Dictionary name: **cif_ms.dic**
Dictionary version: 1.0
Dictionary last updated: 2002-03-04

`_atom_site_displace_modulation_flag` (*char*)

A code that signals if the structural model includes the modulation of the positional coordinates of a given atomic site.

`yes`	displacive modulation
`y`	abbreviation for "yes"
`no`	no displacive modulation
`n`	abbreviation for "no"

Appears in list containing `_atom_site_label`. Where no value is given, the assumed value is `'no'`. [`atom_site`]

`_atom_site_occ_modulation_flag` (*char*)

A code that signals if the structural model includes the modulation of the occupation of a given atomic site.

`yes`	occupational modulation
`y`	abbreviation for "yes"
`no`	no occupational modulation
`n`	abbreviation for "no"

Appears in list containing `_atom_site_label`. Where no value is given, the assumed value is `'no'`. [`atom_site`]

`_atom_site_subsystem_code` (*char*)

A code that links a given atom or rigid-group site to one of the subsystems present in a composite. This code provides an alternative description for composites less explicit than that based on linked data blocks (see the description in this dictionary of `_audit_link_[ms]`). It must match one of the labels specified for `_cell_subsystem_code`.

Appears in list containing `_atom_site_label`. **Must** match data name `_cell_subsystem_code`. [`atom_site`]

`_atom_site_U_modulation_flag` (*char*)

A code that signals if the structural model includes the modulation of the thermal parameters of a given atomic site.

`yes`	modulation of thermal parameters
`y`	abbreviation for "yes"
`no`	no modulation of thermal parameters
`n`	abbreviation for "no"

Appears in list containing `_atom_site_label`. Where no value is given, the assumed value is `'no'`. [`atom_site`]

`_atom_site_displace_Fourier_[]`

Data items in the ATOM_SITE_DISPLACE_FOURIER category record details about the Fourier components of the displacive modulation of an atom site in a modulated structure. In the case of rigid groups items in this category would only include the translational part of the modulation. The rotational part would appear in a separate list of items belonging to the ATOM_SITE_ROT_FOURIER category. The (in general complex) coefficients of each Fourier component belong to the category ATOM_SITE_DISPLACE_FOURIER_PARAM and are listed separately.

Example 1 - extracted from van Smaalen [(1991). J. Phys.: Condens. Matter 3, 1247–1263.]

```
loop_
   _atom_site_Fourier_wave_vector_seq_id
   _atom_site_Fourier_wave_vector_x
   _atom_site_Fourier_wave_vector_description
        1       0.568           'First harmonic'
        2       1.136           'Second harmonic'
loop_
   _atom_site_displace_Fourier_id
   _atom_site_displace_Fourier_atom_site_label
   _atom_site_displace_Fourier_axis
   _atom_site_displace_Fourier_wave_vector_seq_id
        Nb1z1   Nb1   z   1
        Nb1x2   Nb1   x   2
        Nb1y2   Nb1   y   2
        S1x1    S1    x   1
        S1y1    S1    y   1
        S1z1    S1    z   1
        S1x2    S1    x   2
        S1y2    S1    y   2
        S1z2    S1    z   2
```

Example 2 - extracted from van Smaalen [(1991). J. Phys.: Condens. Matter 3, 1247–1263.]

```
# NbS2 subsystem has been chosen as reference, i.e. its
# W matrix is the unit matrix.
loop_
   _cell_subsystem_code
   _cell_subsystem_description
   _cell_subsystem_matrix_W_1_1
   _cell_subsystem_matrix_W_1_4
   _cell_subsystem_matrix_W_2_2
   _cell_subsystem_matrix_W_3_3
   _cell_subsystem_matrix_W_4_1
   _cell_subsystem_matrix_W_4_4
        NbS2   '1st subsystem'  1 0 1 1 0 1
        LaS    '2nd subsystem'  0 1 1 1 1 0
# The modulation wave vectors are referred to the reciprocal
# basis of each subsystem. They are related to the
# reciprocal basis used to index the whole diffraction
# pattern through the W matrices.
loop_
   _atom_site_Fourier_wave_vector_seq_id
   _atom_site_Fourier_wave_vector_x
   _atom_site_Fourier_wave_vector_z
   _atom_site_Fourier_wave_vector_description
        1      0.568     0      'First harmonic'
        2      1.136     0      'Second harmonic'
        3      1.761     0.5    'First harmonic'
        4      3.522     1.0    'Second harmonic'
# The modulation coefficients given below are referred to
# each subsystem.
loop_
   _atom_site_displace_Fourier_id
   _atom_site_displace_Fourier_atom_site_label
   _atom_site_displace_Fourier_axis
   _atom_site_displace_Fourier_wave_vector_seq_id
        Nb1z1_NbS2    Nb1     z    1
        Nb1x2_NbS2    Nb1     x    2
        Nb1y2_NbS2    Nb1     y    2
        S1x1_NbS2     S1      x    1
        S1y1_NbS2     S1      y    1
        S1z1_NbS2     S1      z    1
        S1x2_NbS2     S1      x    2
        S1y2_NbS2     S1      y    2
        S1z2_NbS2     S1      z    2
        La1x3_LaS     La1     x    3
        La1y3_LaS     La1     y    3
        La1z3_LaS     La1     z    3
        La1x4_LaS     La1     x    4
        La1y4_LaS     La1     y    4
        La1z4_LaS     La1     z    4
        S2x3_LaS      S2      x    3
        S2y3_LaS      S2      y    3
        S2z3_LaS      S2      z    3
        S2x4_LaS      S2      x    4
        S2y4_LaS      S2      y    4
        S2z4_LaS      S2      z    4
```

Example 3 - extracted from van Smaalen [(1991). J. Phys.: Condens. Matter 3, 1247–1263.]

```
# The same structural data but expressed using a set of
# linked data blocks
# Items concerning the modulated structure of the first
# subsystem
data_LaSNbS2_MOD_NbS2
_audit_block_code       1997-07-24|LaSNbS2|G.M.|_MOD_NbS2
loop_
   _audit_link_block_code
   _audit_link_block_description
1997-07-24|LaSNbS2|G.M.|
              'common experimental and publication data'
1997-07-24|LaSNbS2|G.M.|_REFRNCE
                    'reference structure (common data)'
1997-07-21|LaSNbS2|G.M.|_MOD
                    'modulated structure (common data)'
1997-07-24|LaSNbS2|G.M.|_REFRNCE_NbS2
                   'reference structure (1st subsystem)'
.                  'modulated structure (1st subsystem)'
1997-07-24|LaSNbS2|G.M.|_REFRNCE_LaS
                   'reference structure (2nd subsystem)'
1997-07-21|LaSNbS2|G.M.|_MOD_LaS
                   'modulated structure (2nd subsystem)'
loop_
   _atom_site_Fourier_wave_vector_seq_id
   _atom_site_Fourier_wave_vector_x
   _atom_site_Fourier_wave_vector_description
        1      0.568     'First harmonic'
        2      1.136     'Second harmonic'
loop_
   _atom_site_displace_Fourier_id
   _atom_site_displace_Fourier_atom_site_label
   _atom_site_displace_Fourier_axis
   _atom_site_displace_Fourier_wave_vector_seq_id
        Nb1z1   Nb1   z     1       Nb1x2   Nb1   x     2
        Nb1y2   Nb1   y     2       S1x1    S1    x     1
        S1y1    S1    y     1       S1z1    S1    z     1
        S1x2    S1    x     2       S1y2    S1    y     2
        S1z2    S1    z     2
#### End of modulated structure first subsystem data ####
# Items concerning the modulated structure of the second
# subsystem
data_LaSNbS2_MOD_LaS
_audit_block_code       1997-07-24|LaSNbS2|G.M.|_MOD_LaS
loop_
   _audit_link_block_code
   _audit_link_block_description
1997-07-24|LaSNbS2|G.M.|
              'common experimental and publication data'
1997-07-24|LaSNbS2|G.M.|_REFRNCE
                    'reference structure (common data)'
1997-07-21|LaSNbS2|G.M.|_MOD
                    'modulated structure (common data)'
1997-07-24|LaSNbS2|G.M.|_REFRNCE_NbS2
                   'reference structure (1st subsystem)'
1997-07-21|LaSNbS2|G.M.|_MOD_NbS2
                   'modulated structure (1st subsystem)'
1997-07-24|LaSNbS2|G.M.|_REFRNCE_LaS
                   'reference structure (2nd subsystem)'
.                  'modulated structure (2nd subsystem)'
loop_
   _atom_site_Fourier_wave_vector_seq_id
   _atom_site_Fourier_wave_vector_x
   _atom_site_Fourier_wave_vector_z
   _atom_site_Fourier_wave_vector_description
        1      1.761   0.5   'First harmonic',
        2      3.522   1.0   'Second harmonic'
loop_
   _atom_site_displace_Fourier_id
   _atom_site_displace_Fourier_atom_site_label
   _atom_site_displace_Fourier_axis
   _atom_site_displace_Fourier_wave_vector_seq_id
        La1x1   La1   x     1       La1y1   La1   y     1
        La1z1   La1   z     1       La1x2   La1   x     2
        La1y2   La1   y     2       La1z2   La1   z     2
        S2x1    S2    x     1       S2y1    S2    y     1
        S2z1    S2    z     1       S2x2    S2    x     2
        S2y2    S2    y     2       S2z2    S2    z     2
#### End of modulated structure second subsystem data ####
```

Example 4 - extracted from Baudour & Sanquer [(1983). Acta Cryst. B39, 75–84.] Note the entry from the ATOM_SITES_DISPLACE_FOURIER category to describe collective information relating to all the atom sites.

```
_atom_sites_displace_Fourier_axes_description
;  a1 and a2 are respectively the long molecular axis
   and the axis normal to the mean molecular plane.
;
loop_
   _atom_site_displace_Fourier_id
   _atom_site_displace_Fourier_atom_site_label
   _atom_site_displace_Fourier_axis
   _atom_site_displace_Fourier_wave_vector_seq_id
        Byphenyl_a1_1    Biphenyl  a1    1
```

`_atom_site_displace_Fourier_atom_site_label` (*char*)

Modulation parameters are usually looped in separate lists. Modulated parameters are the atomic positions (displacive modulation), the atomic occupation (occupational modulation) and/or the atomic anisotropic (or isotropic) displacement parameters (referred to as modulation of thermal parameters since the term 'displacement parameters' is ambiguous in this context). `_atom_site_displace_Fourier_atom_site_label` is the code that identifies an atom or rigid group in a loop where the Fourier components of its displacive modulation are being listed. In the case of a rigid group this list would only include the translational part of its displacive modulation. The rotational part (if any) would appear in a separate list (see `_atom_site_rot_Fourier_atom_site_label`). This code must match the `_atom_site_label` of the associated coordinate list and conform to the rules described in `_atom_site_label`.

Appears in list containing `_atom_site_displace_Fourier_id`. **Must** match data name `_atom_site_label`.

[atom_site_displace_Fourier]

`_atom_site_displace_Fourier_axis` (*char*)

A label identifying the displacement component of a given atom or rigid group that is being parameterized by Fourier series. **a**, **b** and **c** are the basic lattice vectors of the reference structure. For composites they refer to the reference structure of each subsystem. $\mathbf{a}_1$, $\mathbf{a}_2$ and $\mathbf{a}_3$ are defined by `_atom_site_displace_Fourier_axes_description`.

x	displacement along the **a** axis
y	displacement along the **b** axis
z	displacement along the **c** axis
a1	displacement along an arbitrary $\mathbf{a}_1$ axis
a2	displacement along an arbitrary $\mathbf{a}_2$ axis
a3	displacement along an arbitrary $\mathbf{a}_3$ axis

Appears in list containing `_atom_site_displace_Fourier_id`.

[atom_site_displace_Fourier]

`_atom_site_displace_Fourier_id` (*char*)

A code identifying each component of the displacive modulation of a given atom or rigid group when it is expressed in terms of Fourier series. In the case of a rigid group it applies only to the translational part of the distortion.

Appears in list as essential element of loop structure. May match subsidiary data name(s): `_atom_site_displace_Fourier_param_id`.

[atom_site_displace_Fourier]

`_atom_site_displace_Fourier_wave_vector_seq_id` (*numb*)

A numeric code identifying the wave vectors of the Fourier terms used in the structural model to describe the displacive modulation of an atom or rigid group. In the case of a rigid group it applies only to the translational part of the distortion. This code must match `_atom_site_Fourier_wave_vector_seq_id`.

Appears in list containing `_atom_site_displace_Fourier_id`. **Must** match data name `_atom_site_Fourier_wave_vector_seq_id`.

[atom_site_displace_Fourier]

`_atom_site_displace_Fourier_param_[]`

Data items in the ATOM_SITE_DISPLACE_FOURIER_PARAM category record details about the coefficients of the Fourier series used to describe the displacive modulation of an atom or rigid group. In the case of rigid groups items in this category would only include the translational part of the modulation. The rotational part would appear in a separate list of items belonging to the ATOM_SITE_ROT_FOURIER_PARAM category. The Fourier components are defined in the category ATOM_SITE_FOURIER and are listed separately.

