Example 3.4.4.2. *Representation of two mutually incommensurate subsystems.*

```
_exptl_crystal_type_of_structure        'comp'
_cell_subsystems_number                  2
_cell_modulation_dimension               1

_cell_reciprocal_basis_description
; a1*,b1*,c1* (reciprocal basis spanning the
  reciprocal basis of the first subsystem),
  a2* reciprocal axis corresponding to the
  second subsystem.
;

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

_diffrn_symmetry_description
; The whole diffraction pattern shows orthorhombic
  symmetry. The following extinction rules were
  detected:
     hklm   h+k+m=odd
     hklm   h+l=odd
     hklm   k+l+m=odd
     hk0m   h+k=odd
     hk0m   m=odd
  Extinction rules are compatible with the superspace
  groups:
     P:Fmmm:-11s(\a,0,0)
     P:Fm2m:-1-1s(\a,0,0)
;
```

Example 3.4.4.3. *Symmetry description of a superspace group.*

```
_space_group_ssg_name_WJJ   'P:P n a m:-1 s s'
_space_group_ssg_name_IT    'P n m a (\a 0 0) 0 s s'

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
```

In the particular case of K_2SeO_4, the superspace group is $P^{Pnma}_{\bar{1}\,s\,s}$ (de Wolff *et al.*, 1981) or $Pnma(\alpha 00)0ss$ (Janssen *et al.*, 2004). This information would appear in a CIF as shown in Example 3.4.4.3.

Example 3.4.4.4. *Atomic displacements as translations and rigid rotations.*

```
loop_
  _atom_site_description
  _atom_site_label
  _atom_site_occupancy
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
; SeO4 is a tetrahedral group formed by the atoms
  Se, O1, O2, O3 and O1p. O1p is related to O1 by the
  mirror plane perpendicular to the c axis. The
  coordinates given by _atom_site_fract_ correspond
  to the centre of mass.
;
     SeO4 1.0  0.22346    0.41868    0.250000
  .  Se   1.0  0.22216(4) 0.41861(3) 0.250000
  .  K1   1.0  0.1670(1)  0.08069(7) 0.250000
  .  K2   1.0 -0.0013(1)  0.70766(4) 0.250000
  .  O1   1.0  0.2890(3)  0.3413(2)  0.0277(3)
  .  O2   1.0  0.3130(4)  0.5621(2)  0.250000
  .  O3   1.0  0.0092(4)  0.4304(3)  0.250000

_refine_ls_mod_func_description
; Displacive modulation. Fourier series. Modulation
  of SeO4 group described in terms of rigid
  translations and rotations.
;

loop_
  _atom_site_Fourier_wave_vector_seq_id
  _atom_site_Fourier_wave_vector_x
  _atom_site_Fourier_wave_vector_description
     1   0.318(5)   'First 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
     K1_z_1   K1     z   1
     K2_z_1   K2     z   1
     SeO_z_1  SeO4   z   1

loop_
  _atom_site_displace_Fourier_param_id
  _atom_site_displace_Fourier_param_cos
  _atom_site_displace_Fourier_param_sin
     K1_z_1    0.0080(4)  -0.0106(5)
     K2_z_1    0.0159(4)   0.0071(6)
     SeO_z_1  -0.0089(2)  -0.0058(2)

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
     SeO_x_1   SeO4   x   1
     SeO_y_1   SeO4   y   1

loop_
  _atom_site_rot_Fourier_param_id
  _atom_site_rot_Fourier_param_cos
  _atom_site_rot_Fourier_param_sin
     SeO_x_1  -4.2(1)   0.91(3)
     SeO_y_1   4.3(1)   0.
```

