4.3. Modulated and composite structures dictionary (msCIF)

BY G. MADARIAGA

This is version 1.0.1 of the modulated and composite structures CIF dictionary (msCIF). The data names defined in this dictionary complement and/or extend those in the core CIF dictionary (Chapter 4.1) to cover the specific structural features of modulated and composite structures. The msCIF dictionary includes 19 new categories and extends 18 that already exist in the core CIF dictionary. A commentary on the use of this dictionary may be found in Chapter 3.4.

Categories are described in alphabetic order; data items are arranged alphabetically within each category.

ATOM_SITE

Data items in the ATOM_SITE category record details about the atom sites in a crystal structure, such as the positional coordinates, atomic displacement parameters, and magnetic moments and directions. This category exists in the core CIF dictionary but is extended in this dictionary by the addition of some items that may appear in the main looped list of atom-site information.

_atom_site_displace_modulation_flag (*char*)

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

Appears in list containing **_atom_site_label**.

The data value must be one of the following:

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

Where no value is given, the assumed value is 'no'. **[atom_site]**

_atom_site_occ_modulation_flag (*char*)

A code that signals whether the structural model includes the modulation of the occupation of a given atom site.

Appears in list containing **_atom_site_label**.

The data value must be one of the following:

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

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 which is less explicit than that based on linked data blocks (see the description in this dictionary of AUDIT_LINK). It must match one of the labels specified for **_cell_subsystem_code.**

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

_atom_site_U_modulation_flag (*char*)

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

Appears in list containing **_atom_site_label**.

The data value must be one of the following:

yes	modulation of thermal parameters
y	abbreviation for 'yes'
no	no modulation of thermal parameters
n	abbreviation for 'no'

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 – based on the modulated structure of inorganic misfit layer $(LaS)_{1.14}NbS_2$ [Smaalen, S. van (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 – based on the modulated structure of inorganic misfit layer $(LaS)_{1.14}NbS_2$ [Smaalen, S. van (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
```

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```
# 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 – based on the modulated structure of inorganic misfit layer $(LaS)_{1.14}NbS_2$ *[Smaalen, S. van (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 [Acta Cryst. (1983), B****39****, 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 atom 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 in which the Fourier components of its displacive modulation are 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 parent 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_sites_displace_Fourier_axes_description**.

Appears in list containing **_atom_site_displace_Fourier_id**.

The data value must be one of the following:

x	displacement along the *a* axis
y	displacement along the *b* axis
z	displacement along the *c* axis
a1	displacement along an arbitrary a_1 axis
a2	displacement along an arbitrary a_2 axis
a3	displacement along an arbitrary a_3 axis

[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 the modulation 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 child 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 parent 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_DISPLACE_FOURIER and are listed separately.

*Example 1 – based on the modulated structure of inorganic misfit layer $(LaS)_{1.14}NbS_2$ [Smaalen, S. van (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 – based on the modulated structure of inorganic misfit layer $(LaS)_{1.14}NbS_2$ [Smaalen, S. van (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 – based on the modulated structure of inorganic misfit layer $(LaS)_{1.14}NbS_2$ [Smaalen, S. van (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 [Acta Cryst. (1983), B**39**, 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, su*)
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 parent data name **_atom_site_displace_Fourier_id**.

[atom_site_displace_Fourier_param]

_atom_site_displace_Fourier_param_modulus (*numb, su*)
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**.

The permitted range is $0.0 \rightarrow \infty$. Where no value is given, the assumed value is '0.0'.

[atom_site_displace_Fourier_param]

_atom_site_displace_Fourier_param_phase (*numb, su*)
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 ($\varphi/2\pi$) 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**.

The permitted range is $-1.0 \rightarrow 1.0$. Where no value is given, the assumed value is '0.0'.

[atom_site_displace_Fourier_param]

_atom_site_displace_Fourier_param_sin (*numb, su*)

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_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 *JANA* suite of programs. Although this approach is far from being general, it has the advantage that the functions are tightly defined and therefore the atomic displacements and occupations can be calculated easily. In this dictionary, only the special functions available in *JANA*2000 have been included. These are: (1) Sawtooth functions for atomic displacive modulation along *x*, *y* and *z*. (2) Crenel functions for the occupational modulation of atoms and rigid groups. Both of these only apply to one-dimensional modulated structures.

Example 1 – extracted from Gao, Coppens, Cox & Moodenbaugh [Acta Cryst. (1993), 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)  -0.270(6)  0.022(9)  0.014(2)  0.42(2)  1.07(2)
```