Example 1 - extracted from van Smaalen [(1991). J. Phys.: Condens. Matter 3, 1247–1263.]

```
loop_
   _atom_site_Fourier_wave_vector_seq_id
   _atom_site_Fourier_wave_vector_x
   _atom_site_Fourier_wave_vector_description
        1       0.568           'First harmonic'
        2       1.136           'Second harmonic'
loop_
   _atom_site_displace_Fourier_id
   _atom_site_displace_Fourier_atom_site_label
   _atom_site_displace_Fourier_axis
   _atom_site_displace_Fourier_wave_vector_seq_id
        Nb1z1   Nb1   z     1       Nb1x2   Nb1   x     2
        Nb1y2   Nb1   y     2       S1x1    S1    x     1
        S1y1    S1    y     1       S1z1    S1    z     1
        S1x2    S1    x     2       S1y2    S1    y     2
        S1z2    S1    z     2
loop_
   _atom_site_displace_Fourier_param_id
   _atom_site_displace_Fourier_param_cos
   _atom_site_displace_Fourier_param_sin
Nb1z1 -0.0006(2)   0.          Nb1x2  0.          0.0078(17)
Nb1y2 -0.0014(7)   0.          S1x1   0.         -0.0134(85)
S1y1  -0.0022(12)  0.          S1z1   0.0014(14)  0.
S1x2   0.         -0.0129(27)  S1y2  -0.0073(27)  0.
S1z2  -0.0012(3)   0.
```

Example 2 - extracted from van Smaalen [(1991). J. Phys.: Condens. Matter 3, 1247–1263.]

```
# NbS2 subsystem has been chosen as reference, i.e. its
# W matrix is the unit matrix.
loop_
   _cell_subsystem_code
   _cell_subsystem_description
   _cell_subsystem_matrix_W_1_1
   _cell_subsystem_matrix_W_1_4
   _cell_subsystem_matrix_W_2_2
   _cell_subsystem_matrix_W_3_3
   _cell_subsystem_matrix_W_4_1
   _cell_subsystem_matrix_W_4_4
        NbS2   '1st subsystem'  1 0 1 1 0 1
        LaS    '2nd subsystem'  0 1 1 1 1 0
# The modulation wave vectors are referred to the reciprocal
# basis of each subsystem. They are related to the
# reciprocal basis used to index the whole diffraction
# pattern through the W matrices.
loop_
   _atom_site_Fourier_wave_vector_seq_id
   _atom_site_Fourier_wave_vector_x
   _atom_site_Fourier_wave_vector_z
   _atom_site_Fourier_wave_vector_description
        1      0.568     0      'First harmonic'
        2      1.136     0      'Second harmonic'
        3      1.761     0.5    'First harmonic'
        4      3.522     1.0    'Second harmonic'
# The modulation coefficients given below are referred to
# each subsystem.
loop_
   _atom_site_displace_Fourier_id
   _atom_site_displace_Fourier_atom_site_label
   _atom_site_displace_Fourier_axis
   _atom_site_displace_Fourier_wave_vector_seq_id
        Nb1z1_NbS2  Nb1   z  1     Nb1x2_NbS2  Nb1   x  2
        Nb1y2_NbS2  Nb1   y  2     S1x1_NbS2   S1    x  1
        S1y1_NbS2   S1    y  1     S1z1_NbS2   S1    z  1
        S1x2_NbS2   S1    x  2     S1y2_NbS2   S1    y  2
        S1z2_NbS2   S1    z  2     La1x3_LaS   La1   x  3
        La1y3_LaS   La1   y  3     La1z3_LaS   La1   z  3
        La1x4_LaS   La1   x  4     La1y4_LaS   La1   y  4
        La1z4_LaS   La1   z  4     S2x3_LaS    S2    x  3
        S2y3_LaS    S2    y  3     S2z3_LaS    S2    z  3
        S2x4_LaS    S2    x  4     S2y4_LaS    S2    y  4
        S2z4_LaS    S2    z  4
loop_
   _atom_site_displace_Fourier_param_id
   _atom_site_displace_Fourier_param_cos
   _atom_site_displace_Fourier_param_sin
Nb1z1_NbS2 -0.0006(2)   0.   Nb1x2_NbS2  0.     0.0078(17)
Nb1y2_NbS2 -0.0014(7)   0.   S1x1_NbS2   0.    -0.0134(85)
S1y1_NbS2  -0.0022(12)  0.   S1z1_NbS2   0.0014(14)  0.
S1x2_NbS2   0.   -0.0129(27) S1y2_NbS2  -0.0073(27)  0.
S1z2_NbS2  -0.0012(3)   0.   La1x3_LaS   0.    -0.0010(22)
La1y3_LaS   0.0174(4)   0.   La1z3_LaS  -0.0005(3)   0.
La1x4_LaS   0.    0.0144(7)  La1y4_LaS   0.0001(14)  0.
La1z4_LaS   0.0008(3)   0.   S2x3_LaS    0.     0.0059(70)
S2y3_LaS    0.0081(16)  0.   S2z3_LaS    0.0009(12)  0.
S2x4_LaS    0.   -0.0030(30) S2y4_LaS    0.0002(56)  0.
S2z4_LaS    0.0007(10)  0.
```

Example 3 - extracted from van Smaalen [(1991). J. Phys.: Condens. Matter 3, 1247–1263.]

```
# The same structural data but expressed using a set of
# linked data blocks
# Items concerning the modulated structure of the first
# subsystem
data_LaSNbS2_MOD_NbS2
_audit_block_code       1997-07-24|LaSNbS2|G.M.|_MOD_NbS2
loop_
_audit_link_block_code
_audit_link_block_description
1997-07-24|LaSNbS2|G.M.|
              'common experimental and publication data'
1997-07-24|LaSNbS2|G.M.|_REFRNCE
                    'reference structure (common data)'
1997-07-21|LaSNbS2|G.M.|_MOD
                    'modulated structure (common data)'
1997-07-24|LaSNbS2|G.M.|_REFRNCE_NbS2
                   'reference structure (1st subsystem)'
.                  'modulated structure (1st subsystem)'
1997-07-24|LaSNbS2|G.M.|_REFRNCE_LaS
                   'reference structure (2nd subsystem)'
1997-07-21|LaSNbS2|G.M.|_MOD_LaS
                   'modulated structure (2nd subsystem)'
loop_
   _atom_site_Fourier_wave_vector_seq_id
   _atom_site_Fourier_wave_vector_x
   _atom_site_Fourier_wave_vector_description
        1      0.568     'First harmonic'
        2      1.136     'Second harmonic'
loop_
   _atom_site_displace_Fourier_id
   _atom_site_displace_Fourier_atom_site_label
   _atom_site_displace_Fourier_axis
   _atom_site_displace_Fourier_wave_vector_seq_id
        Nb1z1   Nb1   z     1       Nb1x2   Nb1   x     2
        Nb1y2   Nb1   y     2       S1x1    S1    x     1
        S1y1    S1    y     1       S1z1    S1    z     1
        S1x2    S1    x     2       S1y2    S1    y     2
        S1z2    S1    z     2
loop_
   _atom_site_displace_Fourier_param_id
   _atom_site_displace_Fourier_param_cos
   _atom_site_displace_Fourier_param_sin
Nb1z1 -0.0006(2)   0.          Nb1x2  0.          0.0078(17)
Nb1y2 -0.0014(7)   0.          S1x1   0.         -0.0134(85)
S1y1  -0.0022(12)  0.          S1z1   0.0014(14)  0.
S1x2   0.         -0.0129(27)  S1y2  -0.0073(27)  0.
S1z2  -0.0012(3)   0.
#### End of modulated structure first subsystem data ####
# Items concerning the modulated structure of the second
# subsystem
data_LaSNbS2_MOD_LaS
_audit_block_code       1997-07-24|LaSNbS2|G.M.|_MOD_LaS
loop_
   _audit_link_block_code
   _audit_link_block_description
1997-07-24|LaSNbS2|G.M.|
              'common experimental and publication data'
1997-07-24|LaSNbS2|G.M.|_REFRNCE
                    'reference structure (common data)'
1997-07-21|LaSNbS2|G.M.|_MOD
                    'modulated structure (common data)'
1997-07-24|LaSNbS2|G.M.|_REFRNCE_NbS2
                   'reference structure (1st subsystem)'
1997-07-21|LaSNbS2|G.M.|_MOD_NbS2
                    'modulated structure (1st subsystem)'
1997-07-24|LaSNbS2|G.M.|_REFRNCE_LaS
                   'reference structure (2nd subsystem)'
.                  'modulated structure (2nd subsystem)'
loop_
   _atom_site_Fourier_wave_vector_seq_id
   _atom_site_Fourier_wave_vector_x
   _atom_site_Fourier_wave_vector_z
   _atom_site_Fourier_wave_vector_description
        1      1.761   0.5   'First harmonic'
        2      3.522   1.0   'Second harmonic'
loop_
   _atom_site_displace_Fourier_id
   _atom_site_displace_Fourier_atom_site_label
   _atom_site_displace_Fourier_axis
   _atom_site_displace_Fourier_wave_vector_seq_id
        La1x1   La1   x     1       La1y1   La1   y     1
        La1z1   La1   z     1       La1x2   La1   x     2
        La1y2   La1   y     2       La1z2   La1   z     2
        S2x1    S2    x     1       S2y1    S2    y     1
        S2z1    S2    z     1       S2x2    S2    x     2
        S2y2    S2    y     2       S2z2    S2    z     2
loop_
   _atom_site_displace_Fourier_param_id
   _atom_site_displace_Fourier_param_cos
   _atom_site_displace_Fourier_param_sin
La1x1  0.         -0.0010(22)  La1y1 0.0174(4)   0.
La1z1 -0.0005(3)   0.          La1x2 0.          0.0144(7)
La1y2  0.0001(14)  0.          La1z2 0.0008(3)   0.
S2x1   0.          0.0059(70)  S2y1  0.0081(16)  0.
S2z1   0.0009(12)  0.          S2x2  0.         -0.0030(30)
S2y2   0.0002(56)  0.          S2z2  0.0007(10)  0.
#### End of modulated structure second subsystem data ####
```

Example 4 - extracted from Baudour & Sanquer [(1983). Acta Cryst. B39, 75–84.] Note the entry from the ATOM_SITES_DISPLACE_FOURIER category to describe collective information relating to all the atom sites.

```
_atom_sites_displace_Fourier_axes_description
;  a1 and a2 are respectively the long molecular axis
   and the axis normal to the mean molecular plane.
;
loop_
_atom_site_displace_Fourier_id
_atom_site_displace_Fourier_atom_site_label
_atom_site_displace_Fourier_axis
_atom_site_displace_Fourier_wave_vector_seq_id
Byphenyl_a1_1    Biphenyl  a1    1
loop_
_atom_site_displace_Fourier_param_id
_atom_site_displace_Fourier_param_modulus
_atom_site_displace_Fourier_param_phase
Byphenyl_a1_1    0.035(5)       0.
```

`_atom_site_displace_Fourier_param_cos` (*numb*)

The displacive distortion of a given atom or rigid group (see also `_atom_site_rot_Fourier_param_cos`) is usually parameterized by Fourier series. Each term of the series commonly adopts two different representations: the sine–cosine form

$$A_c \cos(2\pi\mathbf{kr}) + A_s \sin(2\pi\mathbf{kr})$$

and the modulus–argument form

$$|A| \cos(2\pi\mathbf{kr} + \varphi)$$

where **k** is the wave vector of the term and **r** is the atomic average position. `_atom_site_displace_Fourier_param_cos` is the cosine coefficient (A_c) corresponding to the Fourier term defined by `_atom_site_displace_Fourier_atom_site_label`, `_atom_site_displace_Fourier_axis`, and `_atom_site_displace_Fourier_wave_vector_seq_id`. Atomic or rigid group displacements must be expressed as fractions of the unit cell or in ångströms if the modulations are referred to some special axes defined by `_atom_sites_displace_Fourier_axes_description`.

Appears in list containing `_atom_site_displace_Fourier_param_id`. Where no value is given, the assumed value is '`0.0`'. [`atom_site_displace_Fourier_param`]

`_atom_site_displace_Fourier_param_id` (*char*)

A code identifying the (in general complex) coefficient of each term present in the Fourier series describing the displacive modulation of a given atom or rigid group. In the case of a rigid group it applies only to the translational part of the distortion. This code must match `_atom_site_displace_Fourier_id`.

Appears in list as essential element of loop structure. **Must** match data name `_atom_site_displace_Fourier_id`.
[`atom_site_displace_Fourier_param`]

`_atom_site_displace_Fourier_param_modulus` (*numb*)

The displacive distortion of a given atom or rigid group (see also `_atom_site_rot_Fourier_param_modulus`) is usually parameterized by Fourier series. Each term of the series commonly adopts two different representations: the sine–cosine form

$$A_c \cos(2\pi\mathbf{kr}) + A_s \sin(2\pi\mathbf{kr})$$

and the modulus–argument form

$$|A| \cos(2\pi\mathbf{kr} + \varphi)$$

where **k** is the wave vector of the term and **r** is the atomic average position. `_atom_site_displace_Fourier_param_modulus` is the modulus ($|A|$) of the complex amplitude corresponding to the Fourier term defined by `_atom_site_displace_Fourier_atom_site_label`, `_atom_site_displace_Fourier_axis`, and `_atom_site_displace_Fourier_wave_vector_seq_id`. Atomic or rigid group displacements must be expressed as fractions of the unit cell or in ångströms if the modulations are referred to some special axes defined by `_atom_sites_displace_Fourier_axes_description`.