3.4.4.3. Description of the structure

A modulated structure is described by a reference periodic structure and the atomic modulation functions. Such functions are periodic and are normally expanded as Fourier series. The modulated parameters may apply to the atom positions (displacive modulation), the site occupancies (occupational modulation) and/or the temperature factors. In composite structures, each substructure is referred to the crystallographic basis defined by the W matrices [see equation (3.4.4.2)]. The simplest case corresponds to a one-dimensional displacive modulated structure. In this case, the atomic modulation functions are given by

$$u^{\mu}_{\alpha} = \sum_{n=1}^{\infty} U^{\mu}_{n\alpha} \cos\left(2\pi n\mathbf{q}\cdot\mathbf{r} + \varphi^{\mu}_{n\alpha}\right), \qquad (3.4.4.3)$$

where $(U^{\mu}_{n\alpha}, \varphi^{\mu}_{n\alpha})$ is the complex amplitude of each Fourier term; μ labels the atoms; $\alpha = x, y, z$; $\mathbf{r}$ is the average atom position; and $n\mathbf{q}$ represents the successive harmonics of the modulation. At present, displacive modulations along axes other than a, b and c can be calculated with the restriction stated in Section 3.4.2.

Example 3.4.4.5. *Relationship between data blocks in an msCIF.*

```
_audit_block_code      1997-07-24|LaSNbS2|G.M.|

loop_
  _audit_link_block_code
  _audit_link_block_description
    .    'common experimental and publication data'
    1997-07-24|LaSNbS2|G.M.|_REFRNCE
         'reference structure (global data)'
    1997-07-21|LaSNbS2|G.M.|_MOD
         'modulated structure (global 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)'
    1997-07-21|LaSNbS2|G.M.|_MOD_LaS
         'modulated structure (2nd subsystem)'
```

Atomic displacements can also be expressed as rigid rotations and translations. The incommensurate phase of K_2SeO_4 is one-dimensional displacive and sinusoidal (at least over a wide range of temperature), *i.e.* $n = 1$ in equation (3.4.4.3). The tetrahedral SeO_4 groups behave as rigid bodies. Symmetry considerations restrict the possible translations to occur along **c** where the only allowed rigid rotations are around the *a* and *b* axes. The incommensurate structure is then expressed as shown in Example 3.4.4.4.

Alternatively, equation (3.4.4.3) can be expressed as a Fourier series with real amplitudes. This form is also covered by the msCIF dictionary. Note that there is a global phase, which is irrelevant in the incommensurate case but fixes the space group if the modulated structure is commensurate. Global phases are also defined in the dictionary.

3.4.4.4. Block pointers

CIFs for modulated and (in particular) composite structures often need several linked data blocks. For example, the average structure of a modulated phase refined using only the main reflections could be reported in one data block and then the results of the refinement of the complete structure using all the reflections could be added as a separate data block at a later stage. Similarly, each substructure in a composite structure can be fully described in a separate data block. It is therefore essential to keep all these blocks together, since all of them together describe the composite structure. Block pointers are described in the core CIF dictionary, but they need to be used with particular care in msCIFs. Therefore, the msCIF dictionary gives additional guidelines for naming the data blocks, as the aim (as in pdCIF) is to define unique names. Example 3.4.4.5 shows how the structure of $(LaS)_{1.14}NbS_2$ can be represented using several data blocks. In this example, the block named `1997-07-24|LaSNbS2|G.M.|` is linked to those in the loop below.

3.4.4.5. Other information

The msCIF and core CIF dictionaries also include items for *R* factors for different reflection classes (for example, for the main reflections and for the satellite reflections; see Section 3.2.3) and for describing the variation of interatomic distances due to the modulation. msCIF can be used to create a complete record of the determination of a modulated or composite structure suitable for submitting as an article to an academic journal or for archiving in a database. The obvious next step in the development of msCIF is to adapt or write software that can filter and manage msCIF data and that can generate msCIFs automatically.

Appendix 3.4.1
Category structure of the msCIF dictionary

Table A3.4.1.1 shows all categories that are represented in the msCIF dictionary.

Table A3.4.1.1. *Categories in the modulated structures CIF dictionary*

Numbers in parentheses refer to the section of this chapter in which each category is described in detail.