_atom_site_displace_special_func_atom_site_label (*char*)

The code that identifies an atom in a loop in which the special function that describes 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 parent 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, su*)

_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:

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

for x_4 belonging to the interval $[c - (w/2), c + (w/2)]$, 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 is the centre of the function in internal space. u_x, u_y and u_z must be expressed in relative units. The use of this function is restricted to one-dimensional modulated structures. For more details, see the manual for *JANA*2000 (Petříček & Dušek, 2000).

Reference: Petříček, V. & Dušek, M. (2000). *JANA*2000. *The crystallographic computing system*. Institute of Physics, Prague, Czech Republic.

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_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 – based on the modulated structure of inorganic misfit layer $(LaS)_{1.14}NbS_2$ [Smaalen, S. van (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: '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 child 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

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, Zúñiga, Paciorek & Bocanegra [Acta Cryst. (1990), B**46**, 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_atom_site_label (*char*)
Modulation parameters are usually looped in separate lists. Modulated parameters are the atom 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 in which the Fourier components of its occupational modulation are 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 parent 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 the modulation is expressed in terms of Fourier series.
Appears in list as essential element of loop structure. May match child 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 parent data name **_atom_site_Fourier_wave_vector_seq_id**.
[atom_site_occ_Fourier]

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, Zúñiga, Paciorek & Bocanegra [Acta Cryst. (1990), B**46**, 620–628].*

```
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, su*)
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 $\mathbf{k}$ is the wave vector of the term and $\mathbf{r}$ 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 parent data name **_atom_site_occ_Fourier_id**. **[atom_site_occ_Fourier_param]**

_atom_site_occ_Fourier_param_modulus (*numb, su*)
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**.
The permitted range is $0.0 \rightarrow \infty$. Where no value is given, the assumed value is '0.0'.
[atom_site_occ_Fourier_param]

_atom_site_occ_Fourier_param_phase (*numb, su*)
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 ($\delta/2\pi$) 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**.
The permitted range is $-1.0 \rightarrow 1.0$. Where no value is given, the assumed value is '0.0'.
[atom_site_occ_Fourier_param]

_atom_site_occ_Fourier_param_sin (*numb, su*)
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_OCC_SPECIAL_FUNC

Data items in the ATOM_SITE_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 *JANA* suite of programs. Although this approach is far from being general, it has the advantage that the functions are tightly defined and therefore the atomic displacements and occupations can be calculated easily. In this dictionary, only the special functions available in *JANA*2000 have been included. These are: (1) Sawtooth functions for atomic displacive modulation along *x*, *y* and *z*. (2) Crenel functions for the occupational modulation of atoms and rigid groups. Both of these only apply to one-dimensional modulated structures.

*Example 1 – extracted from Elding-Pontén, Stenberg, Lidin, Madariaga & Pérez-Mato [Acta Cryst. (1997), B**53**, 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 in which the parameters of the special function that describes its occupational modulation are 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 parent 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, su*)
_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 is the centre of the function in internal space and w is its width. The use of this function is restricted to one-dimensional modulated structures. For more details, see the manual for *JANA*2000 (Petříček & Dušek, 2000).

Reference: Petříček, V. & Dušek, M. (2000). *JANA*2000. *The crystallographic computing system.* Institute of Physics, Prague, Czech Republic.

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_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.

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 [Acta Cryst. (1983), B**39**, 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_phason_atom_site_label (*char*)

The code that identifies an atom or rigid group in a loop in which the phason coefficients are 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 parent data name **_atom_site_label**. **[atom_site_phason]**

_atom_site_phason_coeff (*numb, su*)

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**.

The permitted range is $0.0 \rightarrow \infty$. Where no value is given, the assumed value is '0.0'.

[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_**).

Appears in list containing **_atom_site_phason_atom_site_label**.

The data value must be one of the following:

Axe	Axe, J. D. (1980). *Phys. Rev. B*, **21**, 4181–4190.
Ovr	Overhauser, A. W. (1971). *Phys. Rev. B*, **3**, 3173–3182.

[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.

_atom_site_rot_Fourier_atom_site_label (*char*)

Modulation parameters are usually looped in separate lists. Modulated parameters are the atom 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 in which the Fourier components of the rotational part of its displacive modulation are 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 parent 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**.

Appears in list containing **_atom_site_rot_Fourier_id**.

The data value must be one of the following:

x	rotation around the *a* axis
y	rotation around the *b* axis
z	rotation around the *c* axis
a1	rotation around an arbitrary a_1 axis
a2	rotation around an arbitrary a_2 axis
a3	rotation around an arbitrary a_3 axis

[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 the modulation is expressed in terms of Fourier series.

Appears in list as essential element of loop structure. May match child 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 parent data name **_atom_site_Fourier_wave_vector_seq_id**.
[atom_site_rot_Fourier]

_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 parent data name **_atom_site_rot_Fourier_id**. **[atom_site_rot_Fourier_param]**

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.

