Magnetic CIF Dictionary

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The magCIF dictionary provides CIF infrastructure for the presentation of both commensurate and incommensurate magnetic structures exhibiting long-range three-dimensional magnetic order. Tools for treating short-range order could be added in the future, but have not yet been discussed in earnest. Incommensurate magnetic structures are to be presented using magnetic superspace groups in a manner analogous to incommensurate non-magnetic structures. Commensurate magnetic structures can alternatively employ (1) a Belov–Neronova–Smirnova (BNS) setting, (2) an Opechowski–Guccione (OG) setting, (3) an arbitrary non-standard setting, or (4) an incommensurate (wave) description in some appropriate magnetic-superspace-group setting.

MAGNETIC

This category is the parent of all categories in the dictionary. Head categories from other dictionaries are reparented to this category.

ATOM_SITE_FOURIER_WAVE_VECTOR

Data items in the ATOM_SITE_FOURIER_WAVE_VECTOR category record details about the wave vectors of the Fourier terms used in the structural model. This category is fully defined in the modulated structures dictionary.

Example 1 – Hypothetical example showing the modulation wave vector components expressed using the array data item ***_atom_site_Fourier_wave_vector_q_coeff.***

```
loop_
    _cell_wave_vector_seq_id
    _cell_wave_vector_x
    _cell_wave_vector_y
    _cell_wave_vector_z
          1   0.30000   0.30000   0.00000
          2  -0.60000   0.30000   0.00000
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_q_coeff
        1   -0.30000   0.60000   0.00000  [1   1]
        2   -0.60000   0.30000   0.00000  [0   1]
        3   -0.30000  -0.30000   0.00000  [-1  0]
```

Example 2 – As example 1, but using separate data items for each individual component of the modulation wave vector.

```
loop_
_cell_wave_vector_seq_id
_cell_wave_vector_x
_cell_wave_vector_y
_cell_wave_vector_z
  1   0.30000   0.30000   0.00000
  2  -0.60000   0.30000   0.00000
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
_atom_site_Fourier_wave_vector_q2_coeff
1   -0.30000   0.60000   0.00000  1  1
2   -0.60000   0.30000   0.00000  0  1
3   -0.30000  -0.30000   0.00000 -1  0
```

_atom_site_Fourier_wave_vector.q_coeff (*Integer*[])
For a given incommensurate modulation that contributes to the structure, the wave vector of the modulation can be expressed as an integer linear combination of the d independent wave vectors that define the $(3 + d)$-dimensional superspace. This tag holds each of the integer coefficients as an array. At the time of this writing, no examples with more than three independent wave vectors are known, though there is no theoretical limit to the number that could occur. These tags are not explicitly magnetic; they are equally applicable to any incommensurate modulation.

_atom_site_Fourier_wave_vector.q1_coeff (*Integer*)
For a given incommensurate modulation that contributes to the structure, the wave vector of the modulation can be expressed as an integer linear combination of the d independent wave vectors that define the $(3+d)$-dimensional superspace. The **q1_coeff** tag holds the integer coefficient of the contribution of the first independent wave vector, the **q2_coeff** tag holds the integer coefficient of the contribution of the second independent wave vector, and so on. At the time of this writing, no examples with more than three independent wave vectors are known, though there is no theoretical limit to the number that could occur. These tags are not explicitly magnetic; they are equally applicable to any incommensurate modulation.

_atom_site_Fourier_wave_vector.q2_coeff (*Integer*)
For a given incommensurate modulation that contributes to the structure, the wave vector of the modulation can be expressed as an integer linear combination of the d independent wave vectors that define the $(3+d)$-dimensional superspace. The **q1_coeff** tag holds the integer coefficient of the contribution of the first independent wave vector, the **q2_coeff** tag holds the integer coefficient of the contribution of the second independent wave vector, and so on. At the time of this writing, no examples with more than three independent wave vectors are known, though there is no theoretical limit to the number that could occur. These tags are not explicitly magnetic; they are equally applicable to any incommensurate modulation.

_atom_site_Fourier_wave_vector.q3_coeff (*Integer*)
For a given incommensurate modulation that contributes to the structure, the wave vector of the modulation can be expressed as an integer linear combination of the d independent wave vectors that define the $(3+d)$-dimensional superspace. The **q1_coeff** tag holds the integer coefficient of the contribution of the first independent wave vector, the **q2_coeff** tag holds the integer coefficient of the contribution of the second independent wave vector, and so on. At the time of this writing, no examples with more than three independent wave vectors are known, though there is no theoretical limit to the number that could occur. These tags are not explicitly magnetic; they are equally applicable to any incommensurate modulation.

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ATOM_SITE_MOMENT

This category provides a loop for presenting the magnetic moments of atoms in one of several coordinate systems. This is a child category of the ATOM_SITE category, so that the magnetic moments can either be listed alongside the non-magnetic atom properties in the main ATOM_SITE loop, or be listed in a separate loop.

Category key(s): **_atom_site_moment.label**

_atom_site_moment.Cartn (*Real*[3]; μ_B)
The atom-site magnetic moment vector specified according to a set of orthogonal Cartesian axes where $x||a$ and $z||c*$ with y completing a right-hand set.

_atom_site_moment.Cartn_x (*Real*; μ_B)
The x component of the atom-site magnetic moment vector (see **_atom_site_moment.Cartn**).

_atom_site_moment.Cartn_y (*Real*; μ_B)
The y component of the atom-site magnetic moment vector (see **_atom_site_moment.Cartn**).

_atom_site_moment.Cartn_z (*Real*; μ_B)
The z component of the atom-site magnetic moment vector (see **_atom_site_moment.Cartn**).

_atom_site_moment.crystalaxis (*Real*[3]; μ_B)
The atom-site magnetic moment vector specified using components parallel to each of the unit cell axes. This is the recommended coordinate system for most magnetic structures.

_atom_site_moment.crystalaxis_x (*Real*; μ_B)
The component of the atom-site magnetic-moment vector parallel to the first unit-cell axis. See **_atom_site_moment.crystalaxis**.

_atom_site_moment.crystalaxis_y (*Real*; μ_B)
The component of the atom-site magnetic-moment vector parallel to the second unit-cell axis. See **_atom_site_moment.crystalaxis**.

_atom_site_moment.crystalaxis_z (*Real*; μ_B)
The component of the atom-site magnetic-moment vector parallel to the third unit-cell axis. See **_atom_site_moment.crystalaxis**.

_atom_site_moment.label (*Code*)
This label is a unique identifier for a particular site in the asymmetric unit of the crystal unit cell.

Values must match those for the following item(s):
_atom_site.label

_atom_site_moment.magnitude (*Real*; μ_B)
The magnitude of a magnetic moment vector.

_atom_site_moment.modulation_flag (*Code*)
A code that signals whether the structural model includes the modulation of the magnetic moment of a given atom site.

The data value must be one of the following:

yes	magnetic modulation
y	abbreviation for 'yes'
no	no magnetic modulation
n	abbreviation for 'no'

_atom_site_moment.refinement_flags_magnetic (*Code*)
The constraints/restraints placed on the magnetic moment during model refinement.

The data value must be one of the following:

.	no constraint on magnetic moment
S	special position constraint on magnetic moment
M	modulus restraint on magnetic moment
A	direction restraints on magnetic moment
SM	superposition of S and M constraints/restraints
SA	superposition of S and A constraints/restraints
MA	superposition of M and A constraints/restraints
SMA	superposition of S, M and A constraints/restraints

_atom_site_moment.spherical_azimuthal (*Real*; radians)
The azimuthal angle of the atom-site magnetic moment vector specified in spherical coordinates relative to a set of orthogonal Cartesian axes where $x||a$ and $z||c*$ with y completing a right-hand set. The azimuthal angle is a right-handed rotation around the $+z$ axis starting from the $+x$ side of the x–z plane.

_atom_site_moment.spherical_modulus (*Real*; μ_B)
The modulus of the atom-site magnetic moment vector specified in spherical coordinates relative to a set of orthogonal Cartesian axes where $x||a$ and $z||c*$ with y completing a right-hand set.

_atom_site_moment.spherical_polar (*Real*; radians)
The polar angle of the atom-site magnetic moment vector specified in spherical coordinates relative to a set of orthogonal Cartesian axes where $x||a$ and $z||c*$ with y completing a right-hand set. The polar angle is measured relative to the $+z$ axis.

_atom_site_moment.symmform (*Text*)
A symbolic expression that indicates the symmetry-restricted form of the components of the magnetic moment vector of the atom. Unlike the positional coordinates of an atom, its magnetic moment has no translational component to be represented.

Examples: 'mx,my,mz' (no symmetry restrictions), 'mx,-mx,0' (y component equal and opposite to x component with z component zero), 'mx,0,mz' (y component zero)

ATOM_SITE_MOMENT_FOURIER

Data items in the ATOM_SITE_MOMENT_FOURIER category record details about the Fourier components of the magnetic modulation of an atom site in a modulated structure. The (in general complex) coefficients of each Fourier component belong to the child category ATOM_SITE_MOMENT_FOURIER_PARAM, which may be listed separately.