ATOM group (§3.4.4.3.3)	AUDIT group (§3.4.4.3.4)
ATOM_SITE (§3.4.4.3.3.1(*a*)) ¶	AUDIT (§3.4.4.3.4(*a*)) ‡
ATOM_SITE_DISPLACE_FOURIER (§3.4.4.3.3.2(*a*))	AUDIT_LINK (§3.4.4.3.4(*b*)) ‡
ATOM_SITE_DISPLACE_FOURIER_PARAM (§3.4.4.3.3.2(*b*))	CELL group (§3.4.4.3.1.1)
ATOM_SITE_DISPLACE_SPECIAL_FUNC (§3.4.4.3.3.3(*a*))	CELL (§3.4.4.3.1.1(*a*)) ¶
ATOM_SITE_FOURIER_WAVE_VECTOR (§3.4.4.3.3.2(*c*))	CELL_SUBSYSTEM (§3.4.4.3.1.1(*b*))
ATOM_SITE_OCC_FOURIER (§3.4.4.3.3.2(*d*))	CELL_SUBSYSTEMS (§3.4.4.3.1.1(*c*))
ATOM_SITE_OCC_FOURIER_PARAM (§3.4.4.3.3.2(*e*))	CELL_WAVE_VECTOR (§3.4.4.3.1.1(*d*))
ATOM_SITE_OCC_SPECIAL_FUNC (§3.4.4.3.3.3(*b*))	CELL_WAVE_VECTORS (§3.4.4.3.1.1(*e*))
ATOM_SITE_PHASON (§3.4.4.3.3.1(*b*))	DIFFRN group (§3.4.4.3.1.2)
ATOM_SITE_ROT_FOURIER (§3.4.4.3.3.2(*f*))	DIFFRN_REFLN (§3.4.4.3.1.2(*a*)) ¶
ATOM_SITE_ROT_FOURIER_PARAM (§3.4.4.3.3.2(*g*))	DIFFRN_REFLNS (§3.4.4.3.1.2(*b*)) ¶
ATOM_SITE_U_FOURIER (§3.4.4.3.3.2(*h*))	DIFFRN_STANDARD_REFLN (§3.4.4.3.1.2(*c*)) ¶
ATOM_SITE_U_FOURIER_PARAM (§3.4.4.3.3.2(*i*))	EXPTL group (§3.4.4.3.1.3)
ATOM_SITES_DISPLACE_FOURIER (§3.4.4.3.3.2(*j*))	EXPTL_CRYSTAL (§3.4.4.3.1.3(*a*)) ¶
ATOM_SITES_MODULATION (§3.4.4.3.3.2(*k*))	EXPTL_CRYSTAL_FACE (§3.4.4.3.1.3(*b*)) ¶
ATOM_SITES_ROT_FOURIER (§3.4.4.3.3.2(*l*))	GEOM group (§3.4.4.3.3.4)
	GEOM_ANGLE (§3.4.4.3.3.4(*a*)) ¶
	GEOM_BOND (§3.4.4.3.3.4(*b*)) ¶
	GEOM_CONTACT (§3.4.4.3.3.4(*c*)) ¶
	GEOM_TORSION (§3.4.4.3.3.4(*d*)) ¶
	REFINE group (§3.4.4.3.2.1)
	REFINE (§3.4.4.3.2.1) ¶
	REFLN group (§3.4.4.3.2.2)
	REFLN (§3.4.4.3.2.2(*a*)) ¶
	REFLNS (§3.4.4.3.2.2(*b*)) ¶
	SYMMETRY group (§3.4.4.3.3.5)
	SPACE_GROUP (§3.4.4.3.3.5(*a*)) ¶
	SPACE_GROUP_SYMOP (§3.4.4.3.3.5(*b*)) ¶

¶ Categories already defined in the core CIF dictionary but containing new items.
‡ A stricter definition than that given in the core CIF dictionary.

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