spinCIF: Preliminary definitions

[for full list, see index (on the left)]

(to be detailed further)

(just a first attempt at getting some of this formalized so that it can be accurately implemented in Jmol)

(for reference, see the magCIF dic). xyz

TODO:

- Check categories are correct (click to show link)
    - _atom_site_spin_moment
    - _space_group_spin
    - _space_group_symop_spin_lattice
    - _space_group_symop_spin_operation
-
- Check keys for correct names
- Check for missing categories or keys
- Check for already-obsolete preliminary keys

CIF Categories are **Heading 2**; CIF objects are **Heading 3**.

** _atom_site_spin_moment

_definition.id	ATOM_SITE_SPIN_MOMENT
_definition.scope	Category
_description.text	

;

This category provides a loop for presenting magnetic moments of spin origin

This is a similar category to atom_site_moment used in magCIF for the loop that specifies the magnetic moments without resolving the contributions of spin and orbital origin. Here the difference is that the magnetic moments given are supposed not to have any contribution of orbital orbital origin, as the transformation properties of moments of orbital origin for the SpSG operations are different. The atomic magnetic moments of orbital origin, if known, must be specified in a different loop of a different category, say atom_site_orbital_moment, which for the moment we do not develop, because experimentally it is quite difficult to resolve the spin and orbital contributions to the total moments, and there are no clear examples of this separation. The SpSGs are being applied so far assuming that the magnetic moments are fully of spin origin, having no orbital contribution.

This tag can also be used for descriptions using a MSGif the spin and orbital contribution to the moments is resolved.

(The name of this category is VERY provisional. The people from COMCIF should be consulted and probably it would be better in the end to have something shorter, to make it a direct child category of atom_site, as it is atom_site_ moment. For instance it could be atom_site_spinmoment and for the moments of orbital origin a similar category atom_site_orbitalmoment . It would be then convenient to introduce as alias this alternative for the name of this category)

Examples:

```
loop_
_atom_site_spin_moment.label
_atom_site_spin_moment.axis_u
_atom_site_spin_moment.axis_v
_atom_site_spin_moment.axis_w
_atom_site_spin_moment.symmform_uvw
_atom_site_spin_moment.magnitude
Pr1 1.53 0.0 0.95 ? 1.80
```

```
loop_
_atom_site_spin_moment.label
_atom_site_spin_moment.axis_u
_atom_site_spin_moment.axis_v
_atom_site_spin_moment.axis_w
```

_atom_site_spin_moment.symmform_uvw
_atom_site_spin_moment.magnitude
Mn1 3.0 0.0 0.0 u,0,0 3.0

;

* _atom_site_spin_moment.axis_u

_description.text
;

The component of the atom-site magnetic-moment vector parallel to the first axis of the spin basis.

Type: real

Units: Bohr magnetons

;

_name.category_id	atom_site_spin_moment
_name.object_id	axis_u

* _atom_site_spin_moment.axis_v

_description.text
;

The component of the atom-site magnetic-moment vector parallel to the second axis of the spin basis.

Type: real

Units: Bohr magnetons

;

_name.category_id	atom_site_spin_moment
_name.object_id	axis_v

* _atom_site_spin_moment.axis_w

_description.text

;

_atom_site_spin_moment.axis_w

The component of the atom-site magnetic-moment vector parallel to the third axis of the spin basis.

Type: real

Units: Bohr magnetons

;

_name.category_id	atom_site_spin_moment
_name.object_id	axis_w

* _atom_site_spin_moment.label

_description.text

;

Label of the atom for which the spin-moment is specified. The atom label must be a reference to a value of _atom_site.label.

;

_name.category_id	atom_site_spin_moment
_name.object_id	label

* _atom_site_spin_moment.magnitude

_description.text

;

The magnitude of the spin-magnetic moment vector of the atom-site

Type: real

Units: Bohr magnetons

;
    _name.category_id atom_site_spin_moment
    _name.object_id magnitude

* _atom_site_spin_moment.symmform_uvw

    _description.text
;

A symbolic expression that indicates the symmetry-restricted form of the components of the spin-magnetic moment vector of the atom, described in the spin basis. In the case of collinear structures, it does not bring any additional information, except in the case of the moment being forced to be identically cero, otherwise it is reasonable to have it unfilled, as in the collinear case the spin and lattice basis coincide.