Category key(s): **_atom_site_moment_Fourier.id**

_atom_site_moment_Fourier.atom_site_label (*Code*)
This string uniquely identifies the atom for which the Fourier modulation components are to be specified. The Fourier modulation components are always presented in a separate loop (not in the ATOM_SITE loop). This string must match an **_atom_site.label** from the ATOM_SITE loop, and otherwise conform to the rules for **_atom_site_label**.

Values must match those for the following item(s):
_atom_site_moment.label

_atom_site_moment_Fourier.axis (*Code*)
Specifies the coordinate system in which the Fourier modulation components are to be presented and an axis in that coordinate system.

Analogous tags: msCIF: **_atom_site_displace_Fourier.axis**, msCIF: **_atom_site_rot_Fourier.axis**, msCIF: **_atom_site_U_Fourier.tens_elem**

The data value must be one of the following:

Cx	Cartesian *x* coordinate
Cy	Cartesian *y* coordinate
Cz	Cartesian *z* coordinate
x	crystal *a*-axis coordinate
y	crystal *b*-axis coordinate
z	crystal *c*-axis coordinate
mod	length part of spherical coordinate
pol	polar angle in spherical coordinates
azi	azimuthal angle in spherical coordinates
a1	user-defined coordinate 1
a2	user-defined coordinate 2
a3	user-defined coordinate 3

_atom_site_moment_Fourier.id (*Text*)
An arbitrary code that uniquely identifies each of the components of each of the magnetic Fourier modulations of each of the atoms in the structure. It will typically include an atom name, a wave-vector id, and a coordinate axis. A sequence of positive integers could also be used.

Examples: 'K2_1_z', 'Se1_2_x'

_atom_site_moment_Fourier.wave_vector_seq_id (*Text*)
An arbitrary code that uniquely identifies the wave vector for which magnetic Fourier modulation components are to be described within the ATOM_SITE_MOMENT_FOURIER loop. It must match one of the **_atom_site_Fourier_wave_vector.seq_id** values in the ATOM_SITE_FOURIER_WAVE_VECTOR loop.

Analogous tags:
msCIF: **_atom_site_displace_Fourier_wave_vector.seq_id**,
msCIF: **_atom_site_rot_Fourier_wave_vector.seq_id**,
msCIF: **_atom_site_occ_Fourier_wave_vector.seq_id**,
msCIF: **_atom_site_U_Fourier_wave_vector.seq_id**

ATOM_SITE_MOMENT_FOURIER_PARAM

Data items in this category record details about the coefficients of the Fourier series used to describe the magnetic modulation of an atom. This is a child category of the ATOM_SITE_MOMENT_FOURIER category; so that magnetic Fourier components can either be listed within the ATOM_SITE_MOMENT_FOURIER loop, or else listed in a separate loop.

Analogous tags: **_atom_site_displace_Fourier_param**.*, **_atom_site_rot_Fourier_param**.*, **_atom_site_occ_Fourier_param**.*, **_atom_site_U_Fourier_param**.*

Category key(s): **_atom_site_moment_Fourier_param.id**

Example 1 – Hypothetical example showing the symmetry-restricted form of cosine and sine components of the modulation vector for a specific Wyckoff site.

```
loop_
    _cell_wave_vector_seq_id
    _cell_wave_vector_x
    _cell_wave_vector_y
    _cell_wave_vector_z
          1   0.30000   0.30000   0.00000
          2  -0.60000   0.30000   0.00000
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
    _atom_site_Fourier_wave_vector_q2_coeff
        1   -0.30000   0.60000   0.00000  1  1
        2   -0.60000   0.30000   0.00000  0  1
        3   -0.30000  -0.30000   0.00000 -1  0
loop_
    _atom_site_moment_Fourier.id
    _atom_site_moment_Fourier.atom_site_label
    _atom_site_moment_Fourier.wave_vector_seq_id
    _atom_site_moment_Fourier.axis
    _atom_site_moment_Fourier_param.cos
    _atom_site_moment_Fourier_param.sin
    _atom_site_moment_Fourier_param.cos_symmform
    _atom_site_moment_Fourier_param.sin_symmform
        1  Fe_1 1 x  0.00000  0.84852  0              mxs
        2  Fe_1 1 y  0.00000  0.42426  0      0.50000*mxs
        3  Fe_1 1 z  0.00000  0.00000  0               0
        4  Fe_1 2 x  0.00000 -0.42426  0     -0.50000*mxs
        5  Fe_1 2 y  0.00000 -0.84852  0            -mxs
        6  Fe_1 2 z  0.00000  0.00000  0               0
        7  Fe_1 3 x -0.42426  0.00000 -0.50000*mxs   0
        8  Fe_1 3 y  0.42426  0.00000  0.50000*mxs   0
        9  Fe_1 3 z  0.00000  0.00000  0               0
```

_atom_site_moment_Fourier_param.cos (*Real*; μ_B)
The cosine component of the magnetic Fourier modulation of a specific atom, wave vector and coordinate axis. It is always used together with the sine component, but not with the modulus or phase components.

Analogous tags:
msCIF: **_atom_site_displace_Fourier_param.cos**,
msCIF: **_atom_site_rot_Fourier_param.cos**,
msCIF: **_atom_site_occ_Fourier_param.cos**,
msCIF: **_atom_site_U_Fourier_param.cos**
Also see the technical descriptions of the analogous tags.

_atom_site_moment_Fourier_param.cos_symmform (*Text*)
A symbolic expression that indicates the symmetry-restricted form of this modulation component for the affected Wyckoff site. The expression can include a zero, a symbol, or a symbol multiplied ('*') by a numerical prefactor. An allowed symbol is a string that contains the following parts. (1) The 1st character is '*m*' for magnetic. (2) The 2nd character is one of '*x*', '*y*' or '*z*', to indicate the magnetic component to be modulated. (3) The 3rd character is one of '*m*' for modulus, '*p*' for phase, '*c*' for cosine, or '*s*' for sine. (4) The 4th character is an integer that indicates the modulation vector. To use the same symbol with modulation components belonging to symmetry related axes and/or wave vectors, is to point out symmetry relationships amongst them. Obviously, modulation components belonging to symmetry-distinct atoms, axes, or wave vectors cannot be related by symmetry.

Analogous tags: none, though analogous tags are needed for displace, occ, *U*, and aniso waves.

_atom_site_moment_Fourier_param.id (*Text*)
An arbitrary code that uniquely identifies each of the components of each of the magnetic Fourier modulations of each of the atoms in the structure. It will typically include an atom name, a wave-vector id, and a coordinate axis. A sequence of positive integers could also be used. This tag is only used when the magnetic Fourier modulation components are split off into a separate loop, which is less typical. When used, its value must match one of the **_atom_site_moment_Fourier.id** values in the ATOM_SITE_MOMENT_FOURIER loop.

Values must match those for the following item(s):
_atom_site_moment_Fourier.id

_atom_site_moment_Fourier_param.modulus (*Real*; μ_B)
The modulus component of the magnetic Fourier modulation of a specific atom, wave vector and coordinate axis. It is always used together with the phase component, but not with the cosine or sine components.

Analogous tags:
msCIF: **_atom_site_displace_Fourier_param.modulus**,
msCIF: **_atom_site_rot_Fourier_param.modulus**,
msCIF: **_atom_site_occ_Fourier_param.modulus**,
msCIF: **_atom_site_U_Fourier_param.modulus**
Also see the technical descriptions of the analogous tags.

_atom_site_moment_Fourier_param.modulus_symmform (*Text*)
See the description and example given for the **_atom_site_moment_Fourier_param.cos_symmform** item.

_atom_site_moment_Fourier_param.phase (*Real*; cycles)
The phase component of the magnetic Fourier modulation of a specific atom, wave vector and coordinate axis. It is always used together with the modulus component, but not with the cosine or sine components. This parameter will be unitless regardless of the coordinate system used.

Analogous tags:
msCIF: **_atom_site_displacive_Fourier_param.phase**,
msCIF: **_atom_site_rot_Fourier_param.phase**,
msCIF: **_atom_site_occ_Fourier_param.phase**,
msCIF: **_atom_site_U_Fourier_param.phase**
Also see the technical descriptions of the analogous tags.

_atom_site_moment_Fourier_param.phase_symmform (*Text*)
See the description and example given for the **_atom_site_moment_Fourier_param.cos_symmform** item.

_atom_site_moment_Fourier_param.sin (*Real*; μ_B)
The sine component of the magnetic Fourier modulation of a specific atom, wave vector and coordinate axis. It is always used together with the cosine component, but not with the modulus or phase components.

Analogous tags:
msCIF: **_atom_site_displace_Fourier_param.sin**,
msCIF: **_atom_site_rot_Fourier_param.sin**,
msCIF: **_atom_site_occ_Fourier_param.sin**,
msCIF: **_atom_site_U_Fourier_param.sin**
Also see the technical descriptions of the analogous tags.