```
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 [Acta Cryst. (1983), B**39**, 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_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, su*)
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_modulus (*numb, su*)
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**.
The permitted range is $0.0 \rightarrow \infty$. Where no value is given, the assumed value is '0.0'.
[atom_site_rot_Fourier_param]

_atom_site_rot_Fourier_param_phase (*numb, su*)
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 ($\psi/2\pi$) 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**.
The permitted range is $-1.0 \rightarrow 1.0$. Where no value is given, the assumed value is '0.0'.
[atom_site_rot_Fourier_param]

_atom_site_rot_Fourier_param_sin (*numb, su*)
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 [Acta Cryst. (1994), B**50**, 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 atom 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 in which the Fourier components of its thermal-parameters modulation are 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 parent 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 child 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.

Appears in list containing **_atom_site_U_Fourier_id**.

The data value must be one of the following:

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 $U_{\text{isotropic}}$

[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 parent 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_PARAM 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 [Acta Cryst. (1994), B**50**, 333–343].*

```
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, su*)
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**, **_atom_site_U_Fourier_tens_elem** and **_atom_site_U_Fourier_wave_vector_seq_id**.

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 parent data name **_atom_site_U_Fourier_id**. **[atom_site_U_Fourier_param]**

_atom_site_U_Fourier_param_modulus (*numb, su*)

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**, **_atom_site_U_Fourier_tens_elem** and **_atom_site_U_Fourier_wave_vector_seq_id**.

Appears in list containing **_atom_site_U_Fourier_param_id**.

The permitted range is $0.0 \rightarrow \infty$. Where no value is given, the assumed value is '0.0'. **[atom_site_U_Fourier_param]**

_atom_site_U_Fourier_param_phase (*numb, su*)

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 $(\chi/2\pi)$ in cycles of the complex amplitude corresponding to the Fourier term defined by **_atom_site_U_Fourier_atom_site_label**, **_atom_site_U_Fourier_tens_elem** and **_atom_site_U_Fourier_wave_vector_seq_id**.

Appears in list containing **_atom_site_U_Fourier_param_id**.

The permitted range is $-1.0 \rightarrow 1.0$. Where no value is given, the assumed value is '0.0'. **[atom_site_U_Fourier_param]**

_atom_site_U_Fourier_param_sin (*numb, su*)

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**, **_atom_site_U_Fourier_tens_elem** and **_atom_site_U_Fourier_wave_vector_seq_id**.

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_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 [Acta Cryst. (1983), B**39**, 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:

```
; 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 Perez-Mato, Madariaga, Zuñiga & Garcia Arribas (1987) or van Smaalen (1995)]. Note 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 van Smaalen (1995).

References: Perez-Mato, J. M., Madariaga, G., Zuñiga, F. J. & Garcia Arribas, A. (1987). *Acta Cryst.* A**43**, 216–226. Smaalen, S. van (1995). *Crystallogr. Rev.* **4**, 79–202.

The permitted range is $-1.0 \rightarrow 1.0$. 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 [Acta Cryst. (1983), B**39**, 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:

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

AUDIT_LINK

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 file or in a different file related to the current data block. The value of **_audit_block_code** should be unique.

It is recommended that data blocks are named as follows:

<*string*>: The name of the data block containing those items that, for a particular material, are independent of the specific structure (modulated, reference *etc.*). For example, the experimental set-up or publication details would be described here.