Examples:

0,0,0

u,u,0

0,0,w

;
    _name.category_id atom_site_spin_moment
    _name.object_id symmform_uvw

** _space_group_spin

_description.text
;
[description here]
;
_definition.id SPACE_GROUP_SPIN
_definition.scope Category

* _space_group_spin.collinear_direction

_description.text
;

Indicates that the described structure and its SpSG are collinear and optionally also its direction or a plane where this direction is located. This tag is mandatory in collinear structures. The spin direction is specified with respect to the lattice unit cell. If the meaning is that the value can be any orientation, the string literal “nx,ny,nz” should be used. If the spin direction is known to lie on some specific plane, this tag can indicate this plane using (nx,ny,nz) components with respect to the lattice unit cell. For instance, “nx,ny,0” means the spin direction is known to lie on the xy plane. If the spin direction is known, the tag indicates this direction, for instance “0,0,nz” if the direction is along c.

Examples:

_space_group_spin.collinear_direction “nx,2nx, nz”
_space_group_spin.collinear_directio n “nx, nx, 0”
_space_group_spin.collinear_direction “nx, 0, nz”
_space_group_spin.collinear_direction “0, 0, nz”

;
_name.category_id space_group_spin
_name.object_id collinear_direction

* _space_group_spin.coplanar_perp_uvw

_description.text

;

It indicates that the described structure and its SpSG are coplanar. This tag is mandatory in coplanar structures. It specifies the direction of the normal to the spin plane. The direction is given in the spin basis with integers as components. By convention this direction is normally chosen “0,0,1”, but other choices are allowed, as long as the U spin operations are given consistently with this choice.

Examples:

_space_group_spin.coplanar_perp_uvw “0,0,1”
_space_group_spin.coplanar_perp_uvw “1,1,0”

;

_name.category_id space_group_spin
_name.object_id coplanar_perp_uvw

* _space_group_spin.name_SpSG_Chen

_description.text

;

So-called international symbol of the SpSG, as proposed in Chen et al. (2024), with the collinear or coplanar character of the SpSG indicated with “.L” or “.P”, instead of the symbols of the trivial spin-only subgroups. (the notation for type 4 collinear groups and the groups with spin lattice groups will probably require yet further changes)

Examples:

_space_group_spin.name_SpSG_Chen “P(3)63/(1)m(2)m(2)c.P”

;

_name.category_id space_group_spin
_name.object_id name_SpSG_Chen

* _space_group_spin.number_SpSG_Chen

_description.text

;

Four-index numerical label of the nontrivial SpSG, as proposed in Chen et al. (2024), completed with ".L" or ".P" in the case of being a collinear or a coplanar SpSG, respectively.

Examples:

_space_group_spin.number_SpSG_Chen "11.194.1.6.P"

;

_name.category_id space_group_spin
_name.object_id number_SpSG_Chen

* _space_group_spin.rotation_angle

_description.text

;

Specifies the angle (in degrees) of the rotation to be applied to the spins around the axis specified in the tag **_space_group_spin.rotation_axis,** in order to obtain the final structure.

Examples:

_space_group_spin.rotation_angle 60

;

_name.category_id space_group_spin
_name.object_id rotation_angle

* _space_group_spin.rotation_axis_xyz

_description.text

;

The direction of the axis with respect to the lattice unit cell (with integers as components) around which a rotation of an angle specified by the tag _space_group_spin.rotation_angle must be applied to the spin arrangement in order to obtain the final structure.

Any spin vector **M** in the structure, with components (mx, my, mz) in the lattice basis, is then transformed to its final form **M'**, with components (m'x, m'y, m'z), according to the equation:

$$\mathbf{M_r'} = \mathbf{T}(\mathbf{n}, [\text{theta}]) \, . \, \mathbf{M_r}$$

where $\mathbf{M_r}$ and $\mathbf{M_r'}$ are spin vectors expressed as columns in relative components: (mx/a, my/b, mz/c) and (m'x/a, m'y/b, m'z/c), and **T**(**n**, [theta]) is the matrix form of an axis-angle representation.

Examples:

_space_group_spin.rotation_axis_xyz "0,0,1"
_space_group_spin.rotation_axis_xyz "1,2,0"

;

_name.category_id	space_group_spin
_name.object_id	rotation_axis_xyz

* _space_group_spin.rotation_axis_cartn

_description.text

;

The unit vector, defined as a three-element white-space separated CIF 2 list [ax ay az] describing the Euler axis of rotation of the spin frame relative to a Cartesian frame.