_atom_site_moment_Fourier_param.sin_symmform (*Text*)
See the description and example given for the **_atom_site_moment_Fourier_param.cos_symmform** item.

ATOM_SITE_MOMENT_SPECIAL_FUNC

Data items in the ATOM_SITE_MOMENT_SPECIAL_FUNC category record details about the magnetic modulation of an atom site in a modulated structure when it is not described by Fourier series. Special functions are effective in some cases where the modulations are highly anharmonic, since the number of parameters is drastically reduced. However, they are in general discontinuous or with discontinuous derivatives and therefore these functions describe an ideal situation that never occurs in a real modulated crystal. Up to now, only a few types of special functions have been used and all of them come from the *JANA* suite of programs. Although this approach is far from being general, it has the advantage that the functions are tightly defined and therefore the relevant parameters can be calculated easily. In this dictionary, only the special functions available in *JANA*2000 have been included. These are: (1) Sawtooth functions for atomic displacive modulation along x, y and z. (2) Crenel functions for the occupational modulation of atoms and rigid groups. Both of these only apply to one-dimensional modulated structures.

Analogous tags: **_atom_site_displace_special_func.***, **_atom_site_occ_special_func.***

Category key(s): **_atom_site_moment_special_func.atom_site_label**

_atom_site_moment_special_func.atom_site_label (*Code*)
This label is a unique identifier for a particular site in the asymmetric unit of the crystal unit cell.
Values must match those for the following item(s):
_atom_site.label

_atom_site_moment_special_func.sawtooth_ax (*Real*; μ_B)
_atom_site_moment_special_func.sawtooth_ items are the adjustable parameters of a magnetic sawtooth function. A magnetic sawtooth function is only used when working in the crystal-axis coordinate system. It is defined along the internal space direction as follows:

$$\begin{aligned} m_x &= 2ax[(x_4 - c)/w] \\ m_y &= 2ay[(x_4 - c)/w] \\ m_z &= 2az[(x_4 - c)/w] \end{aligned}$$

with x_4 belonging to the interval $[c-(w/2), c+(w/2)]$, where a_x, a_y and a_z are the amplitudes (maximum magnetic moments) along each crystallographic axis, w is its width, x_4 is the internal coordinate and c is the centre of the function in internal space. The use of this function is restricted to one-dimensional modulated structures. For more details, see the manual for *JANA*2000 (Petricek & Dusek, 2000). Calculated parameters m_x, m_y and m_z must be in Bohr-magneton units and can vary in the range $(-\infty, \infty)$.

Ref: Petricek, V. & Dusek, M. (2000). *JANA*2000. *The crystallographic computing system.* Institute of Physics, Prague, Czech Republic.

Analogous tags:
_atom_site_displace_special_func.sawtooth_*,
_atom_site_occ_special_func.cresnel_*

_atom_site_moment_special_func.sawtooth_ay (*Real*; μ_B)
_atom_site_moment_special_func.sawtooth_ items are the adjustable parameters of a magnetic sawtooth function. A magnetic sawtooth function is only used when working in the crystal-axis coordinate system. It is defined along the internal space direction as follows:

$$\begin{aligned} m_x &= 2ax[(x_4 - c)/w] \\ m_y &= 2ay[(x_4 - c)/w] \\ m_z &= 2az[(x_4 - c)/w] \end{aligned}$$

with x_4 belonging to the interval $[c-(w/2), c+(w/2)]$, where a_x, a_y and a_z are the amplitudes (maximum magnetic moments) along each crystallographic axis, w is its width, x_4 is the internal coordinate and c is the centre of the function in internal space. The use of this function is restricted to one-dimensional modulated structures. For more details, see the manual for *JANA*2000 (Petricek & Dusek, 2000). Calculated parameters m_x, m_y and m_z must be in Bohr-magneton units and can vary in the range $(-\infty, \infty)$.

Ref: Petricek, V. & Dusek, M. (2000). *JANA*2000. *The crystallographic computing system.* Institute of Physics, Prague, Czech Republic.

Analogous tags:
_atom_site_displace_special_func.sawtooth_*,
_atom_site_occ_special_func.cresnel_*

_atom_site_moment_special_func.sawtooth_az
(*Real*; μ_B)

_atom_site_moment_special_func.sawtooth_ items are the adjustable parameters of a magnetic sawtooth function. A magnetic sawtooth function is only used when working in the crystal-axis coordinate system. It is defined along the internal space direction as follows:

$$\begin{aligned} m_x &= 2ax[(x_4-c)/w] \\ m_y &= 2ay[(x_4-c)/w] \\ m_z &= 2az[(x_4-c)/w] \end{aligned}$$

with x_4 belonging to the interval $[c-(w/2), c+(w/2)]$, where a_x, a_y and a_z are the amplitudes (maximum magnetic moments) along each crystallographic axis, w is its width, x_4 is the internal coordinate and c is the centre of the function in internal space. The use of this function is restricted to one-dimensional modulated structures. For more details, see the manual for *JANA*2000 (Petricek & Dusek, 2000). Calculated parameters m_x, m_y and m_z must be in Bohr-magneton units and can vary in the range $(-\infty, \infty)$.

Ref: Petricek, V. & Dusek, M. (2000). *JANA*2000. *The crystallographic computing system.* Institute of Physics, Prague, Czech Republic.

Analogous tags:
_atom_site_displace_special_func.sawtooth_*,
_atom_site_occ_special_func.cresnel_*

_atom_site_moment_special_func.sawtooth_c
(*Real*; μ_B)

_atom_site_moment_special_func.sawtooth_ items are the adjustable parameters of a magnetic sawtooth function. A magnetic sawtooth function is only used when working in the crystal-axis coordinate system. It is defined along the internal space direction as follows:

$$\begin{aligned} m_x &= 2ax[(x_4-c)/w] \\ m_y &= 2ay[(x_4-c)/w] \\ m_z &= 2az[(x_4-c)/w] \end{aligned}$$

with x_4 belonging to the interval $[c-(w/2), c+(w/2)]$, where a_x, a_y and a_z are the amplitudes (maximum magnetic moments) along each crystallographic axis, w is its width, x_4 is the internal coordinate and c is the centre of the function in internal space. The use of this function is restricted to one-dimensional modulated structures. For more details, see the manual for *JANA*2000 (Petricek & Dusek, 2000). Calculated parameters m_x, m_y and m_z must be in Bohr-magneton units and can vary in the range $(-\infty, \infty)$.

Ref: Petricek, V. & Dusek, M. (2000). *JANA*2000. *The crystallographic computing system.* Institute of Physics, Prague, Czech Republic.

Analogous tags:
_atom_site_displace_special_func.sawtooth_*,
_atom_site_occ_special_func.cresnel_*

_atom_site_moment_special_func.sawtooth_w
(*Real*; μ_B)

_atom_site_moment_special_func.sawtooth_ items are the adjustable parameters of a magnetic sawtooth function. A magnetic sawtooth function is only used when working in the crystal-axis coordinate system. It is defined along the internal space direction as follows:

$$\begin{aligned} m_x &= 2ax[(x_4-c)/w] \\ m_y &= 2ay[(x_4-c)/w] \\ m_z &= 2az[(x_4-c)/w] \end{aligned}$$

with x_4 belonging to the interval $[c-(w/2), c+(w/2)]$, where a_x, a_y and a_z are the amplitudes (maximum magnetic moments) along each crystallographic axis, w is its width, x_4 is the internal coordinate and c is the centre of the function in internal space. The use of this function is restricted to one-dimensional modulated structures. For more details, see the manual for *JANA*2000 (Petricek & Dusek, 2000). Calculated parameters m_x, m_y and m_z must be in Bohr-magneton units and can vary in the range $(-\infty, \infty)$.

Ref: Petricek, V. & Dusek, M. (2000). *JANA*2000. *The crystallographic computing system.* Institute of Physics, Prague, Czech Republic.

Analogous tags:
_atom_site_displace_special_func.sawtooth_*,
_atom_site_occ_special_func.cresnel_*

ATOM_SITE_ROTATION

This category provides a loop for presenting atom-site axial-vector rotations in several coordinate systems. Such axial vectors can be applied to describe the rotations of molecular or polyhedral rigid bodies about their pivot atoms or sites, though the use of this category to describe patterns of rotations does not require that rigid bodies be explicitly defined. Because magnetic moments and rotations are both axial rather than polar vectors, their descriptive requirements are highly analogous, except that static rotations are insensitive to time-reversal, so that normal (non-magnetic) symmetry groups are appropriate. This is a child category of the ATOM_SITE category, though pivot-site rotations will typically be listed in a separate loop; the category items mirror those of defined for the ATOM_SITE_MOMENT category.