Appears in list containing `_atom_site_displace_Fourier_param_id`. Where no value is given, the assumed value is '`0.0`'. The permitted range is $0.0 \rightarrow \infty$.
[`atom_site_displace_Fourier_param`]

`_atom_site_displace_Fourier_param_phase` (*numb*)

The displacive distortion of a given atom or rigid group (see also `_atom_site_rot_Fourier_param_phase`) is usually parameterized by Fourier series. Each term of the series commonly adopts two different representations: the sine–cosine form

$$A_c \cos(2\pi\mathbf{kr}) + A_s \sin(2\pi\mathbf{kr})$$

and the modulus–argument form

$$|A| \cos(2\pi\mathbf{kr} + \varphi)$$

where **k** is the wave vector of the term and **r** is the atomic average position. `_atom_site_displace_Fourier_param_phase` is the phase (φ) in cycles of the complex amplitude corresponding to the Fourier term defined by `_atom_site_displace_Fourier_atom_site_label`, `_atom_site_displace_Fourier_axis`, and `_atom_site_displace_Fourier_wave_vector_seq_id`.

Appears in list containing `_atom_site_displace_Fourier_param_id`. Where no value is given, the assumed value is '`0.0`'. The permitted range is $-1.0 \rightarrow 1.0$.
[`atom_site_displace_Fourier_param`]

`_atom_site_displace_Fourier_param_sin` (*numb*)

The displacive distortion of a given atom or rigid group (see also `_atom_site_rot_Fourier_param_sin`) is usually parameterized by Fourier series. Each term of the series commonly adopts two different representations: the sine–cosine form

$$A_c \cos(2\pi\mathbf{kr}) + A_s \sin(2\pi\mathbf{kr})$$

and the modulus–argument form

$$|A| \cos(2\pi\mathbf{kr} + \varphi)$$

where **k** is the wave vector of the term and **r** is the atomic average position. `_atom_site_displace_Fourier_param_sin` is the sine coefficient (A_s) corresponding to the Fourier term defined by `_atom_site_displace_Fourier_atom_site_label`, `_atom_site_displace_Fourier_axis`, and `_atom_site_displace_Fourier_wave_vector_seq_id`. Atomic or rigid group displacements must be expressed as fractions of the unit cell or in ångströms if the modulations are referred to some special axes defined by `_atom_sites_displace_Fourier_axes_description`.

Appears in list containing `_atom_site_displace_Fourier_param_id`. Where no value is given, the assumed value is '`0.0`'.
[`atom_site_displace_Fourier_param`]

`_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.

Example 1 - extracted from van Smaalen [(1991). J. Phys.: Condens. Matter 3, 1247–1263.]

```
loop_
    _atom_site_Fourier_wave_vector_seq_id
    _atom_site_Fourier_wave_vector_x
    _atom_site_Fourier_wave_vector_description
        1       0.568           'First harmonic'
        2       1.136           'Second harmonic'
```

`_atom_site_Fourier_wave_vector_description` (*char*)

A description of the linear combination involved in a given Fourier wave vector used to describe the atomic modulation functions.

Appears in list containing `_atom_site_Fourier_wave_vector_seq_id`.

Example(s): 'q(4)=q(1)+q(2)'
[atom_site_Fourier_wave_vector]

`_atom_site_Fourier_wave_vector_seq_id` (*numb*)

A numeric code identifying the wave vectors defined in `_atom_site_Fourier_wave_vector_`.

Appears in list. May match subsidiary data name(s): `_atom_site_displace_Fourier_wave_vector_seq_id`, `_atom_site_occ_Fourier_wave_vector_seq_id`, `_atom_site_rot_Fourier_wave_vector_seq_id`, `_atom_site_U_Fourier_wave_vector_seq_id`.
[atom_site_Fourier_wave_vector]

`_atom_site_Fourier_wave_vector_x`
`_atom_site_Fourier_wave_vector_y`
`_atom_site_Fourier_wave_vector_z` (*numb*)

Wave vectors of the Fourier terms used in the structural model to describe the atomic modulation functions, expressed with respect to the three-dimensional reciprocal basis that spans the lattice of main reflections. They are linear combinations with integer coefficients of the independent wave vectors given in the `_cell_wave_vector_` list. Therefore a generic Fourier wave vector is expressed as

$$\mathbf{k} = n(1)\mathbf{q}(1) + \ldots + n(p)\mathbf{q}(p)$$

where p is given by `_cell_modulation_dimension`. In the case of composites described in a single data block, these wave vectors are expressed with respect to the three-dimensional reciprocal basis of each subsystem (see `_cell_subsystem_matrix_W_`).

Appears in list containing `_atom_site_Fourier_wave_vector_seq_id`. Where no value is given, the assumed value is '0.0'. [atom_site_Fourier_wave_vector]

`_atom_site_occ_Fourier_atom_site_label` (*char*)

Modulation parameters are usually looped in separate lists. Modulated parameters are the atomic positions (displacive modulation), the atomic occupation (occupational modulation) and/or the atomic anisotropic (or isotropic) displacement parameters (referred to as modulation of thermal parameters since the term 'displacement parameters' is ambiguous in this context). `_atom_site_occ_Fourier_atom_site_label` is the code that identifies an atom in a loop where the Fourier components of its occupational modulation are being listed. This code must match the `_atom_site_label` of the associated coordinate list and conform to the rules described in `_atom_site_label`.

Appears in list. **Must** match data name `_atom_site_label`.
[atom_site_occ_Fourier]

`_atom_site_occ_Fourier_id` (*char*)

A code identifying each component of the occupational modulation of a given atom or rigid group when it is expressed in terms of Fourier series.

Appears in list as essential element of loop structure. May match subsidiary data name(s): `_atom_site_occ_Fourier_param_id`.
[atom_site_occ_Fourier]

`_atom_site_occ_Fourier_wave_vector_seq_id` (*numb*)

A numeric code identifying the wave vectors of the Fourier terms used in the structural model to describe the modulation functions corresponding to the occupational part of the distortion. This code must match `_atom_site_Fourier_wave_vector_seq_id`.

Appears in list containing `_atom_site_occ_Fourier_id`. **Must** match data name `_atom_site_Fourier_wave_vector_seq_id`.
[atom_site_occ_Fourier]

`_atom_site_occ_Fourier_` []

Data items in the ATOM_SITE_OCC_FOURIER category record details about the Fourier components of the occupational modulation of the atom sites in a modulated structure. The (in general complex) coefficients of each Fourier component belong to the category ATOM_SITE_OCC_FOURIER_PARAM and are listed separately.

Example 1 - extracted from Madariaga, G., Zúñiga, F. J., Paciorek, W. A. & Bocanegra, E. H. [(1990). Acta Cryst. B46, 620–628.]

```
loop_
   _atom_site_occ_Fourier_id
   _atom_site_occ_Fourier_atom_site_label
   _atom_site_occ_Fourier_wave_vector_seq_id
       CuBr4_1  CuBr4   1
       NC4_1_1  (NC4)1  1
       NC4_2_1  (NC4)2  1
```

`_atom_site_occ_Fourier_param_` []

Data items in the ATOM_SITE_OCC_FOURIER_PARAM category record details about the coefficients of the Fourier series used to describe the occupational modulation of the atom sites in a modulated structure. The Fourier components are defined in the category ATOM_SITE_OCC_FOURIER and are listed separately.

Example 1 - extracted from Madariaga, G., Zúñiga, F. J., Paciorek, W. A. & Bocanegra, E. H. [(1990). Acta Cryst. B46, 620–628.] The meaning of `_atom_site_occ_Fourier_param_id` *is given in the example of the ATOM_SITE_OCC_FOURIER category.*

```
loop_
   _atom_site_occ_Fourier_param_id
   _atom_site_occ_Fourier_param_modulus
   _atom_site_occ_Fourier_param_phase
       CuBr4_1  0.397(11)    0.392(6)
       NC4_1_1  0.216(42)   -0.047(33)
       NC4_2_1  0.208(48)    0.132(27)
```

`_atom_site_occ_Fourier_param_cos` (*numb*)

The occupational distortion of a given atom or rigid group is usually parameterized by Fourier series. Each term of the series commonly adopts two different representations: the sine–cosine form

$$P_c \cos(2\pi\mathbf{kr}) + P_s \sin(2\pi\mathbf{kr})$$

and the modulus–argument form

$$|P| \cos(2\pi\mathbf{kr} + \delta)$$

where **k** is the wave vector of the term and **r** is the atomic average position. `_atom_site_occ_Fourier_param_cos` is the cosine coefficient (P_c) corresponding to the Fourier term defined by `_atom_site_occ_Fourier_atom_site_label`, and `_atom_site_occ_Fourier_wave_vector_seq_id`.

Appears in list containing `_atom_site_occ_Fourier_param_id`. Where no value is given, the assumed value is `'0.0'`.
[`atom_site_occ_Fourier_param`]

`_atom_site_occ_Fourier_param_id` (*char*)

A code identifying the (in general complex) coefficient of each term present in the Fourier series describing the occupational modulation of a given atom or rigid group. This code must match `_atom_site_occ_Fourier_id`.

Appears in list as essential element of loop structure. **Must** match data name `_atom_site_occ_Fourier_id`.
[`atom_site_occ_Fourier_param`]

`_atom_site_occ_Fourier_param_modulus` (*numb*)

The occupational distortion of a given atom or rigid group is usually parameterized by Fourier series. Each term of the series commonly adopts two different representations: the sine–cosine form

$$P_c \cos(2\pi\mathbf{kr}) + P_s \sin(2\pi\mathbf{kr})$$

and the modulus–argument form

$$|P| \cos(2\pi\mathbf{kr} + \delta)$$

where **k** is the wave vector of the term and **r** is the atomic average position. `_atom_site_occ_Fourier_param_modulus` is the modulus ($|P|$) of the complex amplitude corresponding to the Fourier term defined by `_atom_site_occ_Fourier_atom_site_label`, and `_atom_site_occ_Fourier_wave_vector_seq_id`.

Appears in list containing `_atom_site_occ_Fourier_param_id`. Where no value is given, the assumed value is `'0.0'`. The permitted range is $0.0 \rightarrow \infty$. [`atom_site_occ_Fourier_param`]

`_atom_site_occ_Fourier_param_phase` (*numb*)

The occupational distortion of a given atom or rigid group is usually parameterized by Fourier series. Each term of the series commonly adopts two different representations: the sine–cosine form

$$P_c \cos(2\pi\mathbf{kr}) + P_s \sin(2\pi\mathbf{kr})$$

and the modulus–argument form

$$|P| \cos(2\pi\mathbf{kr} + \delta)$$

where **k** is the wave vector of the term and **r** is the atomic average position. `_atom_site_occ_Fourier_param_phase` is the phase (δ) in cycles corresponding to the Fourier term defined by `_atom_site_occ_Fourier_atom_site_label`, and `_atom_site_occ_Fourier_wave_vector_seq_id`.

Appears in list containing `_atom_site_occ_Fourier_param_id`. Where no value is given, the assumed value is `'0.0'`. The permitted range is $-1.0 \rightarrow 1.0$. [`atom_site_occ_Fourier_param`]

`_atom_site_occ_Fourier_param_sin` (*numb*)

The occupational distortion of a given atom or rigid group is usually parameterized by Fourier series. Each term of the series commonly adopts two different representations: the sine–cosine form

$$P_c \cos(2\pi\mathbf{kr}) + P_s \sin(2\pi\mathbf{kr})$$

and the modulus–argument form,

$$|P| \cos(2\pi\mathbf{kr} + \delta)$$

where **k** is the wave vector of the term and **r** is the atomic average position. `_atom_site_occ_Fourier_param_sin` is the sine coefficient (P_s) corresponding to the Fourier term defined by `_atom_site_occ_Fourier_atom_site_label`, and `_atom_site_occ_Fourier_wave_vector_seq_id`.

Appears in list containing `_atom_site_occ_Fourier_param_id`. Where no value is given, the assumed value is `'0.0'`.
[`atom_site_occ_Fourier_param`]

`_atom_site_phason_[]`

Data items in the ATOM_SITE_PHASON category record details about the atomic phason correction. Although this kind of correction is intended to be overall, some refinement programs (for example *JANA*2000) allow for this (theoretically dubious) atom-dependent phason treatment.

`_atom_site_phason_atom_site_label` (*char*)

The code that identifies an atom or rigid group in a loop where the phason coefficients are being listed. Although this kind of correction is intended to be overall, some refinement programs (for example *JANA*2000) allow an independent phason correction for each atom or rigid group. In this case `_atom_site_phason_formula` and `_atom_site_phason_coeff` should be used (see also `_refine_ls_mod_overall_phason_`). This code must match the `_atom_site_label` of the associated coordinate list and conform to the rules described in `_atom_site_label`.

Appears in list as essential element of loop structure. **Must** match data name `_atom_site_label`. [`atom_site_phason`]

`_atom_site_phason_coeff` (*numb*)

The phason coefficient used to calculate (with the appropriate expression given in `_atom_site_phason_formula`) the atomic phason correction. Although this kind of correction is intended to be overall, some refinement programs (for example *JANA*2000) allow an independent phason correction for each atom or rigid group. In this case `_atom_site_phason_formula` and `_atom_site_phason_coeff` should be used (see also `_refine_ls_mod_overall_phason_`).