Examples:

_space_group_spin.rotation_axis_cartn [0 0 1] _space_group_spin.rotation_axis_cartn [0.6324555320336759 0.6324555320336759 0.4472135954999579]

;
_name.category_id space_group_spin
_name.object_id rotation_axis_cartn

* _space_group_spin.transform_spinframe_P_abc

_description.text
;

This tag is used to define the spin basis and to give it a specific orientation with respect to the lattice. It specifies the transformation from the unit cell used for the description of the atomic positions and the space part, R, of the SpSG symmetry operations to the basis used for the description of spins and the spin part, U, of the symmetry operations. The basis vectors (a_s,b_s,c_s) for the spins are described as linear combinations of the basis vectors (a,b,c) that define the structure unit cell. In principle, the possible linear combinations can be defined as any three linearly independent vectors, but in practice, the spin basis so defined must be consistent with the setting used to describe the spin operations U, and this strongly restricts the possible combinations.

If absent, and no other alternative tag is present that defines the spin basis, the spin basis is assumed to be coincident with the lattice unit cell (a,b,c).

In the case of collinear structures, to define a spin basis different from the lattice unit cell does not bring any advantage. Therefore the spin basis and the lattice basis (unit cell) are assumed to coincide in the description of all collinear structure, so that this tag is not necessary. If the tag is present in the file, it should be filled with “a,b,c”, indicating this coincidence.

[NOTE: The spin basis could be defined without any specific relation with the lattice unit cell, for instance as an orthonormal basis with unspecified orientation with respect to the lattice, as is done in some theoretical papers. We have not yet worked out this approach in the sCIF format. It is not clear that it may have any advantage, because, even in this case, in general, to fully specify a magnetic structure, it is necessary to give a specific orientation of this spin basis with respect to the lattice unit cell, because even if the energy is independent of this orientation assuming null SOC, many other properties – for instance neutron diffraction, most tensor properties – depend on this orientation.]

Examples:

_space_group_spin.transform_spinframe_P_abc 'a,b,c'
_space_group_spin.transform_spinframe_P_abc 'a+b,-a,c'
_space_group_spin.transform_spinframe_P_abc 'a,a+2b,c'
_space_group_spin.transform_spinframe_P_abc 'a,a+2b,c'
;
_name.category_id space_group_spin
_name.object_id tansform_spinframe_P_abc

* _space_group_spin.transform_spinframe_P_matrix

_description.text
;

This tag is an alternative to _space_group_spin.transform_spinframe_P_abc. The value is a CIF 2.0 double list representing

Examples:

_space_group_spin.transform_spinframe_P_abc 'a,b,c'
_space_group_spin.transform_spinframe_P_abc 'a+b,-a,c'
_space_group_spin.transform_spinframe_P_abc 'a,a+2b,c'
;
_name.category_id space_group_spin
_name.object_id tansform_spinframe_P_matrix

** _space_group_symop_spin_lattice

_definition.id SPACE_GROUP_SYMOP_SPIN_LATTICE
_definition.scope Category

;

This category provides a loop for specifying the symmetry operations of the so-called spin translation subgroup of the spin space group. It is formed by the operations that combine a space translation and a spin transformation. The same format is used as in the main loop space_group_symop_spin_operation. As the operations forming the trivial spin-only subgroups are not listed in any case, specifying in this separate loop these operations allow to leave in the main loop only a single representative of all operations having the same space point-group operation. The combination of the operations listed in the two loops produces the full set of representative operations of the nontrivial spin space group. This second loop is optional and it is always possible to include all of the symmetry operations in the main loop. This is a similar category to space_group_symop_magn_centering used in magCIF.