Category key(s): **_atom_site_rotation.label**

_atom_site_rotation.Cartn (*Real*[3]; radians)
The atom-site rotation vector specified according to a set of orthogonal Cartesian axes where $x||a$ and $z||c*$ with y completing a right-hand set.

_atom_site_rotation.Cartn_x (*Real*; radians)
The x component of the atom-site rotation vector (see **_atom_site_rotation.Cartn**).

_atom_site_rotation.Cartn_y (*Real*; radians)
The y component of the atom-site rotation vector (see **_atom_site_rotation.Cartn**).

_atom_site_rotation.Cartn_z (*Real*; radians)
The z component of the atom-site rotation vector (see **_atom_site_rotation.Cartn**).

_atom_site_rotation.crystalaxis (*Real*[3]; radians)
The atom-site rotation vector specified using the components parallel to each of the unit-cell axes. This is the recommended coordinate system for presenting axial rotation vectors.

_atom_site_rotation.crystalaxis_x (*Real*; radians)
The component of the atom-site rotation vector parallel to the first unit-cell axis. See **_atom_site_rotation.crystalaxis**.

_atom_site_rotation.crystalaxis_y (*Real*; radians)
The component of the atom-site rotation vector parallel to the second unit-cell axis. See **_atom_site_rotation.crystalaxis**.

_atom_site_rotation.crystalaxis_z (*Real*; radians)
The component of the atom-site rotation vector parallel to the third unit-cell axis. See **_atom_site_rotation.crystalaxis**.

_atom_site_rotation.label (*Code*)
This label is a unique identifier for a particular site in the asymmetric unit of the crystal unit cell.

Values must match those for the following item(s):
_atom_site.label

_atom_site_rotation.magnitude (*Real*; radians)
The magnitude of a rotation vector.

_atom_site_rotation.modulation_flag (*Code*)
A code that signals whether the structural model includes the modulation of the rotation of a given atom site.

The data value must be one of the following:

yes	rotational modulation
y	abbreviation for 'yes'
no	no rotational modulation
n	abbreviation for 'no'

_atom_site_rotation.refinement_flags_rotational (*Code*)
The constraints/restraints placed on the rotation vector during model refinement.

The data value must be one of the following:

.	no constraint on rotation
S	special position constraint on rotation
M	modulus restraint on rotation
A	direction restraints on rotation
SM	superposition of S and M constraints/restraints
SA	superposition of S and A constraints/restraints
MA	superposition of M and A constraints/restraints
SMA	superposition of S, M and A constraints/restraints

_atom_site_rotation.spherical_azimuthal (*Real*; radians)
The azimuthal angle of the atom-site rotation vector specified in spherical coordinates relative to a set of orthogonal Cartesian axes where $x||a$ and $z||c*$ with y completing a right-hand set. The azimuthal angle is a right-handed rotation around the $+z$ axis starting from the $+x$ side of the x–z plane.

_atom_site_rotation.spherical_modulus (*Real*; radians)
The modulus of the atom-site rotation vector specified in spherical coordinates relative to a set of orthogonal Cartesian axes where $x||a$ and $z||c*$ with y completing a right-hand set.

_atom_site_rotation.spherical_polar (*Real*; radians)
The polar angle of the atom-site rotation vector specified in spherical coordinates relative to a set of orthogonal Cartesian axes where $x||a$ and $z||c*$ with y completing a right-hand set. The polar angle is measured relative to the $+z$ axis.

_atom_site_rotation.symmform (*Text*)
A symbolic expression that indicates the symmetry-restricted form of the components of the rotation vector of the atom. Unlike the positional coordinates of an atom, its rotation has no translational component to be represented.

Examples: '`rx,ry,rz`' (no symmetry restrictions), '`rx,-rx,0`' (y component equal and opposite to x component with z component zero), '`rx,0,rz`' (y component zero)

ATOM_SITES_MOMENT_FOURIER

Data items in the ATOM_SITES_MOMENT_FOURIER category record details common to the magnetic modulations of atom sites in a modulated structure. Details for individual atom sites are described by data items in the ATOM_SITE_MOMENT_FOURIER category.

Analogous tags:
_atom_sites_displace_Fourier.*,
_atom_sites_rot_Fourier.*, **_atom_sites_occ_Fourier.***,
_atom_sites_U_Fourier.*

_atom_sites_moment_Fourier.axes_description (*Text*)
Describes a user-defined coordinate system for which magnetic Fourier modulation components are to be presented. Only used when different from those described by **_atom_site_moment_Fourier.axis**.

Analogous tags: msCIF: **_atom_sites_displace_Fourier.axes_description** It is not difficult to imagine an **_atom_sites_rot_Fourier.axes_description** tag.

```
; a1 and a2 are respectively the long
  molecular axis and the axis normal to
  the mean molecular plane.
  Extracted from Baudour & Sanquer
  [Acta Cryst. (1983), B39, 75-84].
;
```

ATOM_TYPE_SCAT

Data items in the ATOM_TYPE_SCAT category describe atomic scattering information used in crystallographic structure studies. This category is fully defined in the core CIF dictionary.

_atom_type_scat.neutron_magnetic_j0_A1 (*Real*)
First, the parameters are used directly to approximate spatial averages of spherical Bessel functions over the electronic wave functions of unpaired electrons of the given atom type as a function of $s = \sin(\theta)/\lambda$.

$$\begin{aligned}\langle jn(s)\rangle &= [A_1 \exp(-a_2 s^2) + B_1 \exp(-b_2 s^2) \\ &+ C_1 \exp(-c_2 s^2) + D] \\ &\times [1 \text{ if } n = 0, s^2 \text{ if } n = 2, 4, 6]\end{aligned}$$

The $\langle jn(s)\rangle$ are then combined to determine the spin and orbital contributions to the magnetic form factor of the atom. The 'e' parameter is a measure of error in the approximation.

Analogous tags: coreCIF: **_atom_site.scat_Cromer_Mann_***

Ref: *International Tables for Crystallography* (2006). Vol. C, Sections 4.4.5 and 6.1.2.3 (and references therein).

_atom_type_scat.neutron_magnetic_j0_a2 (*Real*; Å^2)
See definition for **_atom_type_scat.neutron_magnetic_j0_A1**

_atom_type_scat.neutron_magnetic_j0_B1 (*Real*)
See definition for **_atom_type_scat.neutron_magnetic_j0_A1**

_atom_type_scat.neutron_magnetic_j0_b2 (*Real*; Å^2)
See definition for **_atom_type_scat.neutron_magnetic_j0_A1**

_atom_type_scat.neutron_magnetic_j0_C1 (*Real*)
See definition for **_atom_type_scat.neutron_magnetic_j0_A1**

_atom_type_scat.neutron_magnetic_j0_c2 (*Real*; Å^2)
See definition for **_atom_type_scat.neutron_magnetic_j0_A1**

_atom_type_scat.neutron_magnetic_j0_D (*Real*)
See definition for **_atom_type_scat.neutron_magnetic_j0_A1**

_atom_type_scat.neutron_magnetic_j0_e (*Real*)
See definition for **_atom_type_scat.neutron_magnetic_j0_A1**

_atom_type_scat.neutron_magnetic_j2_A1 (*Real*)
See definition for **_atom_type_scat.neutron_magnetic_j0_A1**

_atom_type_scat.neutron_magnetic_j2_a2 (*Real*; Å^2)
See definition for **_atom_type_scat.neutron_magnetic_j0_A1**

_atom_type_scat.neutron_magnetic_j2_B1 (*Real*)
See definition for **_atom_type_scat.neutron_magnetic_j0_A1**

_atom_type_scat.neutron_magnetic_j2_b2 (*Real*; Å^2)
See definition for **_atom_type_scat.neutron_magnetic_j0_A1**

_atom_type_scat.neutron_magnetic_j2_C1 (*Real*)
See definition for **_atom_type_scat.neutron_magnetic_j0_A1**

_atom_type_scat.neutron_magnetic_j2_c2 (*Real*; Å^2)
See definition for **_atom_type_scat.neutron_magnetic_j0_A1**

_atom_type_scat.neutron_magnetic_j2_D (*Real*)
See definition for **_atom_type_scat.neutron_magnetic_j0_A1**

_atom_type_scat.neutron_magnetic_j2_e (*Real*)
See definition for **_atom_type_scat.neutron_magnetic_j0_A1**

_atom_type_scat.neutron_magnetic_j4_A1 (*Real*)
See definition for **_atom_type_scat.neutron_magnetic_j0_A1**

_atom_type_scat.neutron_magnetic_j4_a2 (*Real*; Å^2)
See definition for **_atom_type_scat.neutron_magnetic_j0_A1**

_atom_type_scat.neutron_magnetic_j4_B1 (*Real*)
See definition for **_atom_type_scat.neutron_magnetic_j0_A1**

_atom_type_scat.neutron_magnetic_j4_b2 (*Real*; Å^2)
See definition for **_atom_type_scat.neutron_magnetic_j0_A1**