Appears in list containing `_atom_site_phason_atom_site_label`. Where no value is given, the assumed value is `'0.0'`. The permitted range is $0.0 \rightarrow \infty$. [`atom_site_phason`]

`_atom_site_phason_formula` (*char*)

The formula used for the phason correction. Although both kinds of corrections are intended to be overall, some refinement programs (for example *JANA*2000) allow an independent phason correction for each atom or rigid group. In this case `_atom_site_phason_formula` and `_atom_site_phason_coeff` should be used (see also `_refine_ls_mod_overall_phason_`).

`Axe`	Axe, J. D., *Phys. Rev. B***21** (1980), 4181
`Ovr`	Overhauser, A. W., *Phys. Rev. B***3** (1971), 3173

Appears in list containing `_atom_site_phason_atom_site_label`. [`atom_site_phason`]

`_atom_site_rot_Fourier_[]`

Data items in the ATOM_SITE_ROT_FOURIER category record details about the Fourier components present in the rotational part of the displacive modulation of a given rigid group. The translational part would appear in a separate list of items belonging to the ATOM_SITE_DISPLACE_FOURIER category. The (in general complex) coefficients of each Fourier component belong to the category ATOM_SITE_ROT_FOURIER_PARAM and are listed separately.

Example 1 - example corresponding to the one-dimensional incommensurately modulated structure of K_2SeO_4.

```
loop_
   _atom_site_rot_Fourier_id
   _atom_site_rot_Fourier_atom_site_label
   _atom_site_rot_Fourier_axis
   _atom_site_rot_Fourier_wave_vector_seq_id
        SeO4_x_1     SeO4    x       1
        SeO4_y_1     SeO4    y       1
```

Example 2 - extracted from Baudour & Sanquer [(1983). Acta Cryst. B39, 75–84.] Note the entry from the ATOM_SITES_ROT_FOURIER category to describe collective information relating to all the atom sites.

```
_atom_sites_rot_Fourier_axes_description
;  a1 and a2 are respectively the long molecular axis
   and the axis normal to the mean molecular plane.
;
loop_
   _atom_site_rot_Fourier_id
   _atom_site_rot_Fourier_atom_site_label
   _atom_site_rot_Fourier_axis
   _atom_site_rot_Fourier_wave_vector_seq_id
        Ph1_a1_1  Phenyl1   a1    1
        Ph2_a1_1  Phenyl2   a1    1
        Bph_a2_1  Biphenyl  a2    1
```

`_atom_site_rot_Fourier_atom_site_label` (*char*)

Modulation parameters are usually looped in separate lists. Modulated parameters are the atomic positions (displacive modulation), the atomic occupation (occupational modulation) and/or the atomic anisotropic (or isotropic) displacement parameters (referred to as modulation of thermal parameters since the term 'displacement parameters' is ambiguous in this context). `_atom_site_rot_Fourier_atom_site_label` is the code that identifies a rigid group in a loop where the Fourier components of the rotational part of its displacive modulation are being listed. The translational part (if any) would appear in a separate list (see `_atom_site_displace_Fourier_atom_site_label`).

This code must match the `_atom_site_label` of the associated coordinate list and conform to the rules described in `_atom_site_label`.

Appears in list containing `_atom_site_rot_Fourier_id`. **Must** match data name `_atom_site_label`. [`atom_site_rot_Fourier`]

`_atom_site_rot_Fourier_axis` (*char*)

A label identifying the rotation component, around a fixed point of a given rigid group whose modulation is being parameterized by Fourier series. **a**, **b** and **c** are the basic lattice vectors of the reference structure. For composites they refer to the reference structure of each subsystem. $\mathbf{a}_1$, $\mathbf{a}_2$ and $\mathbf{a}_3$ are defined by `_atom_sites_rot_Fourier_axes_description`.

`x`	rotation around the **a** axis
`y`	rotation around the **b** axis
`z`	rotation around the **c** axis
`a1`	rotation around an arbitrary $\mathbf{a}_1$ axis
`a2`	rotation around an arbitrary $\mathbf{a}_2$ axis
`a3`	rotation around an arbitrary $\mathbf{a}_3$ axis

Appears in list containing `_atom_site_rot_Fourier_id`. [`atom_site_rot_Fourier`]

`_atom_site_rot_Fourier_id` (*char*)

A code identifying each component of the rotational modulation of a given rigid group when it is expressed in terms of Fourier series.

Appears in list as essential element of loop structure. May match subsidiary data name(s): `_atom_site_rot_Fourier_param_id`. [`atom_site_rot_Fourier`]

`_atom_site_rot_Fourier_wave_vector_seq_id` (*numb*)

A numeric code identifying the wave vectors of the Fourier terms used in the structural model to describe the modulation functions corresponding to the rotational distortion of a rigid group. This code must match `_atom_site_Fourier_wave_vector_seq_id`.

Appears in list containing `_atom_site_rot_Fourier_id`. **Must** match data name `_atom_site_Fourier_wave_vector_seq_id`. [`atom_site_rot_Fourier`]

`_atom_site_rot_Fourier_param_[]`

Data items in the ATOM_SITE_ROT_FOURIER_PARAM category record details about the coefficients of the Fourier series used to describe the rotational component of the displacive modulation of a given rigid group. The translational part would appear in a separate list of items belonging to the ATOM_SITE_DISPLACE_FOURIER_PARAM category. The Fourier components are defined in the category ATOM_SITE_ROT_FOURIER and are listed separately.

Example 1 - example corresponding to the one-dimensional incommensurately modulated structure of K_2SeO_4. The meaning of `_atom_site_rot_Fourier_param_id` *is given in the examples of the ATOM_SITE_ROT_FOURIER category.*

```
loop_
   _atom_site_rot_Fourier_param_id
   _atom_site_rot_Fourier_param_cos
   _atom_site_rot_Fourier_param_sin
        SeO4_x_1    -4.2(1)   0.91(3)
        SeO4_y_1     4.3(1)   0.
```

Example 2 - extracted from Baudour & Sanquer [(1983). Acta Cryst. B39, 75–84.] Note the entry from the ATOM_SITES_ROT_FOURIER category to describe collective information relating to all the atom sites. The meaning of `_atom_site_rot_Fourier_param_id` *is given in the examples of the ATOM_SITE_ROT_FOURIER category.*

```
_atom_sites_rot_Fourier_axes_description
;  a1 and a2 are respectively the long molecular axis
   and the axis normal to the mean molecular plane.
;
loop_
   _atom_site_rot_Fourier_param_id
   _atom_site_rot_Fourier_param_modulus
   _atom_site_rot_Fourier_param_phase
        Ph1_a1_1  11.0(2)  0.
        Ph2_a1_1  11.0(2)  0.5
        Bph_a2_1   1.0(1)  0.25
```

`_atom_site_rot_Fourier_param_cos` (*numb*)

The displacive distortion of a given rigid group is not completely described by `_atom_site_displace_Fourier_`. The rigid rotation of the group around a given axis passing through a fixed point (for example the centre of mass of the group) is usually parameterized by Fourier series. Each term of the series commonly adopts two different representations: the sine–cosine form

$$R_c \cos(2\pi\mathbf{kr}) + R_s \sin(2\pi\mathbf{kr})$$

and the modulus–argument form

$$|R| \cos(2\pi\mathbf{kr} + \psi)$$

where **k** is the wave vector of the term and **r** is the atomic average position. `_atom_site_rot_Fourier_param_cos` is the cosine coefficient (R_c) in degrees, corresponding to the Fourier term defined by `_atom_site_rot_Fourier_atom_site_label`, `_atom_site_rot_Fourier_axis`, and `_atom_site_rot_Fourier_wave_vector_seq_id`.

Appears in list containing `_atom_site_rot_Fourier_param_id`. Where no value is given, the assumed value is '0.0'. [atom_site_rot_Fourier_param]

`_atom_site_rot_Fourier_param_id` (*char*)

A code identifying the (in general complex) coefficient of each term present in the Fourier series describing the rotational part of the displacive modulation of a given rigid group. This code must match `_atom_site_rot_Fourier_id`.

Appears in list as essential element of loop structure. **Must** match data name `_atom_site_rot_Fourier_id`. [atom_site_rot_Fourier_param]

`_atom_site_rot_Fourier_param_modulus` (*numb*)

The displacive distortion of a given rigid group is not completely described by `_atom_site_displace_Fourier_`. The rigid rotation of the group around a given axis passing through a fixed point (for example the centre of mass of the group) is usually parameterized by Fourier series. Each term of the series commonly adopts two different representations: the sine–cosine form

$$R_c \cos(2\pi\mathbf{kr}) + R_s \sin(2\pi\mathbf{kr})$$

and the modulus–argument form

$$|R| \cos(2\pi\mathbf{kr} + \psi)$$

where **k** is the wave vector of the term and **r** is the atomic average position. `_atom_site_rot_Fourier_param_modulus` is the modulus ($|R|$) in degrees, of the complex amplitude corresponding to the Fourier term defined by `_atom_site_rot_Fourier_atom_site_label`, `_atom_site_rot_Fourier_axis`, and `_atom_site_rot_Fourier_wave_vector_seq_id`.

Appears in list containing `_atom_site_rot_Fourier_param_id`. Where no value is given, the assumed value is '0.0'. The permitted range is $0.0 \rightarrow \infty$. [atom_site_rot_Fourier_param]

`_atom_site_rot_Fourier_param_phase` (*numb*)

The displacive distortion of a given rigid group is not completely described by `_atom_site_displace_Fourier_`. The rigid rotation of the group around a given axis passing through a fixed point (for example the centre of mass of the group) is usually parameterized by Fourier series. Each term of the series commonly adopts two different representations: the sine–cosine form

$$R_c \cos(2\pi\mathbf{kr}) + R_s \sin(2\pi\mathbf{kr})$$

and the modulus–argument form

$$|R| \cos(2\pi\mathbf{kr} + \psi)$$

where **k** is the wave vector of the term and **r** is the atomic average position. `_atom_site_rot_Fourier_param_phase` is the phase (ψ) in cycles, of the complex amplitude corresponding to the Fourier term defined by `_atom_site_rot_Fourier_atom_site_label`, `_atom_site_rot_Fourier_axis`, and `_atom_site_rot_Fourier_wave_vector_seq_id`.

Appears in list containing `_atom_site_rot_Fourier_param_id`. Where no value is given, the assumed value is '0.0'. The permitted range is $-1.0 \rightarrow 1.0$. [atom_site_rot_Fourier_param]

`_atom_site_rot_Fourier_param_sin` (*numb*)

The displacive distortion of a given rigid group is not completely described by `_atom_site_displace_Fourier_`. The rigid rotation of the group around a given axis passing through a fixed point (for example the centre of mass of the group) is usually parameterized by Fourier series. Each term of the series commonly adopts two different representations: the sine–cosine form

$$R_c \cos(2\pi\mathbf{kr}) + R_s \sin(2\pi\mathbf{kr})$$

and the modulus–argument form

$$|R| \cos(2\pi\mathbf{kr} + \psi)$$

where **k** is the wave vector of the term and **r** is the atomic average position. `_atom_site_rot_Fourier_param_sin` is the sine coefficient (R_s) in degrees, corresponding to the Fourier term defined by `_atom_site_rot_Fourier_atom_site_label`,

_atom_site_rot_Fourier_axis, and _atom_site_rot_Fourier_wave_vector_seq_id.

Appears in list containing _atom_site_rot_Fourier_param_id. Where no value is given, the assumed value is '0.0'.
[atom_site_rot_Fourier_param]

_atom_site_U_Fourier_[]

Data items in the ATOM_SITE_U_FOURIER category record details about the Fourier components describing the modulation of the atomic thermal parameters in a modulated structure.

Example 1 - extracted from Meyer, Paciorek, Schenk, Chapuis & Depmeier [(1994). Acta Cryst. B50, 333–343.]

```
loop_
   _atom_site_U_Fourier_id
   _atom_site_U_Fourier_atom_site_label
   _atom_site_U_Fourier_tens_elem
   _atom_site_U_Fourier_wave_vector_seq_id
        Mn_U11_2  Mn  U11  2
        Mn_U22_2  Mn  U22  2
        Mn_U33_2  Mn  U33  2
        Mn_U12_2  Mn  U12  2
        Mn_U13_2  Mn  U13  2
        Mn_U23_2  Mn  U23  2
        Cl1_U11_2 Cl1 U11  2
        Cl1_U22_2 Cl1 U22  2
        Cl1_U33_2 Cl1 U33  2
        Cl1_U12_2 Cl1 U12  2
        Cl1_U13_2 Cl1 U13  2
        Cl1_U23_2 Cl1 U23  2
# - - - - data truncated for brevity - - - -
```

_atom_site_U_Fourier_atom_site_label (*char*)

Modulation parameters are usually looped in separate lists. Modulated parameters are the atomic positions (displacive modulation), the atomic occupation (occupational modulation) and/or the atomic anisotropic (or isotropic) displacement parameters (referred to as modulation of thermal parameters since the term 'displacement parameters' is ambiguous in this context). _atom_site_U_Fourier_atom_site_label is the code that identifies an atom in a loop where the Fourier components of its thermal parameters modulation are being listed. This code must match the _atom_site_label of the associated coordinate list and conform to the rules described in _atom_site_label.