This category contains the following items:

_space_group_symop_spin_lattice.id
_space_group_symop_spin_lattice.xyzt
_space_group_symop_spin_lattice.uvw
_space_group_symop_spin_lattice.uvw_id

Examples:

```
loop_
_space_group_symop_spin_lattice.id
_space_group_symop_spin_lattice.xyzt
_space_group_symop_spin_lattice.uvw
1 x,y,z,+1        u,v,w
2 x,y,z+1/2,-1   -u,-v,-w
```

```
loop_
_space_group_symop_spin_lattice.id
_space_group_symop_spin_lattice.xyzt
_space_group_symop_spin_lattice.uvw
1 x,y,z,+1                    u,v,w
```

2 x+1/3,y,z,+1 -v,u-v,w
3 x,y+1/3,z,+1 -v,u-v,w
4 x+1/3,y+1/3,z,+1 -u+v,-u,w
5 x+2/3,y,z,+1 -u+v,-u,w
6 x,y+2/3,z,+1 -u+v,-u,w
7 x+2/3,y+1/3,z,+1 u,v,w
8 x+1/3,y+2/3,z,+1 u,v,w
9 x+2/3,y+2/3,z,+1 -v,u-v,w
10 x,y,z+1/4,+1 1/sqrt(3)u-2/sqrt(3)v,2/sqrt(3)u-1/sqrt(3)v,w
11 x+1/3,y,z+1/4,+1 -2/sqrt(3)u+1/sqrt(3)v,-1/sqrt(3)u-1/sqrt(3)v,w
12 x,y+1/3,z+1/4,+1 -2/sqrt(3)u+1/sqrt(3)v,-1/sqrt(3)u-1/sqrt(3)v,w
13 x+1/3,y+1/3,z+1/4,+1 1/sqrt(3)u+1/sqrt(3)v,-1/sqrt(3)u+2/sqrt(3)v,w
14 x+2/3,y,z+1/4,+1 1/sqrt(3)u+1/sqrt(3)v,-1/sqrt(3)u+2/sqrt(3)v,w
15 x,y+2/3,z+1/4,+1 1/sqrt(3)u+1/sqrt(3)v,-1/sqrt(3)u+2/sqrt(3)v,w
16 x+2/3,y+1/3,z+1/4,+1 1/sqrt(3)u-2/sqrt(3)v,2/sqrt(3)u-1/sqrt(3)v,w
17 x+1/3,y+2/3,z+1/4,+1 1/sqrt(3)u-2/sqrt(3)v,2/sqrt(3)u-1/sqrt(3)v,w
18 x+2/3,y+2/3,z+1/4,+1 -2/sqrt(3)u+1/sqrt(3)v,-1/sqrt(3)u-1/sqrt(3)v,w
19 x,y,z+1/2,+1 -u,-v,w
20 x+1/3,y,z+1/2,+1 v,-u+v,w
21 x,y+1/3,z+1/2,+1 v,-u+v,w
22 x+1/3,y+1/3,z+1/2,+1 u-v,u,w
23 x+2/3,y,z+1/2,+1 u-v,u,w
24 x,y+2/3,z+1/2,+1 u-v,u,w
25 x+2/3,y+1/3,z+1/2,+1 -u,-v,w
26 x+1/3,y+2/3,z+1/2,+1 -u,-v,w
27 x+2/3,y+2/3,z+1/2,+1 v,-u+v,w
28 x,y,z+3/4,+1 -1/sqrt(3)u+2/sqrt(3)v,-2/sqrt(3)u+1/sqrt(3)v,w
29 x+1/3,y,z+3/4,+1 2/sqrt(3)u-1/sqrt(3)v,1/sqrt(3)u+1/sqrt(3)v,w
30 x,y+1/3,z+3/4,+1 2/sqrt(3)u-1/sqrt(3)v,1/sqrt(3)u+1/sqrt(3)v,w
31 x+1/3,y+1/3,z+3/4,+1 -1/sqrt(3)u-1/sqrt(3)v,1/sqrt(3)u-2/sqrt(3)v,w
32 x+2/3,y,z+3/4,+1 -1/sqrt(3)u-1/sqrt(3)v,1/sqrt(3)u-2/sqrt(3)v,w
33 x,y+2/3,z+3/4,+1 -1/sqrt(3)u-1/sqrt(3)v,1/sqrt(3)u-2/sqrt(3)v,w
34 x+2/3,y+1/3,z+3/4,+1 -1/sqrt(3)u+2/sqrt(3)v,-2/sqrt(3)u+1/sqrt(3)v,w
35 x+1/3,y+2/3,z+3/4,+1 -1/sqrt(3)u+2/sqrt(3)v,-2/sqrt(3)u+1/sqrt(3)v,w
36 x+2/3,y+2/3,z+3/4,+1 2/sqrt(3)u-1/sqrt(3)v,1/sqrt(3)u+1/sqrt(3)v,w

(This is an example of 90 degrees spin rotations, described in the lattice basis, which is hexagonal. Probably it would be more efficient for such cases to allow the format to define an independent orthonormal spin basis, and use a single tag to specify the orientation of this basis with respect to the lattice. How to define this tag, and which kind of parameterization should be use for specifying this orientation, is something to be discussed yet)

;

* _space_group_symop_spin_lattice.id

_description.text

;

An arbitrary identifier that uniquely labels each operation in a looped list of representative operations of the spin-lattice subgroup of the nontrivial group of the spin space group. Most commonly, a sequence of positive integers is used for this identification.