_atom_type_scat.neutron_magnetic_j4_C1 (*Real*)
See definition for **_atom_type_scat.neutron_magnetic_j0_A1**

_atom_type_scat.neutron_magnetic_j4_c2 (*Real*; Å^2)
See definition for **_atom_type_scat.neutron_magnetic_j0_A1**

_atom_type_scat.neutron_magnetic_j4_D (*Real*)
See definition for **_atom_type_scat.neutron_magnetic_j0_A1**

_atom_type_scat.neutron_magnetic_j4_e (*Real*)
See definition for **_atom_type_scat.neutron_magnetic_j0_A1**

_atom_type_scat.neutron_magnetic_j6_A1 (*Real*)
See definition for **_atom_type_scat.neutron_magnetic_j0_A1**

_atom_type_scat.neutron_magnetic_j6_a2 (*Real*; Å^2)
See definition for **_atom_type_scat.neutron_magnetic_j0_A1**

_atom_type_scat.neutron_magnetic_j6_B1 (*Real*)
See definition for **_atom_type_scat.neutron_magnetic_j0_A1**

_atom_type_scat.neutron_magnetic_j6_b2 (*Real*; Å^2)
See definition for **_atom_type_scat.neutron_magnetic_j0_A1**

_atom_type_scat.neutron_magnetic_j6_C1 (*Real*)
See definition for **_atom_type_scat.neutron_magnetic_j0_A1**

_atom_type_scat.neutron_magnetic_j6_c2 (*Real*; Å^2)
See definition for **_atom_type_scat.neutron_magnetic_j0_A1**

_atom_type_scat.neutron_magnetic_j6_D (*Real*)
See definition for **_atom_type_scat.neutron_magnetic_j0_A1**

_atom_type_scat.neutron_magnetic_j6_e (*Real*)
See definition for **_atom_type_scat.neutron_magnetic_j0_A1**

_atom_type_scat.neutron_magnetic_source (*Text*)
Reference to the source of magnetic neutron scattering factors for a given atom type.

Analogous tags: coreCIF: **_atom_site.scat_source**

Example:

```
; International Tables for Crystallography (2006). Vol. C,
  Section 4.4.5.
;
```

PARENT_PROPAGATION_VECTOR

This looped category allows for the presentation of the fundamental magnetic wave vectors in the setting of the parent structure. In general, there can be more than one fundamental magnetic wave vector. See the PARENT_SPACE_GROUP category for more information about parent space groups.

Category key(s): **_parent_propagation_vector.id**

```
loop_
  _parent_propagation_vector.id
  _parent_propagation_vector.kxkykz
    k1  [0 0 1]
    k2  [0 1 0]
    k3  [1 0 0]
```

_parent_propagation_vector.id (*Text*)
A code that uniquely identifies a fundamental magnetic propagation vector.

_parent_propagation_vector.kxkykz (*Real*[3])
A fundamental magnetic propagation vector in unitless reciprocal-lattice units of the parent space group setting.

PARENT_SPACE_GROUP

This category provides information about the space group and setting of a non-magnetic parent structure which is related to the present magnetic structure by a group–subgroup relationship. In general, the choice of a parent structure is not unique; it could be the lowest-symmetry non-magnetic structure obtained by simply setting all magnetic moments to zero, or a higher-symmetry approximation to this structure which idealizes some of the atomic coordinates. The designation of a parent structure is common but optional for a magnetic-structure description. This category could also be used to designate high-symmetry parent structures of low-symmetry non-magnetic structures. As an alternative to this category, one can define a parent structure in a separate data block, and then relate the parent and child space-group settings by conveying an appropriate inter-data-block basis transformation in each data block.

Analogous tags: none

_parent_space_group.child_transform_Pp_abc
(*Real*[4,4])
This item specifies the transformation (P, p) of the basis vectors and origin of the present setting of the parent space group to those of the present setting of the child space group. The basis vectors (a', b', c') of the child are described as linear combinations of the basis vectors (a, b, c) of the parent, and the origin shift (ox, oy, oz) is displayed in the lattice coordinates of the parent. The Jones–Faithful notation and possible values are identical to those of symCIF: **_space_group.transform_Pp_abc**, except that the point and translational components are separated by a semicolon. If the child structure is incommensurate, the transformation applies to the present setting of the basic space group of the incommensurate structure.

Analogous tags: symCIF: **_space_group.transform_Pp_abc**

_parent_space_group.IT_number (*Text*)
Analogous tags: Perfectly analogous to symCIF: **_space_group.IT_number** except that it applies to the parent structure.

_parent_space_group.name_H-M_alt (*Text*)
Analogous tags: Perfectly analogous to symCIF: **_space_group.name_H-M_alt** except that it applies to the parent structure.

_parent_space_group.reference_setting (*Text*)
Analogous tags: Perfectly analogous to symCIF: **_space_group.reference_setting** except that it applies to the parent structure.

_parent_space_group.transform_Pp_abc (*Real*[4,4])
Analogous tags: Notation and usage is analogous to symCIF: **_space_group.transform_Pp_abc** except that it applies to the parent structure, and that the point and translational components are separated by a semicolon.

SPACE_GROUP_MAGN

The data items in this category provide identifying and/or descriptive information about the relevant magnetic symmetry group and setting.

_space_group_magn.name_BNS (*Text*)
See **_space_group_magn_number_OG** for a description of magnetic space groups (MSGs). The Belov–Neronova–Smirnova (BNS) symbol for a MSG is based on the short Hermann–Mauguin space-group symbol of non-magnetic space group F for MSGs of types 1-3 or its subgroup D for MSGs of type 4. For a type-1 MSG, the symbol for the MSG is identical with the unprimed symbol of F. For a type-2 MSG, its symbol is the symbol of the space group F followed by $1'$. For a type-3 MSG, one starts with the symbol for F and then primes any non-translational generators whose corresponding MSG elements are time reversed. For a type-4 MSG, the non-translational generators are never primed. A subscript always appears on the first (lattice) character of the symbol of a type-4 MSG, and communicates that a pure time-reversal element is included in the point group of the MSG. The value of this subscript indicates the magnetic lattice of the MSG, and specifically indicates the translational part of the generator whose point part is the pure time reversal. Note that OG and BNS symbols are identical for MSGs of types 1-3, but differ substantially for MSGs of type 4.

Analogous tags: symCIF: **_space_group.name_H-M_ref**

Ref: '*Magnetic Group Tables*' by D.B. Litvin at http://www.iucr.org/publ/978-0-9553602-2-0. ISO-MAG tables of H.T. Stokes and B.J. Campbell at http://iso.byu.edu.

Examples: 'P 1', 'P 1 1′', 'P_S 1', 'P -1', 'P -1 1′', 'P -1′', 'P_2s -1', 'I a′ -3 d′'

_space_group_magn.name_OG (*Text*)
See **_space_group_magn.number_OG** for more information on magnetic space groups (MSGs). The Opechowski–Guccione (OG) symbol for an MSG is based on the short Hermann–Mauguin space-group symbol of non-magnetic space group F. For a type-1 MSG, the OG symbol for the MSG is identical with the unprimed symbol of F. For a type-2 MSG, the OG symbol is the symbol of the non-magnetic space group F followed by $1'$. For a type-3 or type-4 MSG, the OG symbol is constructed by starting with the symbol for F and then priming the symbols of any non-translational generators whose corresponding MSG elements are time reversed. When a non-translational generator symbol could potentially represent both time-reversed and non-time-reversed symmetry elements, the prime placement is as described in the '*Magnetic Group Tables*' of Litvin. A subscript always appears on the first (lattice) character of the symbol of a type-4 MSG, and communicates that a pure time-reversal element is included in the point group of the MSG. The value of this subscript indicates the magnetic lattice of the MSG. Note that OG and BNS symbols are identical for MSGs of types 1-3, but differ substantially for MSGs of type 4.

Analogous tags: symCIF: **_space_group.name_H-M_ref**

Ref: '*Magnetic Group Tables*' by D.B. Litvin at http://www.iucr.org/publ/978-0-9553602-2-0. ISO-MAG tables of H.T. Stokes and B.J. Campbell at http://iso.byu.edu.

Examples: 'P 1', 'P 1 1′', 'P_S 1', 'P -1', 'P -1 1′', 'P -1′', 'P_2s -1', 'I a′ -3′ d′'

_space_group_magn.number_BNS (*Text*)

See **_space_group_magn.number_OG** for a description of magnetic space groups (MSGs). The Belov–Neronova–Smirnova (BNS) number for an MSG is composed of two positive integers separated by a period. The first integer lies in the range [1–230] and indicates the non-magnetic space group F for MSGs of types 1-3 or the non-magnetic space group of the subgroup D for MSGs of type 4. The second integer is sequential over all MSGs associated with the same crystal family. There are 1651 distinct equivalence classes of MSGs, each of which has a unique BNS number. These equivalence classes are most accurately referred to as magnetic space-group 'types', following the usage in the *International Tables for Crystallography*. But the word 'type' is also commonly used to indicate the four-fold classification of MSGs presented above. To avoid confusion, the word 'type' is only used in the latter sense here.