Appears in list containing _atom_site_U_Fourier_id. **Must** match data name _atom_site_label. [atom_site_U_Fourier]

_atom_site_U_Fourier_id (*char*)

A code identifying each Fourier component used to describe the modulation of the atomic thermal parameters.

Appears in list as essential element of loop structure. May match subsidiary data name(s): _atom_site_U_Fourier_param_id.
[atom_site_U_Fourier]

_atom_site_U_Fourier_tens_elem (*char*)

A label identifying the temperature tensor element U^{ij} of a given atom or rigid group whose modulation is being parameterized by Fourier series.

U11	modulation of U^{11}
U12	modulation of U^{12}
U13	modulation of U^{13}
U22	modulation of U^{22}
U23	modulation of U^{23}
U33	modulation of U^{33}
Uiso	modulation of U isotropic

Appears in list containing _atom_site_U_Fourier_id.
[atom_site_U_Fourier]

_atom_site_U_Fourier_wave_vector_seq_id (*numb*)

A numeric code identifying the wave vectors of the Fourier terms used to describe the modulation functions corresponding to the temperature factors of an atom or rigid group. This code must match _atom_site_Fourier_wave_vector_seq_id.

Appears in list containing _atom_site_U_Fourier_id. **Must** match data name _atom_site_Fourier_wave_vector_seq_id.
[atom_site_U_Fourier]

_atom_site_U_Fourier_param_[]

Data items in the ATOM_SITE_U_FOURIER category record details about the coefficients of the Fourier series used to describe the modulation of the atomic thermal parameters in a modulated structure. The Fourier components are defined in the category ATOM_SITE_U_FOURIER and are listed separately.

Example 1 - extracted from Meyer, Paciorek, Schenk, Chapuis & Depmeier [(1994). Acta Cryst. B50, 333–343.] The meaning of _atom_site_U_Fourier_param_id is given in the example of the ATOM_SITE_U_FOURIER category.

```
loop_
   _atom_site_U_Fourier_param_id
   _atom_site_U_Fourier_param_modulus
   _atom_site_U_Fourier_param_phase
        Mn_U11_2  0.003(3)  0.0
        Mn_U22_2  0.0       0.0
        Mn_U33_2  0.017(2)  0.0
        Mn_U12_2  0.0       0.0
        Mn_U13_2  0.00(2)   0.5
        Mn_U23_2  0.0       0.0
        Cl1_U11_2 0.003(3)  0.5
        Cl1_U22_2 0.005(3)  0.0
        Cl1_U33_2 0.020(3)  0.0
        Cl1_U12_2 0.008(3)  0.0
        Cl1_U13_2 0.02(2)   0.75
        Cl1_U23_2 0.03(3)   0.25
# - - - - data truncated for brevity - - - -
```

_atom_site_U_Fourier_param_cos (*numb*)

The modulation of the atomic thermal parameters is usually parameterized by Fourier series. Each term of the series commonly adopts two different representations: the sine–cosine form

$$U_c^{ij}\cos(2\pi\mathbf{kr}) + U_s^{ij}\sin(2\pi\mathbf{kr})$$

and the modulus–argument form

$$|U^{ij}|\cos(2\pi\mathbf{kr} + \chi)$$

where **k** is the wave vector of the term and **r** is the atomic average position. _atom_site_U_Fourier_param_cos is the cosine coefficient U_c^{ij}, in ångströms squared, corresponding to the Fourier term defined by _atom_site_U_Fourier_atom_site_label and _atom_site_U_Fourier_wave_vector_seq_id. *_iso refers to the isotropic atomic displacement parameter.

Appears in list containing `_atom_site_U_Fourier_param_id`. Where no value is given, the assumed value is '0.0'. [atom_site_U_Fourier_param]

`_atom_site_U_Fourier_param_id` (*char*)

A code identifying the (in general complex) coefficient of each term present in the Fourier series describing the modulation of the atomic thermal parameters. This code must match `_atom_site_U_Fourier_id`.

Appears in list as essential element of loop structure. **Must** match data name `_atom_site_U_Fourier_id`. [atom_site_U_Fourier_param]

`_atom_site_U_Fourier_param_modulus` (*numb*)

The modulation of the atomic thermal parameters is usually parameterized by Fourier series. Each term of the series commonly adopts two different representations: the sine–cosine form

$$U_c^{ij}\cos(2\pi\mathbf{kr}) + U_s^{ij}\sin(2\pi\mathbf{kr})$$

and the modulus–argument form

$$|U^{ij}|\cos(2\pi\mathbf{kr} + \chi)$$

where **k** is the wave vector of the term and **r** is the atomic average position. `_atom_site_U_Fourier_param_modulus` is the modulus $|U^{ij}|$, in ångströms squared, of the complex amplitudes corresponding to the Fourier term defined by `_atom_site_U_Fourier_atom_site_label` and `_atom_site_U_Fourier_wave_vector_seq_id`. `*_iso` refers to the isotropic atomic displacement parameter.

Appears in list containing `_atom_site_U_Fourier_param_id`. Where no value is given, the assumed value is '0.0'. The permitted range is $0.0 \rightarrow \infty$. [atom_site_U_Fourier_param]

`_atom_site_U_Fourier_param_phase` (*numb*)

The modulation of the atomic thermal parameters is usually parameterized by Fourier series. Each term of the series commonly adopts two different representations: the sine–cosine form

$$U_c^{ij}\cos(2\pi\mathbf{kr}) + U_s^{ij}\sin(2\pi\mathbf{kr})$$

and the modulus–argument form

$$|U^{ij}|\cos(2\pi\mathbf{kr} + \chi)$$

where **k** is the wave vector of the term and **r** is the atomic average position. `_atom_site_U_Fourier_param_phase` is the phase (χ), in cycles, of the complex amplitude corresponding to the Fourier term defined by `_atom_site_U_Fourier_atom_site_label` and `_atom_site_U_Fourier_wave_vector_seq_id`. `*_iso` refers to the isotropic atomic displacement parameter.

Appears in list containing `_atom_site_U_Fourier_param_id`. Where no value is given, the assumed value is '0.0'. The permitted range is $-1.0 \rightarrow 1.0$. [atom_site_U_Fourier_param]

`_atom_site_U_Fourier_param_sin` (*numb*)

The modulation of the atomic thermal parameters is usually parameterized by Fourier series. Each term of the series commonly adopts two different representations: the sine–cosine form

$$U_c^{ij}\cos(2\pi\mathbf{kr}) + U_s^{ij}\sin(2\pi\mathbf{kr})$$

and the modulus–argument form

$$|U^{ij}|\cos(2\pi\mathbf{kr} + \chi)$$

where **k** is the wave vector of the term and **r** is the atomic average position. `_atom_site_U_Fourier_param_sin` is the sine coefficient U_s^{ij}, in ångströms squared, corresponding to the Fourier term defined by `_atom_site_U_Fourier_atom_site_label` and `_atom_site_U_Fourier_wave_vector_seq_id`. `*_iso` refers to the isotropic atomic displacement parameter.

Appears in list containing `_atom_site_U_Fourier_param_id`. Where no value is given, the assumed value is '0.0'. [atom_site_U_Fourier_param]

`_atom_site_displace_special_func_[]`

Data items in the ATOM_SITE_DISPLACE_SPECIAL_FUNC category record details about the displacive 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 suite of programs *JANA*. In this dictionary only the special functions available in *JANA*2000 have been included. Although this approach is far from being general it has the advantage that functions are tightly defined and therefore the atomic displacements and occupations can be easily calculated.

Summarising the special functions included in the dictionary are: 1) Sawtooth functions for atomic displacive modulation along *x*, *y* and *z*. Only applies to one-dimensional modulated structures. 2) Crenel functions for the occupational modulation of atoms and rigid groups. Only applies to one-dimensional modulated structures.

Example 1 - extracted from Gao, Coppens, Cox & Moodenbaugh [(1993). Acta Cryst. A49, 141–148.]

```
# - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
#   In this example the displacive modulation of the O(4)
#   atom was modelled using a sawtooth-shaped function.
# - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
loop_
   _atom_site_displace_special_func_atom_site_label
   _atom_site_displace_special_func_sawtooth_ax
   _atom_site_displace_special_func_sawtooth_ay
   _atom_site_displace_special_func_sawtooth_az
   _atom_site_displace_special_func_sawtooth_c
   _atom_site_displace_special_func_sawtooth_w
        O(4)  -1.46(3)  0.12(5)  0.42(5)  0.42(2)  1.07(2)
```

`_atom_site_displace_special_func_atom_site_label` (*char*)

The code that identifies an atom in a loop where the special function that describe its displacive modulation is being defined. This code must match the `_atom_site_label` of the associated coordinate list and conform to the rules described in `_atom_site_label`.

Appears in list as essential element of loop structure. **Must** match data name `_atom_site_label`. [atom_site_displace_special_func]

```
_atom_site_displace_special_func_sawtooth_ax
_atom_site_displace_special_func_sawtooth_ay
_atom_site_displace_special_func_sawtooth_az
_atom_site_displace_special_func_sawtooth_c
_atom_site_displace_special_func_sawtooth_w
```
(*numb*)

`_atom_site_displace_special_func_sawtooth_` items are the adjustable parameters of a sawtooth function. A displacive sawtooth function along the internal space is defined as follows:

$$u_x = 2a_x\left[\frac{(x_4 - c)}{w}\right] \quad u_y = 2a_y\left[\frac{(x_4 - c)}{w}\right] \quad u_z = 2a_z\left[\frac{(x_4 - c)}{w}\right]$$

where a_x, a_y and a_z are the amplitudes (maximum displacements) along each crystallographic axis, w is its width, x_4 is the internal coordinate and c the center of the function in internal space. u_x, u_y and u_z must be expressed in relative units. Its usage is restricted to one-dimensional modulated structures. For more details see for example the manual of *JANA*2000 (Petricek & Dusek, 2000).

Appears in list containing `_atom_site_displace_special_func_atom_site_label`. Where no value is given, the assumed value is '0.0'. [atom_site_displace_special_func]

`_atom_site_occ_special_func_` []

Data items in the ATOM_SITE_DISPLACE_OCC_SPECIAL_FUNC category record details about the occupational modulation of a given atom or rigid group 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 suite of programs *JANA*. In this dictionary only the special functions available in *JANA*2000 have been included. Although this approach is far from being general it has the advantage that functions are tightly defined and therefore the atomic displacements and occupations can be easily calculated.

Summarising the special functions included in the dictionary are: 1) Sawtooth functions for atomic displacive modulation along *x*, *y* and *z*. Only applies to one-dimensional modulated structures. 2) Crenel functions for the occupational modulation of atoms and rigid groups. Only applies to one-dimensional modulated structures.

Example 1 - extracted from Elding-Pontén, M., Stenberg, L., Lidin, S., Madariaga, G. & Pérez-Mato, J. M. [(1997). Acta Cryst. B53, 364–372.]

```
# - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
#   In this example the occupational modulation of the Mn(2)
#   atom was modelled using a square-wave crenel function.
# - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
loop_
   _atom_site_occ_special_func_atom_site_label
   _atom_site_occ_special_func_crenel_c
   _atom_site_occ_special_func_crenel_w
      Mn(2)    0.25    0.623(4)
```

`_atom_site_occ_special_func_atom_site_label` (*char*)

The code that identifies an atom or rigid group in a loop where the parameters of the special function that describe its occupational modulation are being listed. This code must match the `_atom_site_label` of the associated coordinate list and conform to the rules described in `_atom_site_label`.

Appears in list as essential element of loop structure. **Must** match data name `_atom_site_label`. [atom_site_occ_special_func]

```
_atom_site_occ_special_func_crenel_c
_atom_site_occ_special_func_crenel_w
```
(*numb*)

`_atom_site_occ_special_func_crenel_` items are the adjustable parameters of a crenel function. An occupational crenel function along the internal space is defined as follows:

$p(x_4) = 1$ if x_4 belongs to the interval $[c - w/2, c + w/2]$

$p(x_4) = 0$ if x_4 is outside the interval $[c - w/2, c + w/2]$

where x_4 is the internal coordinate, c the center of the function in internal space and w its width. Its usage is restricted to one-dimensional modulated structures. For more details see for example the manual of *JANA*2000 (Petricek & Dusek, 2000).

Appears in list containing `_atom_site_occ_special_func_atom_site_label`. Where no value is given, the assumed value is '0.0'. [atom_site_occ_special_func]

`_atom_sites_displace_Fourier_` []

Data items in the ATOM_SITES_DISPLACE_FOURIER category record details common to the displacive modulation of atom sites in a modulated structure. Details for individual atom sites are described by data items in the ATOM_SITE_DISPLACE_FOURIER category.

Example 1 - extracted from Baudour & Sanquer [(1983). Acta Cryst. B39, 75–84.]

```
_atom_sites_displace_Fourier_axes_description
;  a1 and a2 are respectively the long molecular axis
   and the axis normal to the mean molecular plane.
;
```

`_atom_sites_displace_Fourier_axes_description`
(*char*)

The definition of the axes used for describing the displacive modulation, parameterized by Fourier series, when they are other than the crystallographic axes.