;

_name.category_id	space_group_spin_lattice
_name.object_id	id

* _space_group_symop_spin_lattice.uvw

_description.text

;

The representation of the spin lattice operation in u,v,w format. An alternative to using _space_group_symop_spin_lattice.uvw_id. See _space_group_symop_spin_upart.uvw.

;

_name.category_id	space_group_spin_lattice
_name.object_id	uvw

* _space_group_symop_spin_lattice.uvw_id

_description.text

;

A reference to _space_group_symop_spin_upart.id.

;

_name.category_id	space_group_spin_lattice
_name.object_id	uvw_id

* _space_group_symop_spin_lattice.xyzt

_description.text

;

A parsable string giving the space part in algebraic form of one of the representative operations (not equivalent by lattice translations) belonging to the spin-lattice subgroup of the nontrivial spin space group. These operations are formed by a space translation together with a spin transformation, with the zero translation only combined with the identity for the spin transformation. The format of such a string is identical to that expected for _space_group_symop_spin_operation.xyzt, except that the rotational part of the operation must always be the identity element, in order to represent a translation.

;

_name.category_id	space_group_spin_lattice
_name.object_id	xyzt

** _space_group_symop_spin_operation

_definition.id SPACE_GROUP_SYMOP_SPIN_OPERATION
_definition.scope Category
_description.text
;

This category provides a loop for specifying the symmetry operations of the spin space group, excluding the trivial spin-only subgroup. It is mandatory and must include all operations of the non-trivial group, which are not related by a lattice translation, except in the case of using the optional loop space_group_symop_spin_lattice (see below). This second auxiliary loop allows to shorten the present loop by listing only a representative of the operations that differ by a (non-lattice) translation. This is a similar category to space_group_symop_magn_operation used in magCIF for the loop that specifies the symmetry operations of the MSG. Here, the difference is that, in addition to the operation for the space coordinates, described with x,y,z symbols, and the "-1" or "+1", to indicate the inclusion or not of time reversal, the spin point-group operation is also separately specified, as it is not determined by the space operation as it happens in a MSG.

This category contains the following items:

_space_group_symop_spin_operation.id
_space_group_symop_spin_operation.xyzt
_space_group_symop_spin_operation.uvw
_space_group_symop_spin_operation.uvw_id

Examples:

```
loop_
_space_group_symop_spin_operation.id
_space_group_symop_spin_operation.xyzt
_space_group_symop_spin_operation.uvw
1 x,y,z,+1      u,v,w
2 -x,-y,z,+1    u,v,w
3 y,x,-z,-1     -u,-v,-w
4 -y,-x,-z,-1   -u,-v,-w
5 -x,-y,-z,+1   u,v,w
6 x,y,-z,+1     u,v,w
7 -y,-x,z,-1    -u,-v,-w
8 y,x,z,-1      -u,-v,-w
9 -y,x,z,-1     -u,-v,-w
10 y,-x,z,-1    -u,-v,-w
```

```
11 x,-y,-z,+1    u,v,w
12 -x,y,-z,+1            u,v,w
13 y,-x,-z,-1    -u,-v,-w
14 -y,x,-z,-1    -u,-v,-w
15 -x,y,z,+1             u,v,w
16 x,-y,z,+1             u,v,w


loop_
_space_group_symop_spin_operation.id
_space_group_symop_spin_operation.xyzt
_space_group_symop_spin_operation.uvw
1 x,y,z,+1       u,v,w
2 x-y,x,z+1/2,+1         -v,u-v,w
3 -y,x-y,z,+1    -u+v,-u,w
4 -x,-y,z+1/2,+1         u,v,w
5 -x+y,-x,z,+1           -v,u-v,w
6 y,-x+y,z+1/2,+1        -u+v,-u,w
7 -x,-y,-z,+1            u,v,w
8 -x+y,-x,-z+1/2,+1  -v,u-v,w
9 y,-x+y,-z,+1           -u+v,-u,w
10 x,y,-z+1/2,+1         u,v,w
11 x-y,x,-z,+1           -v,u-v,w
12 -y,x-y,-z+1/2,+1  -u+v,-u,w
13 x-y,-y,-z,+1          u-v,-v,-w
14 y,x,-z,+1     -u,-u+v,-w
15 -x,-x+y,-z,+1         v,u,-w
16 x,x-y,-z+1/2,+1       v,u,-w
17 -x+y,y,-z+1/2,+1   u-v,-v,-w
18 -y,-x,-z+1/2,+1       -u,-u+v,-w
19 -x+y,y,z,+1           u-v,-v,-w
20 -y,-x,z,+1            -u,-u+v,-w
21 x,x-y,z,+1            v,u,-w
22 -x,-x+y,z+1/2,+1   v,u,-w
23 x-y,-y,z+1/2,+1       u-v,-v,-w
24 y,x,z+1/2,+1          -u,-u+v,-w
```

