_wave_vector_seq_id** is a pointer to the description of the separate modulation wave vectors and must match one of the identifiers **_atom_site_Fourier_wave_vector_seq_id** listed separately in the ATOM_SITE_FOURIER_WAVE_VECTOR category. Likewise, the ***_atom_site_label** data item must match a value of **_atom_site_label** in the main list of atom positions. This is how the modulation is linked to the atom list. The item **_atom_site_displace_Fourier_id** is the formal key for the ATOM_SITE_DISPLACE_FOURIER category. It is used to locate the matching Fourier coefficients in the ATOM_SITE_DISPLACE_FOURIER_PARAM category. The coefficients may be reported in a sine–cosine (**_atom_site_displace_Fourier_param_sin**, ***_cos**) or modulus–argument (_mod**, ***_phase**) representation.

Where a group of atoms is treated as a rigid group, the categories above describe only the translational part of the positional distortion. ATOM_SITE_ROT_FOURIER and ATOM_SITE_ROT_FOURIER_PARAM are used to describe the rotational components.

ATOM_SITE_OCC_FOURIER and ATOM_SITE_U_FOURIER, and their associated *_PARAM categories, are the analogous categories for the modulation of site occupation and thermal parameters.

All the categories above describe the properties of individual atom sites. Larger-scale descriptions of the displacive modulation or of the rotational component of a rigid group are covered by the categories ATOM_SITES_DISPLACE_FOURIER and ATOM_SITES_ROT_FOURIER, each of which at present contains one descriptive data item.

The ATOM_SITES_MODULATION category contains data items describing the initial phases of the modulation waves, which are essential for determining the space group of the commensurate superstructure. More details are given in the dictionary.

3.4.3.3.3. *Special modulation functions*

Data items in these categories are as follows:

(*a*) ATOM_SITE_DISPLACE_SPECIAL_FUNC

```
• _atom_site_displace_special_func_atom_site_label
        → _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
```

(*b*) ATOM_SITE_OCC_SPECIAL_FUNC

```
• _atom_site_occ_special_func_atom_site_label
        → _atom_site_label
  _atom_site_occ_special_func_crenel_c
  _atom_site_occ_special_func_crenel_w
```

The bullet (•) *indicates a category key. The arrow* (→) *is a reference to a parent data item.*

Several data items cover modulation functions that are not expressed as Fourier expansions. The examples in the current msCIF dictionary are restricted to the one-dimensional modulations (sawtooth displacive and occupational crenel functions) implemented in the program *JANA2000* (see Section 3.4.2).

3.4.3.3.4. *Molecular or packing geometry*

New data items in these categories are as follows:

(*a*) GEOM_ANGLE

```
_geom_angle_av
_geom_angle_max
_geom_angle_min
_geom_angle_site_ssg_symmetry_1
_geom_angle_site_ssg_symmetry_2
_geom_angle_site_ssg_symmetry_3
```

(*b*) GEOM_BOND

```
_geom_bond_distance_av
_geom_bond_distance_max
_geom_bond_distance_min
_geom_bond_site_ssg_symmetry_1
_geom_bond_site_ssg_symmetry_2
```

(*c*) GEOM_CONTACT

```
_geom_contact_distance_av
_geom_contact_distance_max
_geom_contact_distance_min
_geom_contact_site_ssg_symmetry_1
_geom_contact_site_ssg_symmetry_2
```

(*d*) GEOM_TORSION

```
_geom_torsion_av
_geom_torsion_max
_geom_torsion_min
_geom_torsion_site_ssg_symmetry_1
_geom_torsion_site_ssg_symmetry_2
_geom_torsion_site_ssg_symmetry_3
_geom_torsion_site_ssg_symmetry_4
```

For each of the geometry categories, there are two groups of extensions. One set covers maximum, minimum and average values of bonds, contact distances, angles and torsion angles. The other extends the symmetry-operation code used in geometry listings in the core CIF dictionary (see Section 3.2.4.3.2) to the higher-dimensional superspace form.

3.4.3.3.5. *Symmetry information*

New data items in these categories are as follows:

(*a*) SPACE_GROUP

```
_space_group_ssg_IT_number
_space_group_ssg_name
_space_group_ssg_name_IT
_space_group_ssg_name_WJJ
_space_group_ssg_WJJ_code
```

(*b*) SPACE_GROUP_SYMOP

```
_space_group_symop_ssg_id
_space_group_symop_ssg_operation_algebraic
```

At present, the msCIF dictionary extends the core CIF dictionary symmetry categories to describe superspace groups for one-dimensional modulated structures in four ways: as the superspace-group number in Janssen *et al.* (2004) (**_space_group_ssg_IT_number**), as the *International Tables* superspace-group symbol (***_ssg_name_IT**), as one of the notations from de Wolff *et al.* (1981) (***_ssg_name_WJJ**, ***_ssg_WJJ_code**), or in some other formalism (***_ssg_name**). At present, superspace-group names for higher dimensions can only be indicated using **_space_group_ssg_name**.

Symmetry operations in the superspace group are specified in the SPACE_GROUP_SYMOP category by an obvious extension to the method used in the core dictionary. These items must always be present in a CIF corresponding to a modulated or composite structure.

3.4.3.4. File metadata

The categories modified in the msCIF dictionary to formalize the construction of a multi-block description of modulated or composite structures are as follows:

AUDIT group

AUDIT ¶

AUDIT_LINK ¶

Categories marked with ¶ *are already defined in the core CIF dictionary.*