Example(s):
```
; a1 and a2 are respectively the long molecular axis
  and the axis normal to the mean molecular plane.
;
```
[atom_sites_displace_Fourier]

`_atom_sites_modulation_` []

Data items in the ATOM_SITES_MODULATION category record details common to the modulation of atom sites in a modulated structure.

_atom_sites_modulation_global_phase_t_1
_atom_sites_modulation_global_phase_t_2
_atom_sites_modulation_global_phase_t_3
_atom_sites_modulation_global_phase_t_4
_atom_sites_modulation_global_phase_t_5
_atom_sites_modulation_global_phase_t_6
_atom_sites_modulation_global_phase_t_7
_atom_sites_modulation_global_phase_t_8 (*numb*)

The initial phases in cycles of the modulation waves. For incommensurate structures they are irrelevant. However they are essential for the description of commensurate structures within the superspace formalism since they determine the space group of the commensurate superstructure [see Pérez-Mato, J. M., Madariaga, G., Zuñiga, F. J. & Garcia Arribas, A. (1987), *Acta Cryst. A***43**, 216–226 or van Smaalen, S. (1995), *Cryst. Rev.* **4**, 79–202]. Notice that for composites described using a single data block the initial phases for each subsystem are derived using the *W* matrices (see _cell_subsystem_matrix_W_) from a unique set of global phases whose values are assigned to _atom_sites_modulation_global_phase_t_. Detailed information can be found in the above cited reference of van Smaalen.

The permitted range is −1.0→1.0. Where no value is given, the assumed value is '0.0'. [atom_sites_modulation]

_atom_sites_rot_Fourier_[]

Data items in the ATOM_SITES_ROT_FOURIER category record details about the rotational component of the displacive modulation of a given rigid group as a whole. Details for individual atom sites are described by data items in the ATOM_SITES_ROT_FOURIER category.

Example 1 - extracted from Baudour & Sanquer [(1983). Acta Cryst. B39, 75–84.]

```
_atom_sites_rot_Fourier_axes_description
;  a1 and a2 are respectively the long molecular axis
   and the axis normal to the mean molecular plane.
;
```

_atom_sites_rot_Fourier_axes_description (*char*)

The definition of the axes used for describing the rotational part of the displacive modulation of a given rigid group, parameterized by Fourier series, when they are other than the crystallographic axes.

Example(s):

```
; a1 and a2 are respectively the long molecular axis
  and the axis normal to the mean molecular plane.
;                                [atom_sites_rot_Fourier]
```

_audit_link_[ms]

This category description does *not* introduce a new category; instead, it describes the recommended practice for using block codes as described in the core AUDIT_LINK category for descriptions of modulated structures. The value of _audit_block_code may be associated with a data block in the same or a different file related to the current data block. For an appropriate use of this item, _audit_block_code should be unique.

A recommended way for naming data blocks is the following:

<*string*> For the data block that includes those items that, given a certain material, are independent of a specific structure (modulated, reference, *etc.*). Consider, for example, the experimental set-up, publication details, *etc.*

<*string*>_REFRNCE For the data block that contains specific details corresponding to the reference (unmodulated) structure if it was refined separately using only main reflections. In the case of composites this data block may gather those items that are common to the reference structures of all subsystems.

<*string*>_MOD For the data block where specific details concerning the modulated structure are defined. Again, in the case of composites this data block may include either those items that are common to the modulated structures of all subsystems or the whole modulated structure if it is described implicitly through the *_subsystem_code pointers.

A trailing code following the reserved words MOD or REFRNCE would indicate that the corresponding data block includes structural information corresponding to the modulated or reference structures of the subsystem labelled by _cell_subsystem_code. A good format for <*string*> can be found in the definitions of _pd_block_[pd] and _pd_block_id that belong to the dictionary extension cif_pd.dic (http://www.iucr.org/iucr-top/cif/pd/index.html).

Example 1 - example file for the one-dimensional incommensurately modulated structure of K_2SeO_4.

```
loop_
  _audit_link_block_code
  _audit_link_block_description
    .               'publication details'
    K2SEO4_COM
       'experimental data common to ref./mod. structures'
    K2SEO4_REFRNCE  'reference structure'
    K2SEO4_MOD      'modulated structure'
```

Example 2 - example with a trailing string referencing a modulated structure of the subsystem labelled by _cell_subsystem_code.

```
_audit_link_block_code      'PbSVS2_MOD_VS2'
```

_cell_modulation_dimension (*numb*)

Number of additional reciprocal vectors needed to index the whole diffraction pattern using integer Miller indices.

The permitted range is 1→8. [cell]

_cell_reciprocal_basis_description (*char*)

Definition of the higher-dimensional basis with respect to which the Miller indices are defined. The three-dimensional basis used to index the additional wave vectors should be clearly indicated.

Example(s):

```
; a*,b*,c* (reciprocal basis spanning the lattice
  of main reflections) and q (incommensurate
  with respect to a*,b*,c*)
;
```

(Example 1 - Typical choice for a one-dimensional incommensurate structure),

```
; The diffraction pattern can be indexed with four
  integers based on the reciprocal vectors
  a*~1~=a*~11~, a*~2~=a*~12~, a*~3~=a*~13~,
  a*~4~=a*~21~. a*~1j~ (j=1,2,3) index the
  main reflections of the 1st subsystem. a*~21~ is
  incommensurate with a*~11~.
;
```

(Example 2 - Common choice for a misfit layer compound composed of two subsystems that have in common two reciprocal vectors. Extracted from van Smaalen [(1995). *Cryst. Rev.*, **4**, 79–202]) [cell]

_cell_subsystem_[ms]

Data items in the CELL_SUBSYSTEM category record details about the crystallographic cell parameters of each subsystem present in a composite.

Example 1 - extracted from van Smaalen [(1991). J. Phys.: Condens. Matter 3, 1247–1263.]

```
_cell_subsystems_number                 2
loop_
   _cell_subsystem_code
   _cell_subsystem_description
   _cell_subsystem_matrix_W_1_1
   _cell_subsystem_matrix_W_1_4
   _cell_subsystem_matrix_W_2_2
   _cell_subsystem_matrix_W_3_3
   _cell_subsystem_matrix_W_4_1
   _cell_subsystem_matrix_W_4_4
          NbS2           '1st subsystem'  1 0 1 1 0 1
          LaS            '2nd subsystem'  0 1 1 1 1 0
```

_cell_subsystem_description (*char*)

Description of each subsystem defining structurally a composite. Number of definitions must match the number given in _cell_subsystems_number.

Appears in list.

Example(s):

```
'NbS2 part of the layer compound (LaS)~1.14~NbS~2~'
```

[cell_subsystem]

_cell_subsystem_code (*char*)

The code identifying uniquely a certain composite subsystem. This code is used to identify the data blocks that contain the structural information associated with the subsystem.

Appears in list.

Example(s): 'NbS2' [cell_subsystem]

_cell_subsystem_matrix_W_1_1
_cell_subsystem_matrix_W_1_2
_cell_subsystem_matrix_W_1_3
_cell_subsystem_matrix_W_1_4
_cell_subsystem_matrix_W_1_5
_cell_subsystem_matrix_W_1_6
_cell_subsystem_matrix_W_1_7
_cell_subsystem_matrix_W_1_8
_cell_subsystem_matrix_W_1_9
_cell_subsystem_matrix_W_1_10
_cell_subsystem_matrix_W_1_11
_cell_subsystem_matrix_W_2_1
_cell_subsystem_matrix_W_2_2
_cell_subsystem_matrix_W_2_3
_cell_subsystem_matrix_W_2_4
_cell_subsystem_matrix_W_2_5
_cell_subsystem_matrix_W_2_6
_cell_subsystem_matrix_W_2_7
_cell_subsystem_matrix_W_2_8
_cell_subsystem_matrix_W_2_9
_cell_subsystem_matrix_W_2_10
_cell_subsystem_matrix_W_2_11
_cell_subsystem_matrix_W_3_1
_cell_subsystem_matrix_W_3_2
_cell_subsystem_matrix_W_3_3
_cell_subsystem_matrix_W_3_4
_cell_subsystem_matrix_W_3_5
_cell_subsystem_matrix_W_3_6
_cell_subsystem_matrix_W_3_7
_cell_subsystem_matrix_W_3_8
_cell_subsystem_matrix_W_3_9
_cell_subsystem_matrix_W_3_10
_cell_subsystem_matrix_W_3_11
_cell_subsystem_matrix_W_4_1
_cell_subsystem_matrix_W_4_2
_cell_subsystem_matrix_W_4_3
_cell_subsystem_matrix_W_4_4
_cell_subsystem_matrix_W_4_5
_cell_subsystem_matrix_W_4_6
_cell_subsystem_matrix_W_4_7
_cell_subsystem_matrix_W_4_8
_cell_subsystem_matrix_W_4_9
_cell_subsystem_matrix_W_4_10
_cell_subsystem_matrix_W_4_11
_cell_subsystem_matrix_W_5_1
_cell_subsystem_matrix_W_5_2
_cell_subsystem_matrix_W_5_3
_cell_subsystem_matrix_W_5_4
_cell_subsystem_matrix_W_5_5
_cell_subsystem_matrix_W_5_6
_cell_subsystem_matrix_W_5_7
_cell_subsystem_matrix_W_5_8
_cell_subsystem_matrix_W_5_9
_cell_subsystem_matrix_W_5_10
_cell_subsystem_matrix_W_5_11
_cell_subsystem_matrix_W_6_1
_cell_subsystem_matrix_W_6_2
_cell_subsystem_matrix_W_6_3
_cell_subsystem_matrix_W_6_4
_cell_subsystem_matrix_W_6_5
_cell_subsystem_matrix_W_6_6
_cell_subsystem_matrix_W_6_7
_cell_subsystem_matrix_W_6_8
_cell_subsystem_matrix_W_6_9
_cell_subsystem_matrix_W_6_10
_cell_subsystem_matrix_W_6_11
_cell_subsystem_matrix_W_7_1
_cell_subsystem_matrix_W_7_2
_cell_subsystem_matrix_W_7_3
_cell_subsystem_matrix_W_7_4
_cell_subsystem_matrix_W_7_5
_cell_subsystem_matrix_W_7_6
_cell_subsystem_matrix_W_7_7
_cell_subsystem_matrix_W_7_8
_cell_subsystem_matrix_W_7_9
_cell_subsystem_matrix_W_7_10
_cell_subsystem_matrix_W_7_11
_cell_subsystem_matrix_W_8_1

```
_cell_subsystem_matrix_W_8_2
_cell_subsystem_matrix_W_8_3
_cell_subsystem_matrix_W_8_4
_cell_subsystem_matrix_W_8_5
_cell_subsystem_matrix_W_8_6
_cell_subsystem_matrix_W_8_7
_cell_subsystem_matrix_W_8_8
_cell_subsystem_matrix_W_8_9
_cell_subsystem_matrix_W_8_10
_cell_subsystem_matrix_W_8_11
_cell_subsystem_matrix_W_9_1
_cell_subsystem_matrix_W_9_2
_cell_subsystem_matrix_W_9_3
_cell_subsystem_matrix_W_9_4
_cell_subsystem_matrix_W_9_5
_cell_subsystem_matrix_W_9_6
_cell_subsystem_matrix_W_9_7
_cell_subsystem_matrix_W_9_8
_cell_subsystem_matrix_W_9_9
_cell_subsystem_matrix_W_9_10
_cell_subsystem_matrix_W_9_11
_cell_subsystem_matrix_W_10_1
_cell_subsystem_matrix_W_10_2
_cell_subsystem_matrix_W_10_3
_cell_subsystem_matrix_W_10_4
_cell_subsystem_matrix_W_10_5
_cell_subsystem_matrix_W_10_6
_cell_subsystem_matrix_W_10_7
_cell_subsystem_matrix_W_10_8
_cell_subsystem_matrix_W_10_9
_cell_subsystem_matrix_W_10_10
_cell_subsystem_matrix_W_10_11
_cell_subsystem_matrix_W_11_1
_cell_subsystem_matrex_W_11_2
_cell_subsystem_matrix_W_11_3
_cell_subsystem_matrix_W_11_4
_cell_subsystem_matrix_W_11_5
_cell_subsystem_matrix_W_11_6
_cell_subsystem_matrix_W_11_7
_cell_subsystem_matrix_W_11_8
_cell_subsystem_matrix_W_11_9
_cell_subsystem_matrix_W_11_10
_cell_subsystem_matrix_W_11_11          (numb)
```

In the case of composites, for each subsystem the matrix W as defined in van Smaalen [(1991), *Phys. Rev. B***43**, 11330; see also van Smaalen (1995). *Cryst. Rev.* **4**, 79–202]. Its dimension must match (`_cell_modulation_dimension` + 3) × (`_cell_modulation_dimension` + 3).