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

<*string*>_MOD: The name of the data block in which specific details of the modulated structure are given. 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 indicates that the corresponding data block includes structural information corresponding to the modulated or reference structures of the subsystem labelled by **_cell_subsystem_code**. A recommended format for <*string*> is given in the definitions of PD_BLOCK and **_pd_block_id** in the dictionary extension cif_pd.dic (Chapter 4.2).

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

Data items in the CELL category record details about the crystallographic cell parameters and their measurement. This category is already defined in the core CIF dictionary but is extended in this dictionary by the addition of some items that are specific for modulated and composite structures.

_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.

Examples:

```
; a*,b*,c* (reciprocal basis spanning the lattice of main
  reflections) and q (incommensurate with respect to a*,b*,c*)
;  (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~.
;  (Common choice for a misfit layer compound composed of two subsystems that have in
common two reciprocal vectors. Extracted from van Smaalen [*Crystallogr. Rev.* (1995), **4**,
79–202].)                                                    [cell]
```

CELL_SUBSYSTEM

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

*Example 1 – based on the modulated structure of inorganic misfit layer $(LaS)_{1.14}NbS_2$ [Smaalen, S. van (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_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: 'NbS2'. **[cell_subsystem]**

_cell_subsystem_description (*char*)
Description of each subsystem defining a composite structurally. The number of definitions must match the number given in **_cell_subsystems_number**.
Appears in list.
Example: 'NbS2 part of the layer compound (LaS)~1.14~NbS~2~'.
[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_matrix_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); see also van Smaalen (1995). 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 index-

ing 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 as 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 of 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. Atomic coordinates are only referred to a common basis when interatomic distances are calculated. Usually, the reciprocal vectors $\{\mathbf{a}^*, \mathbf{b}^*$ and $\mathbf{c}^*\}$ span the lattice of main reflections of one of the subsystems 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.

References: Smaalen, S. van (1991). *Phys. Rev. B*, **43**, 11330–11341. Smaalen, S. van (1995). *Crystallogr. Rev.* **4**, 79–202.

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

CELL_SUBSYSTEMS

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

*Example 1 – based on the modulated structure of inorganic misfit layer $(LaS)_{1.14}NbS_2$ [Smaalen, S. van (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 $2 \rightarrow \infty$. **[cell_subsystems]**

CELL_WAVE_VECTOR

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_seq_id (*numb*)
A numeric code to identify each independent wave vector. These codes define uniquely the reciprocal basis and, therefore, force the order of the Miller indices assigned to intensities, crystal faces *etc.*
Appears in list. **[cell_wave_vector]**

_cell_wave_vector_x
_cell_wave_vector_y
_cell_wave_vector_z (*numb, su*)
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 (**_cell_modulation_dimension** + 3) $\times$ (**_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_VECTORS

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 about the method used to determine the independent modulation wave vector(s).
[cell_wave_vectors]

_cell_wave_vectors_pressure_max
_cell_wave_vectors_pressure_min (*numb, su*)
The maximum and minimum values of the pressure in kilopascals defining the interval within which 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, su*)
The maximum and minimum values of the temperature in kelvins defining the interval within which 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

Data items in the DIFFRN_REFLN category record details about the intensities measured in the diffraction experiment. The DIFFRN_REFLN data items refer to individual intensity measurements and must be included in looped lists. (The DIFFRN_REFLNS data items specify the parameters that apply to all intensity measurements. The DIFFRN_REFLNS data items are not looped.) Data items in this category are extensions of the core CIF dictionary definitions to the indexing of diffraction intensities by higher-dimensional components.

_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

$$\mathbf{H} = h^*\mathbf{a}^* + k^*\mathbf{b}^* + l^*\mathbf{c}^* + m_1^*\mathbf{q}_1 + ... + m_8^*\mathbf{q}_8,$$

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 occurred.
Appears in list containing **_diffrn_refln_index_h**, **_diffrn_refln_index_k**, **_diffrn_refln_index_l**. **[diffrn_refln]**

DIFFRN_REFLNS

Data items in the DIFFRN_REFLNS category record details about the set of intensities measured in the diffraction experiment. The DIFFRN_REFLNS data items specify the parameters that apply to all intensity measurements. The DIFFRN_REFLNS data items are not looped. (The DIFFRN_REFLN data items refer to individual intensity measurements and must be included in looped lists.) Data items in this category extend the core CIF dictionary definitions providing independent checks on the range of values recorded for each of the additional Miller indices given in the DIFFRN_REFLN category.