;

* _space_group_symop_spin_operation.id

_description.text

;

An arbitrary identifier that uniquely labels each symmetry operation in a looped list of spin space-group symmetry operations. Most commonly, a sequence of positive integers is used for this identification.

;

_name.category_id space_group_spin_operation
_name.object_id id

* _space_group_symop_spin_operation.uvw

_description.text

;

The representation of the spin operation in u,v,w format. An alternative to using _space_group_symop_spin_operation.uvw_id. See _space_group_symop_spin_upart.uvw.

;

_name.category_id space_group_spin_operation
_name.object_id uvw

* _space_group_symop_spin_operation.uvw_id

_description.text

;

A reference to _space_group_symop_spin_Upart.id.

;

_name.category_id space_group_spin_operation
_name.object_id uvw_id

* _space_group_symop_spin_operation.xyzt

_description.text

;

A parsable string giving in algebraic form the part of the symmetry operation of the spin space group corresponding to the transformation of a general position in space, completed with the information of the inclusion or not of time reversal. The analogy with non-magnetic symmetry operations is perfect, except for the fact that it ends with an additional piece of information ("-1" or "+1") indicating that the operation is or is not time-reversed, respectively.

;

_name.category_id space_group_spin_operation

_name.object_id xyzt

** _space_group_symop_spin_Upart

_definition.id SPACE_GROUP_SYMOP_SPIN_UPART

_definition.scope Category

_description.text

;

This category allows for efficiently referencing spin operation u,v,w representations from the categories _space_group_spin_operation and _space_group_spin_lattice. This discussion also describes the required format for _space_group_symop_spin_lattice.uvw and _space_group_symop_spin_operation.uvw.

The uvw representation is a parsable string giving in algebraic form describing the part of the symmetry operation of the spin space group corresponding to the transformation of the spins. The spin operation is indicated using coordinates u,v,w, which refer to the spin basis, which in general may be different from the lattice unit cell.

In the case that the spin operation combines spin components corresponding to basis vectors of the spin basis of different magnitude, the u,v,w components in the expression should be interpreted as relative components, i.e. as U/a_s, V/b_s and W/c_s, where U,V,W are the absolute components of the spin in the basis (a_s, b_s, c_s). In any other case, the result is the same if the operation is interpreted as valid for absolute or relative spin components.

The determinant of the spin transformation described by this string must be consistent with the time reversal presence or not (-1 or 1) in the associated value for tags _space_group_symop_spin_lattice.xyzt and _space_group_symop_spin_operation.xyzt being necessarily -1, in the first case.

The format to express this spin part of the operation allows the presence of symbols like sqrt(..), cos(…), sin(…), tan(…), “+”, “-“, “*”, “/” to represent obvious operations or functions. In general, the presence in the expression of u, v or w is preceded by some factor, where these symbols can be used. Arguments of trigonometric functions should be degrees (to be completed)

;

* _space_group_symop_spin_Upart.id

_description.text

;

The key for this category.

;

_name.category_id space_group_spin_Upart
_name.object_id id

* _space_group_symop_spin_Upart.uvw

_description.text

;

The representation of the spin operation in u,v,w format.

;

_name.category_id space_group_spin_lattice
_name.object_id uvw_id