Analogous tags: symCIF: **_space_group.number_IT**

Ref: '*Magnetic Group Tables*' by D.B. Litvin at http://www.iucr.org/publ/978-0-9553602-2-0. ISO-MAG tables of H.T. Stokes and B.J. Campbell at http://iso.byu.edu.

Examples: '1.1', '1.2', '1.3', '2.4', '2.5', '2.6', '2.7', '230.149'

_space_group_magn.OG_wavevector_kxkykz (*Real*[3])

The magnetic propagation vector (**k**) of the OG(**k**)-supercell description, which determines the time-reversal component of each translation vector (**x**) of the OG lattice (including the centering vectors if a centered setting is used) according to the expression $\cos(2\pi\mathbf{k}.\mathbf{x}) = \pm 1$, where **x** is defined in the unitless coordinates of the direct-space OG lattice and **k** is defined in the unitless coordinates of the corresponding reciprocal-space lattice. If $2\mathbf{k}.\mathbf{x}$ has a non-integer value for any OG lattice (or centering) translation, the definition of **k** is incorrect. The value of OG wave vector is essential to the OG(**k**) description of the magnetic space group symmetry; it cannot be omitted from such a description without ambiguity.

_space_group_magn.point_group_name (*Text*)

Any magnetic point group (MPG) can be constructed by starting with a non-magnetic point group P, and then by adding a time-reversal component to some or all or none of its elements. For a type-1 MPG, $M = P$, there are no time-reversed elements. For a type-2 MPG, $M = P + P1'$, there is both a time-reversed and a non-time-reversed copy of each element in P. For a type-3 MPG, $M = Q + (P - Q)1'$, there is a subgroup Q of P of index 2 whose elements are not time reversed, whereas the remaining elements in $P - Q$ are time reversed. For a type-1 MPG, the symbol is identical with the symbol for the non-magnetic point group P. For a type-2 MPG, the symbol is the symbol for P followed by the symbol $1'$. For a type-3 MPG, the symbol is that of P with a prime added to each time-reversed generator.

Analogous tags: symCIF: **_space_group.point_group_H-M**

Ref: '*Magnetic Group Tables*' by D.B. Litvin at http://www.iucr.org/publ/978-0-9553602-2-0

Examples: '1', '1 1'', '-1', '-1 1'', '-1'', '4 m m', '4' m' m', '4' m m''

_space_group_magn.point_group_number (*Text*)

Each of the 122 crystallographic magnetic point groups can be associated with exactly one crystallographic non-magnetic space group by removing the time-reversal component from each group operator. The identifying number for each such group is taken from the 'Survey of 3-dimensional magnetic point group types' from the '*Magnetic Group Tables*' of D.B. Litvin. This number is composed of three integers: (1) an integer from 1 to 32 that corresponds to the non-magnetic point group; (2) an integer that runs sequentially over each of the magnetic point groups associated with a given non-magnetic point group; and (3) a redundant third integer that runs from 1 to 122.

Ref: '*Magnetic Group Tables*' by D.B. Litvin at http://www.iucr.org/publ/978-0-9553602-2-0

Examples: '1.1.1', '32.5.122'

_space_group_magn.ssg_name (*Text*)

The Belov–Neronova–Smirnova (BNS) symbol for a magnetic superspace group (MSSG) is based on the symbol of the non-magnetic superspace group (SSG) obtained by eliminating all time-reversed operators from the group, as listed in the ISO$(3 + d)$D tables of Stokes and Campbell. If the magnetic basic space group (MBSG) is of type-1 or type-3 (also known as type-3a), its BNS symbol merely replaces that of the basic space-group (BSG). If the MBSG is of type-2 or type-4 (also known as type-3b), an additional phase-shift symbol associated with the time-reversal generator is added to each modulation vector. If the MBSG is of type-4, the BNS symbol of the MSSG is further modified to explicitly show the time-reversal generator $(1')$ at the end, and the anti-centering subscript is moved from the lattice symbol to the 1' so as to clearly indicate the fractional external-space translation of this generator. The examples are based on SSG 47.1.9.3 Pmmm(0,0,g)ss0 in (3+1)D.

Analogous tags: msCIF: **_space_group.ssg_name**

Ref: ISO-MAG tables of H.T. Stokes and B.J. Campbell at http://iso.byu.edu. ISO$(3 + d)$D tables of H.T. Stokes and B.J. Campbell at http://iso.byu.edu.

Examples: 'Pmmm(0,0,g)ss0' (type-1 MBSG Pmmm), 'Pmmm1'(0,0,g)ss00' (type-2 MBSG *Pmmm*$1'$, with no basic-cell or modulated moments allowed), 'Pmmm1'(0,0,g)ss0s' (type-2 MBSG *Pmmm*$1'$, with magnetic modulations allowed, but not basic-cell moments), 'Pm'm'm(0,0,g)ss0' (type-3 MBSG $Pm'm'm$), 'Pmmm1'_a(0,0,g)ss00' (type-4 MBSG *P_ammm* with purely external anti-centering), 'Pmmm1'_a(0,0,g)ss0s' (type-4 MBSG *P_ammm* with superspace anti-centering)

_space_group_magn.ssg_number (*Text*)

The Belov–Neronova–Smirnova (BNS) number for a magnetic superspace group. This tag is being held in reserve until a future numbering scheme is approved.

Analogous tags: msCIF: **_space_group.ssg_number**

_space_group_magn.transform_BNS_Pp (*Text*[4,4])

This item specifies the transformation matrix Pp of the basis vectors and origin of the current setting to those of the Belov–Neronova–Smirnova setting presented in the ISO-MAG tables. The basis vectors (a', b', c') of the BNS setting are obtained as (a',b',c',1) = Pp (a,b,c,1) where (a, b, c) are the current basis vectors.

Ref: ISO-MAG tables of H.T. Stokes and B.J. Campbell at http://iso.byu.edu; Wondratschek, H., Aroyo, M. I., Souvignier, B. and Chapuis, G. Transformation of coordinate systems. In *International Tables for Crystallography* (2016). Volume A, *Space-group symmetry*, edited by M. Aroyo, 6th ed. ch 1.5. Chichester: Wiley. ;

Examples:

```
; [[1 0 0 0.25]
   [0 1 0 0   ]
   [0 0 1 0   ]
   [0 0 0 1   ]]
;
```

(Transformation from OG 5.6.24 C_P2' to BNS 4.12 P_C2_1)

```
; [[0  0 1 0   ]
   [0 -1 0 0.25]
   [1  0 0 0   ]
   [0  0 0 1   ]]
;
```

(Transformation from OG 8.7.44 C_Pm' to BNS 7.31 P_Ac)

_space_group_magn.transform_BNS_Pp_abc (*Text*)
This item specifies the transformation (P, p) of the basis vectors and origin of the current setting to those of the Belov–Neronova–Smirnova setting presented in the ISO-MAG tables. The basis vectors (a', b', c') of the BNS setting are described as linear combinations of the current basis vectors (a, b, c), and the origin shift (ox, oy, oz) is displayed in the lattice coordinates of the current setting. The Jones–Faithful notation and possible values are identical to those of symCIF: **_space_group.transform_Pp_abc**, except that the point and translational components are separated by a semicolon.

Analogous tags: symCIF: **_space_group.transform_Pp_abc**

Ref: ISO-MAG tables of H.T. Stokes and B.J. Campbell at http://iso.byu.edu

_space_group_magn.transform_OG_Pp (*Text*[4,4])
This item specifies the transformation (P, p) of the basis vectors and origin of the current setting to those of the Opechowski–Guccione setting presented in the '*Magnetic Group Tables*' of D.B. Litvin. The basis vectors (a', b', c') of the OG setting are obtained as (a',b',c',1) = Pp (a,b,c,1) where (a, b, c) are the current basis vectors.

Ref: '*Magnetic Group Tables*' by D.B. Litvin at http://www.iucr.org/publ/978-0-9553602-2-0; Wondratschek, H., Aroyo, M. I., Souvignier, B. and Chapuis, G. Transformation of coordinate systems. In *International Tables for Crystallography* (2016). Volume A, *Space-group symmetry*, edited by M. Aroyo, 6th ed. ch 1.5. Chichester: Wiley.

_space_group_magn.transform_OG_Pp_abc (*Text*)
This item specifies the transformation (P, p) of the basis vectors and origin of the current setting to those of the Opechowski–Guccione setting presented in the '*Magnetic Group Tables*' of D.B. Litvin. The basis vectors (a', b', c') of the reference setting are described as linear combinations of the current basis vectors (a, b, c), and the origin shift (ox, oy, oz) is displayed in the lattice coordinates of the current setting. The Jones–Faithful notation and possible values are identical to those of symCIF: **_space_group.transform_Pp_abc**, except that the point and translational components are separated by a semicolon.