_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_**. The number of ranges must match **_cell_modulation_dimension**. The 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

Data items in the DIFFRN_STANDARD_REFLN category record details about the reflections treated as standards during the measurement of diffraction intensities. Note that these are the individual standard reflections, not the results of the analysis of the standard reflections. Data items in this category are extensions of the core CIF dictionary definitions to the indexing of standard reflections by higher-dimensional components.

_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 vectors of the 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_h**, **_diffrn_standard_refln_index_k**, **_diffrn_standard_refln_index_l**.

[diffrn_standard_refln]

EXPTL_CRYSTAL

Data items in the EXPTL_CRYSTAL category record details about experimental measurements on the crystal or crystals used, such as shape, size and density. The new data item added to this category specifies whether the structure is crystalline, modulated or composite.

_exptl_crystal_type_of_structure (*char*)

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

The data value must be one of the following:

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

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

EXPTL_CRYSTAL_FACE

Data items in the EXPTL_CRYSTAL_FACE category record details of the crystal faces. Data items in this category are extensions of the core CIF dictionary definitions to the indexing of crystal faces by higher-dimensional components.

_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). The order of the indices must be consistent with the codes given in **_cell_wave_vector_seq_id**.

Appears in list containing **_exptl_crystal_face_index_h**, **_exptl_crystal_face_index_k**, **_exptl_crystal_face_index_l**.

[exptl_crystal_face]

GEOM_ANGLE

Data items in the GEOM_ANGLE category record details about the bond angles, as calculated from the ATOM, CELL and SYMMETRY data. These extensions to the core CIF dictionary definitions record the maximum, minimum and average values of angles and extend the symmetry-operation code used in angle listings to the higher-dimensional superspace form.

_geom_angle_max
_geom_angle_min
_geom_angle_av (*numb, su*)

Maximum, minimum and average angles in degrees bounded by **_geom_angle_atom_site_label_1**, *_2, and *_3. The 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 full stop '.' is used.

Appears in list containing **_geom_angle_atom_site_label_**.

Examples: '.' (no symmetry or translation to site), '4' (4th symmetry operation applied), '7_6455' (7th symmetry position; +**a** on *x*, -**b** on *y*). **[geom_angle]**

GEOM_BOND

Data items in the GEOM_BOND category record details about bonds, as calculated from the ATOM, CELL and SYMMETRY data. These extensions to the core CIF dictionary definitions record the maximum, minimum and average lengths of bonds and extend the symmetry-operation code used in bond listings to the higher-dimensional superspace form.

_geom_bond_distance_max
_geom_bond_distance_min
_geom_bond_distance_av (*numb, su*)

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 $0.0 \rightarrow \infty$. **[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 bond. 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 full stop '.' is used.

Appears in list containing **_geom_bond_atom_site_label_**.

Examples: '. ' (no symmetry or translation to site), '4' (4th symmetry operation applied), '7_6455' (7th symmetry position; +**a** on *x*, -**b** on *y*). **[geom_bond]**

GEOM_CONTACT

Data items in the GEOM_CONTACT category record details about interatomic contacts, as calculated from the ATOM, CELL and SYMMETRY data. These extensions to the core CIF dictionary definitions record the maximum, minimum and average values of contact distances and extend the symmetry-operation code used in contact-distance listings to the higher-dimensional superspace form.

_geom_contact_distance_max
_geom_contact_distance_min
_geom_contact_distance_av (*numb, su*)

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 $0.0 \rightarrow \infty$. **[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 contact. 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 full stop '.' is used.

Appears in list containing **_geom_contact_atom_site_label_**.

Examples: '. ' (no symmetry or translation to site), '4' (4th symmetry operation applied), '7_6455' (7th symmetry position; +**a** on *x*, -**b** on *y*). **[geom_contact]**

GEOM_TORSION

Data items in the GEOM_TORSION category record details about torsion angles, as calculated from the ATOM, CELL and SYMMETRY data. These extensions to the core CIF dictionary definitions record the maximum, minimum and average values of torsion angles and extend the symmetry-operation code used in torsion-angle listings to the higher-dimensional superspace form.

_geom_torsion_max
_geom_torsion_min
_geom_torsion_av (*numb, su*)

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 and Prelog.