Intergrowth compounds are composed of several periodic substructures in which the reciprocal lattices of two different subsystems are incommensurate in at least one direction. The indexation of the whole diffraction diagram with integer indices requires more than three reciprocal basic vectors. However the distinction between main reflections and satellites is not so obvious as in normal incommensurate structures. Indeed true satellites are normally difficult to locate for composites and the modulation wave vectors are reciprocal vectors of the other subsystem(s) referred to the reciprocal basis on one of them. The choice of the enlarged reciprocal basis $\{\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*, \mathbf{q}_1, \ldots, \mathbf{q}_d\}$ is completely arbitrary but the reciprocal basis of each subsystem is always known through the W matrices. These matrices [$(3 + d) \times (3 + d)$-dimensional], one for each subsystem, can be blocked as follows:

$$W^{\nu} = \begin{pmatrix} Z_3^{\nu} & Z_d^{\nu} \\ V_3^{\nu} & V_d^{\nu} \end{pmatrix}$$

the dimension of each block being (3×3), $(3 \times d)$, $(d \times 3)$ and $(d \times d)$ for Z_3^{ν}, Z_d^{ν}, V_3^{ν} and V_d^{ν} respectively. For example, Z^{ν} expresses the reciprocal basis of each subsystem in terms of the basis $\{\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*, \mathbf{q}_1, \ldots, \mathbf{q}_d\}$. W^{ν} also gives the irrational components of the modulation wave vectors of each subsystem in its own three-dimensional reciprocal basis $\{\mathbf{a}_{\nu}^*, \mathbf{b}_{\nu}^*, \mathbf{c}_{\nu}^*\}$ and the superspace group of a given subsystem from the unique superspace group of the composite.

The structure of these materials is always described by a set of incommensurate structures, one for each subsystem. The atomic coordinates, modulation parameters and wave vectors used for describing the modulation(s) are always referred to the (direct or reciprocal) basis of each particular subsystem. Although expressing the structural results in the chosen common basis is possible (using the matrices W) it is less confusing to use this alternative description. Atom coordinates are only put in a common basis when interatomic distances are calculated. Usually the triplet of reciprocal vectors $\{\mathbf{a}^*, \mathbf{b}^*$ and $\mathbf{c}^*\}$ span the lattice of main reflections of one of the subystems and therefore its W matrix is the unit matrix.

For composites described in a single data block using `*_subsystem_code` pointers, the cell parameters, the superspace group and the measured modulation wave vectors (see CELL_WAVE_VECTOR below) correspond to the reciprocal basis described in `_cell_reciprocal_basis_description` and coincide with the reciprocal basis of the specific subsystem (if any) whose W matrix is the unit matrix. The cell parameters and the symmetry of the remaining subsystems can be derived using the appropriate W matrices. In any case (single or multiblock CIF) the values assigned to the items describing the atomic parameters (including the wave vectors used to describe the modulations) are always the same and are referred to the basis of each particular subsystem. Such a basis will be explicitly given in a multiblock CIF or should be calculated (with the appropriate W matrix) in the case of a single block description of the composite.

Appears in list containing `_cell_subsystem_code`. Where no value is given, the assumed value is `'0'`. [cell_subsystem]

`_cell_subsystems_[ms]`

Data items in the CELL_SUBSYSTEMS category describe the gross structure of the subsystems present in a composite.

Example 1 - extracted from van Smaalen [(1991). J. Phys.: Condens. Matter 3, 1247–1263.]

```
_cell_subsystems_number                 2
```

`_cell_subsystems_number` (*numb*)

The number of subsystems used to define the structural model of a composite structure.

The permitted range is 2→∞. [cell_subsystems]

`_cell_wave_vector_[ms]`

Data items in the CELL_WAVE_VECTOR category list the independent modulation wave vectors $\mathbf{q}_i$. The diffraction vectors are indexed in the form $h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^* + \sum_i (m_i \mathbf{q}_i)$. $\sum_i$ is taken over all wave vectors. In this version of the dictionary the index *i* has been restricted to be less than 9.

Example 1 - example corresponding to the one-dimensional incommensurately modulated structure of K_2SeO_4.

```
loop_
   _cell_wave_vector_seq_id
   _cell_wave_vector_x
         1       0.318(5)
```

`_cell_wave_vector_x`
`_cell_wave_vector_y`
`_cell_wave_vector_z` (*numb*)

Independent modulation wave vector(s) with which the whole diffraction pattern is indexed, expressed as fractions of the three reciprocal basis vectors of the reference structure. In the case of composites the modulation wave vectors of each subsystem are expressed in terms of the reciprocal basis of its corresponding reference structure. Their number must match `_cell_modulation_dimension`. In the case of composites described in a single data block, the wave vectors are expressed in the three-dimensional basis chosen as reference in `_cell_reciprocal_basis_description` which would correspond to the subsystem (if any) whose *W* matrix is the $\{(\text{\_cell\_modulation\_dimension} + 3) \times (\text{\_cell\_modulation\_dimension} + 3)\}$ unit matrix. In this case the wave vectors used to describe the modulation of each subsystem are referred to their own reciprocal basis *via* the *W* matrices (for details see `_cell_subsystem_matrix_W_` and `_atom_site_Fourier_wave_vector_`).

Appears in list containing `_cell_wave_vector_seq_id`. Where no value is given, the assumed value is '0.0'. [cell_wave_vector]

`_cell_wave_vector_seq_id` (*numb*)

A numeric code to identify each independent wave vector. These codes define uniquely the reciprocal basis and, therefore, condition the order of the Miller indices assigned to intensities, crystal faces, *etc.*

Appears in list. [cell_wave_vector]

`_cell_wave_vectors_[ms]`

Data items in the CELL_WAVE_VECTORS category record details about the set of independent modulation wave vectors $\mathbf{q}_i$ and their measurement. The diffraction vectors are indexed in the form $h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^* + \sum_i (m_i \mathbf{q}_i)$. $\sum_i$ is taken over all wave vectors. In this version of the dictionary the index *i* has been restricted to be less than 9.

Example 1 - example corresponding to the one-dimensional incommensurately modulated structure of K_2SeO_4.

```
_cell_wave_vectors_meas_details
                'Determined from profiles along q'
```

`_cell_wave_vectors_meas_details` (*char*)

Details concerning the method of determining the independent modulation wave vector(s).

[cell_wave_vectors]

`_cell_wave_vectors_pressure_max`
`_cell_wave_vectors_pressure_min` (*numb*)

The maximum and minimum values of pressure in kilopascals defining the interval where the modulation wave vector(s) were measured.

The permitted range is $0.0 \rightarrow \infty$. [cell_wave_vectors]

`_cell_wave_vectors_temp_max`
`_cell_wave_vectors_temp_min` (*numb*)

The maximum and minimum values of temperature in kelvins defining the interval where the modulation wave vector(s) were measured.

The permitted range is $0.0 \rightarrow \infty$. [cell_wave_vectors]

`_cell_wave_vectors_variation` (*char*)

Details concerning the behaviour (and its experimental detection) of the wave vector(s) with temperature and/or pressure within the ranges specified by `_cell_wave_vectors_pressure_max`, `_cell_wave_vectors_pressure_min`, `_cell_wave_vectors_temp_max` and `_cell_wave_vectors_temp_min`.

[cell_wave_vectors]

`_diffrn_refln_index_m_1`
`_diffrn_refln_index_m_2`
`_diffrn_refln_index_m_3`
`_diffrn_refln_index_m_4`
`_diffrn_refln_index_m_5`
`_diffrn_refln_index_m_6`
`_diffrn_refln_index_m_7`
`_diffrn_refln_index_m_8` (*numb*)

Additional Miller indices needed to write the reciprocal vector of a certain reflection in the basis described in `_cell_reciprocal_basis_description`. Following the usual convention such a vector would be expressed as:

$$\mathbf{H} = h^*\mathbf{a}^* + k^*\mathbf{b}^* + l^*\mathbf{c}^* + m_1^*\mathbf{q}(1) + \cdots + m_8^*\mathbf{q}(8)$$

where h, k, l are the usual `_diffrn_refln_index_`, and $\mathbf{q}(1), \ldots, \mathbf{q}(8)$ represent the independent wave vectors given by `_cell_wave_vector_` and identified by `_cell_wave_vector_seq_id`. Therefore the total number of indices of a given reflection must match (`_cell_modulation_dimension` + 3) and the order of the additional indices must be consistent with the codes given in `_cell_wave_vector_seq_id`. These indices need not match `_refln_index_m_` values if a transformation of the original measured cell has been taken.

Appears in list containing `_diffrn_refln_index_`. [diffrn_refln]

`_diffrn_reflns_limit_index_m_1_max`
`_diffrn_reflns_limit_index_m_1_min`
`_diffrn_reflns_limit_index_m_2_max`
`_diffrn_reflns_limit_index_m_2_min`
`_diffrn_reflns_limit_index_m_3_max`
`_diffrn_reflns_limit_index_m_3_min`
`_diffrn_reflns_limit_index_m_4_max`
`_diffrn_reflns_limit_index_m_4_min`
`_diffrn_reflns_limit_index_m_5_max`

`_diffrn_reflns_limit_index_m_5_min`
`_diffrn_reflns_limit_index_m_6_max`
`_diffrn_reflns_limit_index_m_6_min`
`_diffrn_reflns_limit_index_m_7_max`
`_diffrn_reflns_limit_index_m_7_min`
`_diffrn_reflns_limit_index_m_8_max`
`_diffrn_reflns_limit_index_m_8_min` (*numb*)

Maximum and minimum values of the additional Miller indices appearing in `_diffrn_refln_index_m_`. Number of ranges must match `_cell_modulation_dimension`. Order of the additional indices must be consistent with the codes given in `_cell_wave_vector_seq_id`.

[diffrn_reflns]

`_diffrn_reflns_satellite_order_max` (*numb*)

Maximum order of observed satellites.

[diffrn_reflns]

`_diffrn_standard_refln_index_m_1`
`_diffrn_standard_refln_index_m_2`
`_diffrn_standard_refln_index_m_3`
`_diffrn_standard_refln_index_m_4`
`_diffrn_standard_refln_index_m_5`
`_diffrn_standard_refln_index_m_6`
`_diffrn_standard_refln_index_m_7`
`_diffrn_standard_refln_index_m_8` (*numb*)

Additional Miller indices needed to write the reciprocal vector of standard intensities used in the diffraction measurement process, in the basis described in `_cell_reciprocal_basis_description`. The total number of indices of a given standard reflection must match (`_cell_modulation_dimension` + 3) and the order of the additional indices must be consistent with the codes given in `_cell_wave_vector_seq_id`.

Appears in list containing `_diffrn_standard_refln_index_`.

[diffrn_standard_refln]

`_exptl_crystal_face_index_m_1`
`_exptl_crystal_face_index_m_2`
`_exptl_crystal_face_index_m_3`
`_exptl_crystal_face_index_m_4`
`_exptl_crystal_face_index_m_5`
`_exptl_crystal_face_index_m_6`
`_exptl_crystal_face_index_m_7`
`_exptl_crystal_face_index_m_8` (*numb*)

Additional Miller indices of the crystal face associated with the value `_exptl_crystal_face_perp_dist` when the face is indexed using a multidimensional scheme. The total number of indices must match (`_cell_modulation_dimension` + 3). Order of indices must be consistent with the codes given in `_cell_wave_vector_seq_id`.

Appears in list containing `_exptl_crystal_face_index_`.

[exptl_crystal_face]

`_exptl_crystal_type_of_structure` (*char*)

The type of structure used to check the consistency of a CIF. Expected data blocks and/or certain characteristic parameters depend on whether the material is classified as crystalline (periodic in three dimensions), modulated or composite.

`cryst`	crystalline structure
`mod`	modulated structure
`comp`	composite (misfit) structure

Where no value is given, the assumed value is `'cryst'`. [exptl_crystal]

`_geom_angle_max`
`_geom_angle_min`
`_geom_angle_av` (*numb*)

Maximum, minimum and average angles in degrees bounded by the `_geom_angle_atom_site_label_1`, `*_2`, and `*_3`. Site at `*_2` is at the apex of the angle.

Appears in list containing `_geom_angle_atom_site_label_`.

[geom_angle]

`_geom_angle_site_ssg_symmetry_1`
`_geom_angle_site_ssg_symmetry_2`
`_geom_angle_site_ssg_symmetry_3` (*char*)

The symmetry code of each atom site as the symmetry operation number '*n*' and the higher-dimensional translation '$m_1 \ldots m_p$'. These numbers are combined to form the code '*n* $m_1 \ldots m_p$' or *n*_$m_1 \ldots m_p$. The character string *n*_$m_1 \ldots m_p$ is composed as follows: '*n*' refers to the symmetry operation that is applied to the superspace coordinates. It must match a number given in `_space_group_symop_ssg_id`. '$m_1 \ldots m_p$' refer to the translations that are subsequently applied to the symmetry transformed coordinates to generate the atom used in calculating the angle. These translations $(t_1, \ldots, t_p)$ are related to $(m_1 \ldots m_p)$ by the relations $m_1 = 5 + t_1, \ldots, m_p = 5 + t_p$. By adding 5 to the translations, the use of negative numbers is avoided. The number '*p*' must agree with (`_cell_modulation_dimension` + 3). If there are no cell translations the translation number may be omitted. If no symmetry operations or translations are applicable then a single period '.' may be used.

Appears in list containing `_geom_angle_atom_site_label_`.

Example(s): `'.'` (no symmetry or translation to site), `'4'` (4th symmetry operation applied), `'7_6455'` (7th symm. posn; +*a* on *x*; −*b* on *y*) [geom_angle]

`_geom_bond_distance_max`
`_geom_bond_distance_min`
`_geom_bond_distance_av` (*numb*)

Maximum, minimum and average values of the intramolecular bond distance in ångströms.