Analogous tags: symCIF: **_space_group.transform_Pp_abc**

Ref: '*Magnetic Group Tables*' by D.B. Litvin at http://www.iucr.org/publ/978-0-9553602-2-0

SPACE_GROUP_MAGN_SSG_TRANSFORMS

This loop provides a list of matrix transformations to one or more settings of the magnetic superspace group, including transformations to both standard and non-standard settings. A transformation loop is particularly helpful for magnetic superspace groups, which often have several reference settings of interest.

Analogous tags: transform loops have not yet been approved in other dictionaries.

Category key(s): **_space_group_magn_ssg_transforms.id**

_space_group_magn_ssg_transforms.description (*Text*)
A string that describes the source of a reference setting for the magnetic superspace group. The item **_space_group_magn_ssg_transforms.source** should be used if the reference source is one of those provided in that definition. Otherwise, arbitrary free text can be used to describe reference settings of interest, such as might appear in a specific publication, though care should be taken to make the description clear and unambiguous.

_space_group_magn_ssg_transforms.id (*Text*)
An arbitrary identifier that uniquely labels each setting transformation of interest in a looped list of superspace-group transformations. Most commonly, a sequence of positive integers is used for this identification.

Analogous tags: transform loops have not yet been approved in other dictionaries.

_space_group_magn_ssg_transforms.Pp_superspace (*Text*)
This item specifies the transformation (P, p) of the superspace basis vectors from the current setting (a1,...,a$(3 + d)$) to a reference setting (a1',...,a$(3 + d)$') given by **_space_group_magn_ssg_transforms.description**. The origin shift is presented in the unitless lattice coordinates of the current setting. The notation and usage are analogous to those of **_space_group.transform_Pp_abc**, except that P now represents a superspace point operation, that p now represents a superspace translation, and that the point and translational components are now separated with a semicolon.

Analogous tags: symCIF: **_space_group.transform_Pp_abc**

Examples: '`a1,a2,a3,a4,a5;0,0,0,0,0`' (Identity transformation),
'`-a2,a1,1/2a3,-a1+a5,-1/2a3+a4;1/4,-1/4,0,1/4,0`' (Transforms from a supercentered setting to the ISO$(3 + d)$D setting of 65.2.43.64.m481.1 *Cmmm*$(0, b1, 1/2)000(1, 0, g2)0s0$.)

_space_group_magn_ssg_transforms.source (*Text*)
A string that describes the source of a reference setting for the magnetic superspace group. If the reference source does not appear in the list below, use **_space_group_magn_ssg_transforms.description**

Ref: '*Magnetic Group Tables*' of D.B. Litvin at http://www.iucr.org/publ/978-0-9553602-2-0. ISO-MAG tables of H.T. Stokes and B.J. Campbell at http://iso.byu.edu. ISO$(3 + d)$D tables of H.T. Stokes and B.J. Campbell at http://iso.byu.edu.

The data value must be one of the following:

`ISO(3+d)D-MAG` This superspace transformation simultaneously takes the setting of the basic magnetic space group (BMSG) to the setting of the corresponding entry in the ISO-MAG tables, and takes the setting of the derived non-magnetic superspace group (DNMSG) to within a purely external operation of the setting of the corresponding entry in the ISO$(3 + d)$D tables. The external components of this superspace transformation are those that take the setting of the BMSG to the setting of the corresponding entry in the ISO-MAG tables, while the internal components are those of the transformation that takes the setting of the DNMSG to the setting of the corresponding superspace group in the ISO$(3 + d)$D tables. Such a transformation is unique for any setting of a magnetic superspace group.

SPACE_GROUP_MAGN_TRANSFORMS

This category provides a list of matrix transformations to multiple settings of the magnetic space group, including transformations to both standard and non-standard settings. A transformation loop is particularly helpful for a magnetic space group, which often have several reference settings of interest.

Category key(s): **_space_group_magn_transforms.id**

```
loop_
_space_group_magn_transforms.id
_space_group_magn_transforms.Pp_abc
_space_group_magn_transforms.description
_space_group_magn_transforms.source
   1  'a,b,c;0,0,0'     .                  "data_block_CURRENT"
   2  'a/2,b,c;0,0,0'  "data_block_205763"  .
   3  'a,b,c;0,0,0'     .                  "BNS"
   4  'a/2,b,c;0,0,0'   .                  "OG"
   5  'a/4,b,c;0,0,0'
      "literature citation to a nuclear parent structure"  .
```

_space_group_magn_transforms.description (*Text*)
A string that describes the source of the magnetic-space-group reference setting indicated by the **_space_group_magn_transforms.Pp_abc** tag. **_space_group_magn_transforms.source** should be used if the reference source is one of those provided in that definition. The value string 'data_block_⟨blockname⟩' refers to the setting used in a separate data block named 'blockname' within the same file. Otherwise, arbitrary free text can be used to describe other reference settings of interest, such as might appear in a specific publication, though care should be taken to make the description clear and unambiguous.

_space_group_magn_transforms.id (*Text*)
An arbitrary identifier that uniquely labels each setting transformation of interest in a looped list of space-group transformations.

Analogous tags: transform loops have not been approved in other dictionaries.

_space_group_magn_transforms.Pp (*Text*[4,4])
This item specifies the transformation (P, p) of the basis vectors and origin in the current setting of the CIF file to the reference setting described by the **_space_group_magn_transforms.description** or **_space_group_magn_transforms.source** tags, and should not be used without this description. The basis vectors (a', b', c') of the reference setting are obtained as $(a', b', c', 1) = Pp(a, b, c, 1)$ where (a, b, c) are the current basis vectors.

Ref: Wondratschek, H., Aroyo, M. I., Souvignier, B. and Chapuis, G. Transformation of coordinate systems. In *International Tables for Crystallography* (2016). Volume A, *Space-group symmetry*, edited by M. Aroyo, 6th ed. ch 1.5. Chichester: Wiley.

_space_group_magn_transforms.Pp_abc (*Text*)
This item specifies the transformation (P, p) of the basis vectors and origin in the current setting of the CIF file to the reference setting described by the **_space_group_magn_transforms.description** or **_space_group_magn_transforms.source** tags, and should not be used without this description. The basis vectors (a', b', c') of the reference setting are described as linear combinations of the current basis vectors (a, b, c), and the origin shift (ox, oy, oz) is displayed in the lattice coordinates of the current setting. The Jones–Faithful notation and possible values are identical to those of symCIF: **_space_group_transform_Pp_abc**, except that the point and translational components are separated by a semicolon.

Analogous tags: symCIF: **_space_group.transform_Pp_abc**

_space_group_magn_transforms.source (*Text*)
A string that describes the source of the magnetic space group reference indicated by the **_space_group_magnetic_transforms.Pp_abc** tag. If the reference source does not appear in the list below, use **_space_group_magn_transforms.description**

Ref: '*Magnetic Group Tables*' of D.B. Litvin at http://www.iucr.org/publ/978-0-9553602-2-0. ISO-MAG tables of H.T. Stokes and B.J. Campbell at http://iso.byu.edu. ISO$(3+d)$D tables of H.T. Stokes and B.J. Campbell at http://iso.byu.edu.

The data value must be one of the following:

data_block_CURRENT	The setting used in the current data block. Obviously, the basis transformation to this setting is the identity. The ability to reference the current setting can be useful when communicating the same magnetic propagation vector in multiple settings.
BNS	The Belov–Neronova–Smirnova group setting presented in the ISO-MAG tables.
OG	The Opechowski–Guccione group setting presented in the '*Magnetic Group Tables*' of D.*B*. Litvin.

SPACE_GROUP_SYMOP_MAGN_CENTERING

This loop provides a list of centering or anti-centering translation in a BNS-supercell description of a magnetic space group. Keeping the centering and anti-centering translations in a separate loop leaves only representative point operations in the main SPACE_GROUP_SYMOP_MAGN_OPERATION loop. The direct sum of the two loops produces the full set of representative operations of the magnetic space group. This centering loop is optional, so that it is always possible to include all of the symmetry operations in the main loop. When this centering loop is employed, the representative point operations in the main SPACE_GROUP_SYMOP_MAGN_OPERATION loop may not form a closed subgroup, but instead generate some of the fractional translations of the centering loop. Despite this annoyance, a separate centering loop is important because magnetic structures tend to have a relatively large number of centering and anti-centering translations, which can make the resulting list of operators very long and unintuitive, especially when working in non-standard settings. One could argue that anti-centering operations belong in the main representative- point-operation loop since they are not actually translations of the magnetic lattice. In fact, a pure time reversal is a generator of the magnetic point group of a type-4 magnetic space group. Nevertheless, this centering loop is defined to include the anti-centerings due to the common practice of referring to a 'black and white' lattice of centerings and anti-centerings.