Reference: Klyne, W. & Prelog, V. (1960). *Experientia*, **16**, 521–523.

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 full stop '.' is used.

Appears in list containing **_geom_torsion_atom_site_label_**.

Examples: '. ' (no symmetry or translation to site), '4' (4th symmetry operation applied), '7_6455' (7th symmetry position; +**a** on *x*, -**b** on *y*). **[geom_torsion]**

REFINE

Data items in the REFINE category record details about the structure refinement parameters. The new items in this category extend those of the core CIF dictionary and are specific to the refinement of modulated structures.

_refine_ls_mod_func_description (*char*)

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

Examples: 'Only displacive modulation. Fourier series.',

```
; Modulation of atom S(1) described by a non-standard
  linear sawtooth function
;
```

[refine]

_refine_ls_mod_hydrogen_treatment (*char*)

Treatment of hydrogen-atom modulation parameters in the refinement.

The data value must be one of the following:

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

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

_refine_ls_mod_overall_phason_coeff (*numb, su*)
The phason coefficient used to calculate the overall phason correction.
The permitted range is $0.0 \rightarrow \infty$. Where no value is given, the assumed value is '0.0'.
[refine]

_refine_ls_mod_overall_phason_formula (*char*)
The expression for the overall phason correction, if used.
The data value must be one of the following:

Axe	Axe, J. D. (1980). *Phys. Rev. B*, **21**, 4181–4190.
Ovr	Overhauser, A. W. (1971). *Phys. Rev. B*, **3**, 3173–3182.

[refine]

REFLN

Data items in the REFLN category record details about the reflections used to determine the ATOM_SITE data items. The REFLN data items refer to individual reflections and must be included in looped lists. The REFLNS data items specify the parameters that apply to all reflections. The REFLNS data items are not looped. Data items in this category are extensions of the core CIF dictionary definitions to the indexing of reflections used in the refinement by higher-dimensional components.

_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 particular 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_h**, **_refln_index_k**, **_refln_index_l**.
[refln]

REFLNS

Data items in the REFLNS category record details about the reflections used to determine the ATOM_SITE data items. The REFLN data items refer to individual reflections and must be included in looped lists. The REFLNS data items specify the parameters that apply to all reflections. The REFLNS data items are not looped. Data items in this category extend the core CIF dictionary definitions providing independent checks on the range of values recorded for each of the additional Miller indices given in the REFLN category.

_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_**. The number of ranges must match **_cell_modulation_dimension**. The 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

The SPACE_GROUP category introduced in the symmetry CIF dictionary (cif_sym.dic) 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 (2004). Valid only for one-dimensional modulated structures.

Reference: *International Tables for Crystallography* (2004). Vol. C, Chapter 9.8. Dordrecht: Kluwer Academic Publishers.
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 a separator between the different parts of the superspace-group symbol. Within each part, leave a space between each component. Rules for the notation for Hermann–Mauguin and Hall symbols (if present) are given in the symmetry CIF dictionary (cif_sym.dic) 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: 'Hall's notation W:-P -2xb -2ya:q q'. **[space_group]**

_space_group_ssg_name_IT (*char*)
Superspace-group symbol as given in *International Tables for Crystallography*, Vol. C (2004). Valid only for one-dimensional modulated structures. The symbol is divided into 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 and bars should be given as negative signs. The components of the modulation wave vector (in parentheses) 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.

Reference: *International Tables for Crystallography* (2004). Vol. C, Chapter 9.8. Dordrecht: Kluwer Academic Publishers.

Example: '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 into three parts separated by colons ':': 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 and bars should be given 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.

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

Example: '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.

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

Example: '28a.10.1/2'. **[space_group]**

SPACE_GROUP_SYMOP

The SPACE_GROUP_SYMOP category introduced in the symmetry CIF dictionary (cif_sym.dic) 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_id (*numb*)

A numeric code identifying each entry in the **_space_group_symop_ssg_operation_algebraic** list.

Appears in list. **[space_group_symop]**

_space_group_symop_ssg_operation_algebraic (*char*)

A parsable string giving one of the symmetry operations of the superspace group in algebraic form. These 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. The symbolic notation for coordinates is such that the identity operation is expressed as $x_1, x_2, x_3, \ldots, x_n$. **_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: 'x1,-x2,x3,1/2+x4'. **[space_group_symop]**