Appears in list containing `_geom_bond_atom_site_label_`. The permitted range is 0.0→∞. [geom_bond]

`_geom_bond_site_ssg_symmetry_1`
`_geom_bond_site_ssg_symmetry_2` (*char*)

The symmetry code of each atom site as the symmetry operation number '*n*' and the higher-dimensional translation '$m_1 \ldots m_p$'. These numbers are combined to form the code '*n* $m_1 \ldots m_p$' or *n*_$m_1 \ldots m_p$. The character string *n*_$m_1 \ldots m_p$ is composed as follows: '*n*' refers to the symmetry operation that is applied to the superspace coordinates. It must match a number given in `_space_group_symop_ssg_id`. '$m_1 \ldots m_p$' refer to the translations that are subsequently applied to the symmetry transformed coordinates to generate the atom used in calculating the angle. These translations $(t_1, \ldots, t_p)$ are related to $(m_1 \ldots m_p)$ by the relations $m_1 = 5 + t_1, \ldots, m_p = 5 + t_p$. By adding 5 to the translations, the use of negative numbers is avoided. The number '*p*'

must agree with (_cell_modulation_dimension + 3). If there are no cell translations the translation number may be omitted. If no symmetry operations or translations are applicable then a single period '.' may be used.

Appears in list containing _geom_bond_atom_site_label_.

Example(s): '.' (no symmetry or translation to site), '4' (4th symmetry operation applied), '7_6455' (7th symm. posn; $+a$ on x; $-b$ on y) [geom_bond]

_geom_contact_distance_max
_geom_contact_distance_min
_geom_contact_distance_av (*numb*)

Maximum, minimum and average values of the interatomic contact distance in ångströms.

Appears in list containing _geom_contact_atom_site_label_. The permitted range is 0.0→∞. [geom_contact]

_geom_contact_site_ssg_symmetry_1
_geom_contact_site_ssg_symmetry_2 (*char*)

The symmetry code of each atom site as the symmetry operation number 'n' and the higher-dimensional translation '$m_1 \ldots m_p$'. These numbers are combined to form the code '$n\ m_1 \ldots m_p$' or $n\_m_1 \ldots m_p$. The character string $n\_m_1 \ldots m_p$ is composed as follows: 'n' refers to the symmetry operation that is applied to the superspace coordinates. It must match a number given in _space_group_symop_ssg_id. '$m_1 \ldots m_p$' refer to the translations that are subsequently applied to the symmetry transformed coordinates to generate the atom used in calculating the angle. These translations $(t_1, \ldots, t_p)$ are related to $(m_1 \ldots m_p)$ by the relations $m_1 = 5 + t_1, \ldots, m_p = 5 + t_p$. By adding 5 to the translations, the use of negative numbers is avoided. The number 'p' must agree with (_cell_modulation_dimension + 3). If there are no cell translations the translation number may be omitted. If no symmetry operations or translations are applicable then a single period '.' may be used.

Appears in list containing _geom_contact_atom_site_label_.

Example(s): '.' (no symmetry or translation to site), '4' (4th symmetry operation applied), '7_6455' (7th symm. posn; $+a$ on x; $-b$ on y) [geom_contact]

_geom_torsion_max
_geom_torsion_min
_geom_torsion_av (*numb*)

Maximum, minimum and average torsion angles in degrees bounded by the four atom sites identified by the _geom_torsion_atom_site_label_ codes. These must match labels specified as _atom_site_label in the atom list. The torsion angle definition should be that of Klyne, W. & Prelog, V. (1960). *Endeavour*, **16**, 521–528.

Appears in list containing _geom_torsion_atom_site_label_. [geom_torsion]

_geom_torsion_site_ssg_symmetry_1
_geom_torsion_site_ssg_symmetry_2
_geom_torsion_site_ssg_symmetry_3
_geom_torsion_site_ssg_symmetry_4 (*char*)

The symmetry code of each atom site as the symmetry operation number 'n' and the higher-dimensional translation '$m_1 \ldots m_p$'. These numbers are combined to form the code '$n\ m_1 \ldots m_p$' or $n\_m_1 \ldots m_p$. The character string $n\_m_1 \ldots m_p$ is composed as follows: 'n' refers to the symmetry operation that is applied to the superspace coordinates. It must match a number given in _space_group_symop_ssg_id. '$m_1 \ldots m_p$' refer to the translations that are subsequently applied to the symmetry transformed coordinates to generate the atom used in calculating the angle. These translations $(t_1, \ldots, t_p)$ are related to $(m_1 \ldots m_p)$ by the relations $m_1 = 5 + t_1, \ldots, m_p = 5 + t_p$. By adding 5 to the translations, the use of negative numbers is avoided. The number 'p' must agree with (_cell_modulation_dimension + 3). If there are no cell translations the translation number may be omitted. If no symmetry operations or translations are applicable then a single period '.' may be used.

Appears in list containing _geom_torsion_atom_site_label_.

Example(s): '.' (no symmetry or translation to site), '4' (4th symmetry operation applied), '7_6455' (7th symm. posn; $+a$ on x; $-b$ on y) [geom_torsion]

_refine_ls_mod_hydrogen_treatment (*char*)

Treatment of hydrogen modulation parameters in the least-squares refinement.

refA	refined H displacive modulation parameters only
refxyzA	refined H coordinates and displacive modulation parameters only
refP	refined H occupational modulation parameters only
refUP	refined H U and occupational modulation parameters only
nomod	no modulation of H parameters

Where no value is given, the assumed value is 'nomod'. [refine]

_refine_ls_mod_func_description (*char*)

Types of modulation present in the structural model and their parameterization.

Example(s):
'Only displacive modulation. Fourier series',
; Modulation of atom S(1) described by a non-standard
  linear sawtooth function
; [refine]

_refine_ls_mod_overall_phason_coeff (*numb*)

The phason coefficient used to calculate the overall phason correction.

Where no value is given, the assumed value is '0.0'.The permitted range is 0.0→∞. [refine]

_refine_ls_mod_overall_phason_formula (*char*)

The expression for the overall phason correction if used.

Axe	Axe, J. D., *Phys. Rev. B***21** (1980), 4181
Ovr	Overhauser, A. W., *Phys. Rev. B***3** (1971), 3173

[refine]

_refln_index_m_1
_refln_index_m_2
_refln_index_m_3
_refln_index_m_4
_refln_index_m_5
_refln_index_m_6
_refln_index_m_7
_refln_index_m_8 (*numb*)

Additional Miller indices of a certain reflection in the basis described in `_cell_reciprocal_basis_description`. The total number of indices must match (`_cell_modulation_dimension` + 3). The order of the additional indices must be consistent with the codes given in `_cell_wave_vector_seq_id`.

Appears in list containing `_refln_index_`. [refln]

`_reflns_limit_index_m_1_max`
`_reflns_limit_index_m_1_min`
`_reflns_limit_index_m_2_max`
`_reflns_limit_index_m_2_min`
`_reflns_limit_index_m_3_max`
`_reflns_limit_index_m_3_min`
`_reflns_limit_index_m_4_max`
`_reflns_limit_index_m_4_min`
`_reflns_limit_index_m_5_max`
`_reflns_limit_index_m_5_min`
`_reflns_limit_index_m_6_max`
`_reflns_limit_index_m_6_min`
`_reflns_limit_index_m_7_max`
`_reflns_limit_index_m_7_min`
`_reflns_limit_index_m_8_max`
`_reflns_limit_index_m_8_min` (*numb*)

Maximum and minimum values of the additional Miller indices appearing in `_refln_index_m_`. Number of ranges must match `_cell_modulation_dimension`. Order of the additional indices must be consistent with the codes given in `_cell_wave_vector_seq_id`. These need not be the same as the `_diffrn_reflns_limit_index_m_`.

[reflns]

`_space_group_[ms]`

The SPACE_GROUP category introduced in the symmetry CIF Dictionary (cif_sym.dic 1.0) is intended to replace the original core SYMMETRY category. For modulated structures, superspace group descriptions may be included in the same category, but include the `_ssg_` flag to indicate their dimensionality of > 3.

`_space_group_ssg_IT_number` (*numb*)

Superspace group number from *International Tables for Crystallography*, Vol. C. Valid only for one-dimensional modulated structures.

Ref: *International Tables for Crystallography*, Vol. C, First edition (1992) pp. 797–835, or *International Tables for Crystallography*, Vol. C, Second edition (1999) pp. 899–937.

The permitted range is $1.1 \rightarrow \infty$. [space_group]

`_space_group_ssg_name` (*char*)

Superspace group symbol conforming to an alternative definition from that given in `_space_group_ssg_name_IT` and `_space_group_ssg_name_WJJ` for one-dimensional modulated structures or to the superspace group name for higher dimensions. When necessary indicate the origin and the setting. Use a colon ':' as separator between the different parts of the superspace group symbol. Within each part leave a space between each component. Rules about the notation for Hermann–Mauguin and Hall symbols (if present) are given in the symmetry CIF Dictionary (cif_sym.dic 1.0) and, partially, in `_space_group_ssg_name_IT` and `_space_group_ssg_name_WJJ`. For composites described in a single data block, the superspace group describes the symmetry of the whole structure. The symmetry of each subsystem can be derived using the appropriate *W* matrices.

Example(s): `'Hall's notation W:-P -2xb -2ya:q q'` [space_group]

`_space_group_ssg_name_IT` (*char*)

Superspace group symbol as supplied in *International Tables for Crystallography*, Vol. C. Valid only for one-dimensional modulated structures. The symbol is divided in three parts: the Hermann–Mauguin space group symbol of the reference structure, the modulation wave vector, and the phase shift (or internal translation) associated with each component of the space group. Each component of the space group name is separated by a space. Subscripts should appear without special symbols, bars as negative signs. The components of the modulation wave vector (in parenthesis) and the phase shifts are also separated by a space. For composites described in a single data block, the superspace group describes the symmetry of the whole structure. The symmetry of each subsystem can be derived using the appropriate *W* matrices.

Ref: *International Tables for Crystallography*, Vol. C, First edition (1992) pp. 797–835, or *International Tables for Crystallography*, Vol. C, Second edition (1999) pp. 899–937.

Example(s): `'P n m a (0 0 \g) 0 s 0'` [space_group]

`_space_group_ssg_name_WJJ` (*char*)

Superspace group symbol as given by de Wolff, Janssen & Janner (1981). Valid only for one-dimensional modulated structures. The symbol is divided in three parts separated by a colon ':': The superspace lattice symbol, the Hermann–Mauguin space group symbol of the reference structure, and the phase shift (or internal translation) associated with each component of the space group. Each component of the space group name is separated by a space. Subscripts should appear without special symbols, bars as negative signs. The phase shifts are also separated by a space. For composites described in a single data block, the superspace group describes the symmetry of the whole structure. The symmetry of each subsystem can be derived using the appropriate *W* matrices.

Ref: de Wolff, P. M., Janssen, T. & Janner, A. (1981). *Acta Cryst. A***37**, 625–636

Example(s): `'P:P c m n:s s -1'` [space_group]

`_space_group_ssg_WJJ_code` (*char*)

Superspace group code as given by de Wolff, Janssen & Janner (1981). Valid only for one-dimensional modulated structures.

Ref: de Wolff, P. M., Janssen, T. & Janner, A. (1981). *Acta Cryst. A***37**, 625–636

Example(s): `'28a.10.1/2'` [space_group]

`_space_group_symop_[ms]`

The SPACE_GROUP_SYMOP category introduced in the symmetry CIF dictionary (cif_sym.dic 1.0) is intended to replace the original core SYMMETRY_EQUIV category. It contains information about the symmetry operations of the space group. For modulated structures, superspace group descriptions may be included in the same category, but include the `_ssg_` flag to indicate their dimensionality of > 3.

Example 1 - example corresponding to the one-dimensional incommensurately modulated structure of K_2SeO_4.

```
loop_
  _space_group_symop_ssg_id
  _space_group_symop_ssg_operation_algebraic
         1                      x1,x2,x3,x4
         2                      1/2+x1,1/2-x2,1/2-x3,x4
         3                      1/2-x1,1/2+x2,-x3,1/2-x4
         4                      -x1,-x2,1/2+x3,1/2-x4
         5                      -x1,-x2,-x3,-x4
         6                      1/2-x1,1/2+x2,1/2+x3,-x4
         7                      1/2+x1,1/2-x2,x3,1/2+x4
         8                      x1,x2,1/2-x3,1/2+x4
```

`_space_group_symop_ssg_operation_algebraic` (*char*)

A parsable string giving one of the symmetry operations of the superspace group in algebraic form. This data will generally be repeated in a loop. Use symbols as necessary according to `_cell_modulation_dimension`. All symmetry operations should be entered, including the identity operation, those for lattice centring and a centre of symmetry, if present. Symbolic notation for coordinates is expected to be so that the identity is expressed as $x1, x2, x3, \ldots, xn$. `_space_group_symop_ssg_operation_algebraic` must always be present in a CIF corresponding to a modulated structure.

Appears in list containing `_space_group_symop_ssg_id`.

Example(s): `'x1,-x2,x3,1/2+x4'` [space_group_symop]

`_space_group_symop_ssg_id` (*numb*)

A numeric code identifying the associated set of superspace symmetry operations given in `_space_group_symop_ssg_operation_algebraic`.

Appears in list. [space_group_symop]