Category key(s): **_space_group_symop_magn_centering.id**

```
loop_
   _space_group_symop_magn_centering.id
   _space_group_symop_magn_centering.xyz
   _space_group_symop_magn_centering.description
       1    'x+1/2,y+1/2,z,+1'
        'a non-time-reversed (1/2,1/2,0) translation'
       2    'x+1/2,y+1/2,z,-1'
            'a time-reversed (1/2,1/2,0) translation'
```

_space_group_symop_magn_centering.description (*Text*)
An optional free text description of a particular centering or anti-centering translation in the BNS-supercell description of a magnetic space group.

Example:

```
; "(1|1/2,1/2,0)'", "(1'|1/2,1/2,0)" or
  "(1/2,1/2,0) anti-centering translation"
  would adequately describe
  "x+1/2,y+1/2,z,-1"
;
```

_space_group_symop_magn_centering.id (*Text*)
An arbitrary identifier that uniquely labels each centering or anti-centering translation in a BNS-supercell description of a magnetic space group. Most commonly, a sequence of positive integers is used for this identification.

_space_group_symop_magn_centering.xyz (*Text*)
A parsable string giving one of the centering or anti-centering translations in the BNS-supercell description of a magnetic space group in algebraic form. The form of such a string is identical to that expected for **_space_group_symop_magn_operation.xyz**, except that the rotational part of a translation must always be the identity element.

SPACE_GROUP_SYMOP_MAGN_OG_CENTERING

This loop provides a list of centering translations in an OG(k)-supercell description of a magnetic space group. For an OG(k)-supercell description, this loop is mandatory and entirely distinct from the optional SPACE_GROUP_SYMOP_MAGN_CENTERING loop used to simplify the presentation of a BNS-supercell description. An integer translation in an OG setting of a type-4 magnetic space group may have a time-reversal component of -1, in which case it is actually an anti-translation vector rather than a lattice vector. This loop should include all centering and anti-centering translations, but does not include the time-reversal components, which are instead determined using the value of the **_space_group_magn.OG_wavevector_kxkykz** tag. Because the centering translations are listed in a separate loop in the OG(k) description, only representative point operations remain in the main SPACE_GROUP_SYMOP_MAGN_OPERATION loop.

Category key(s): **_space_group_symop_magn_OG_centering.id**

_space_group_symop_magn_OG_centering.description (*Text*)

An optional free-text description of a particular centering operation from the OG(k)-supercell description of a magnetic space group, without the time-reversal component.

Analogous tags: centering loops have not been approved for other dictionaries.

Example: '`(1/2,1/2,0)`' (Adequately describes $x+1/2, y+1/2, z$)

_space_group_symop_magn_OG_centering.id (*Text*)

An arbitrary loop identifier that uniquely labels each centering translation in an OG(k)-supercell description of a magnetic space group. Most commonly, a sequence of positive integers is used for this identification.

Analogous tags: centering loops have not been approved for other dictionaries.

_space_group_symop_magn_OG_centering.xyz (*Text*)

A parsable string giving one of the centering operations of the OG(k)-supercell description of a magnetic space group in algebraic form. The form of such a string is identical to that expected for **_space_group_symop_operation.xyz**, except that the rotational part of a translation must always be the identity element. The magnetic component of the centering vector is not given in the value of this tag, but should instead be separately established using the value of the **_space_group_magn.OG_wavevector_kxkykz** tag.

Example: '`x+1/2,y+1/2,z`' (a centering translation of (1/2,1/2,0))

SPACE_GROUP_SYMOP_MAGN_OPERATION

A list of magnetic space-group symmetry operations.

Category key(s): **_space_group_symop_magn_operation.id**

_space_group_symop_magn_operation.description (*Text*)

The description of a particular symmetry operation of the magnetic space group, which can be presented in either the geometric notation presented in the *International Tables for Crystallography* (2006), Volume A, section 11.1.2, or the Seitz notation as presented in *Acta Cryst.* (2014), A70, 300-302. This tag is intended for use with the BNS-supercell description of a magnetic structure.

Analogous tags: symCIF: **_space_group_symop.operation_description**

Ref: '*Magnetic Group Tables*' by D.B. Litvin at http://www.iucr.org/publ/978-0-9553602-2-0. ISO-MAG tables of H.T. Stokes and B.J. Campbell at http://iso.byu.edu.

_space_group_symop_magn_operation.id (*Text*)

An arbitrary identifier that uniquely labels each symmetry operation in a looped list of magnetic space-group symmetry operations. Most commonly, a sequence of positive integers is used for this identification. The **_space_group_symop_magn.id** alias provides backwards compatibility with the established magCIF prototype.

_space_group_symop_magn_operation.xyz (*Text*)

A parsable string giving one of the symmetry operations of the magnetic space group in algebraic form. The analogy between parsable labels for magnetic and non-magnetic symmetry operations is perfect except for the fact that a magnetic symop label ends with an additional piece of information ('-1' or '$+1$') indicating that the operation is or is not time-reversed, respectively. This tag is intended for use with the BNS-supercell description of a magnetic structure.

Analogous tags: symCIF: **_space_group_symop.operation_xyz**

Ref: '*Magnetic Group Tables*' by D.B. Litvin at http://www.iucr.org/publ/978-0-9553602-2-0. ISO-MAG tables of H.T. Stokes and B.J. Campbell at http://iso.byu.edu.

Examples: '`x+1/2,y+1/2,z,-1`' (a time-reversed (1/2,1/2,0) translation, i.e. anti-centering vector), '`-y,x,z+1/2,-1`' (a time-reversed 4_2 screw along (00z).), '`-y,x,z+1/2,+1`' (a non-time-reversed 4_2 screw along (00z).)

SPACE_GROUP_SYMOP_MAGN_SSG_CENTERING

This loop provides a list of the centering and anti-centering translations of a magnetic superspace-group.

Category key(s): **_space_group_symop_magn_ssg_centering.id**

_space_group_symop_magn_ssg_centering.algebraic (*Text*)

A parsable string giving one of the centering or anti-centering operations of the magnetic superspace group in algebraic form. The form of such a string is identical to that expected for **_space_group_symop_magn_ssg_operation.algebraic**, except that the rotational part of a translation must always be the identity element. See the description of **_space_group_symop_magn_centering.id** for more information about centering loops. This tag is intended for use with the BNS description of the magnetic basic cell.

Examples:

'`x1,x2,x3,x4,x5,+1`' (the identity element in (3+2)D), '`x1,x2,x3,x4+1/2,-1`' (a time-reversed superspace translation in (3+1)D based on a simple 180-degree phase shift of a single modulation vector'), '`x1+1/2,x2+1/2,x3+1/2,x4,+1`' (a non-time-reversed external body-center translation in (3+1)D), '`x1+1/2,x2,x3,x4,x5,x6+3/2,-1`' (a time-reversed superspace translation in (3+3)D that combines internal and external shifts)

_space_group_symop_magn_ssg_centering.id (*Text*)

An arbitrary identifier that uniquely labels each centering or anti-centering translations in a looped list of magnetic superspace-group symmetry operations. Most commonly, a sequence of positive integers is used for this identification. This tag is intended for use with the BNS description of the magnetic basic cell. Analogous to the case of magnetic space groups, the magCIF dictionary allows the subgroup of time-reversed and non-time-reversed fractional translations of a magnetic superspace group to be split off into a separate loop. See the description of **_space_group_symop_magn_centering.id** for more information about centering loops.

SPACE_GROUP_SYMOP_MAGN_SSG_OPERATION

A looped list of magnetic superspace-group symmetry operations.

Analogous tags: msCIF: **_space_group_symop.ssg_***

Category key(s): **_space_group_symop_magn_ssg_operation.id**

_space_group_symop_magn_ssg_operation.algebraic (*Text*)

A parsable string giving one of the symmetry operations of the magnetic superspace group in algebraic form. The analogy between parsable labels for magnetic and non-magnetic symmetry operations is perfect except for the fact that a magnetic symop label ends with an additional piece of information ('−1' or '+1') indicating that the operation is or is not time-reversed, respectively. This tag is intended for use with the BNS description of the magnetic basic cell.

Analogous tags: msCIF: **_space_group_symop.ssg_operation_algebraic**

Examples: 'x1,x2,x3,x4,x5,x6,+1' (the identity element in (3+3)D.), 'x1,x2,x3,x4+1/2,−1' (a superspace anti-centering translation based on a simple 180-degree phase shift of a single modulation vector), 'x1+1/2,x2+1/2,−x3,−x4,−1' (a time-reversed n-glide perpendicular to a z-axis modulation), 'x1−x2,x1,x3+1/3,x4−1/6,x5,+1' (a non-time-reversed 6_2 screw axis with phase shift along a pair of z-axis modulations)

_space_group_symop_magn_ssg_operation.id (*Text*)

An arbitrary identifier that uniquely labels each symmetry operation in a looped list of magnetic superspace-group symmetry operations. Most commonly, a sequence of positive integers is used for this identification. The **_space_group_symop_magn_ssg.id** alias provides backwards compatibility with the established magCIF prototype.

Analogous tags: msCIF: **_space_group_symop_ssg_id**