom_site_Fourier_wave_vector_q1_coeff
1    0.00000   0.00000  -0.27000  1
```

magCIF: incommensurate case

Magnetic superspace group (MSSG): modulations

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



```
Mn    1 x    0.00000   -3.95980
Mn    1 y    0.00000    0.00000
Mn    1 z   -5.51543    0.00000
```

Implementation progress (Aug 2014)

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)

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

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

TOPAS Academic [C]
Now: magnetic refinement
Hoped: magCIF (r&w)

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

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

Who else should we talk to?

Accelrys

Atoms by ShapeSoftware

Crystal Studio

Crystal Maker

Diamond

DrawXtl

Mercury

???

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AGH University of Science and Tech., Krakow, Poland

Possible developments in magCIF

For OG settings of type-4 MSGs, use magnetic propagation vector as alternative or addition to primary anti-translation.

Irrep-mode description of magnetic structures.

Magnetic twins

Moment-vector distribution for a given site

Magnetic diffraction data

Magnetic structure factor

Magnetic systematic absences

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