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 (§3.4.3.3)	AUDIT group (§3.4.3.4)
ATOM_SITE (§3.4.3.3.1(*a*)) ¶	AUDIT (§3.4.3.4(*a*)) ‡
ATOM_SITE_DISPLACE_FOURIER (§3.4.3.3.2(*a*))	AUDIT_LINK (§3.4.3.4(*b*)) ‡
ATOM_SITE_DISPLACE_FOURIER_PARAM (§3.4.3.3.2(*b*))	CELL group (§3.4.3.1.1)
ATOM_SITE_DISPLACE_SPECIAL_FUNC (§3.4.3.3.3(*a*))	CELL (§3.4.3.1.1(*a*)) ¶
ATOM_SITE_FOURIER_WAVE_VECTOR (§3.4.3.3.2(*c*))	CELL_SUBSYSTEM (§3.4.3.1.1(*b*))
ATOM_SITE_OCC_FOURIER (§3.4.3.3.2(*d*))	CELL_SUBSYSTEMS (§3.4.3.1.1(*c*))
ATOM_SITE_OCC_FOURIER_PARAM (§3.4.3.3.2(*e*))	CELL_WAVE_VECTOR (§3.4.3.1.1(*d*))
ATOM_SITE_OCC_SPECIAL_FUNC (§3.4.3.3.3(*b*))	CELL_WAVE_VECTORS (§3.4.3.1.1(*e*))
ATOM_SITE_PHASON (§3.4.3.3.1(*b*))	DIFFRN group (§3.4.3.1.2)
ATOM_SITE_ROT_FOURIER (§3.4.3.3.2(*f*))	DIFFRN_REFLN (§3.4.3.1.2(*a*)) ¶
ATOM_SITE_ROT_FOURIER_PARAM (§3.4.3.3.2(*g*))	DIFFRN_REFLNS (§3.4.3.1.2(*b*)) ¶
ATOM_SITE_U_FOURIER (§3.4.3.3.2(*h*))	DIFFRN_STANDARD_REFLN (§3.4.3.1.2(*c*)) ¶
ATOM_SITE_U_FOURIER_PARAM (§3.4.3.3.2(*i*))	EXPTL group (§3.4.3.1.3)
ATOM_SITES_DISPLACE_FOURIER (§3.4.3.3.2(*j*))	EXPTL_CRYSTAL (§3.4.3.1.3(*a*)) ¶
ATOM_SITES_MODULATION (§3.4.3.3.2(*k*))	EXPTL_CRYSTAL_FACE (§3.4.3.1.3(*b*)) ¶
ATOM_SITES_ROT_FOURIER (§3.4.3.3.2(*l*))	GEOM group (§3.4.3.3.4)
	GEOM_ANGLE (§3.4.3.3.4(*a*)) ¶
	GEOM_BOND (§3.4.3.3.4(*b*)) ¶
	GEOM_CONTACT (§3.4.3.3.4(*c*)) ¶
	GEOM_TORSION (§3.4.3.3.4(*d*)) ¶
	REFINE group (§3.4.3.2.1)
	REFINE (§3.4.3.2.1) ¶
	REFLN group (§3.4.3.2.2)
	REFLN (§3.4.3.2.2(*a*)) ¶
	REFLNS (§3.4.3.2.2(*b*)) ¶
	SYMMETRY group (§3.4.3.3.5)
	SPACE_GROUP (§3.4.3.3.5(*a*)) ¶
	SPACE_GROUP_SYMOP (§3.4.3.3.5(*b*)) ¶

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

The msCIF dictionary exists thanks to the continuous help and support received from I. David Brown and Brian McMahon. The suggestions and criticisms of Sander van Smaalen, Howard Flack, Juan Manuel Pérez-Mato and, especially, Vaclav Petříček (who has implemented a CIF input/output routine in the program *JANA2000*) were important.

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