EXPTL group
EXPTL_CRYSTAL ¶
EXPTL_CRYSTAL_FACE ¶

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

New data items in these categories are as follows:

(*a*) EXPTL_CRYSTAL

_exptl_crystal_type_of_structure

(*b*) EXPTL_CRYSTAL_FACE

_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

_exptl_crystal_type_of_structure specifies the structure type as `cryst` (crystalline), `mod` (modulated) or `comp` (composite). These are the only three types of structure handled at present by the msCIF dictionary.

The extensions to the EXPTL_CRYSTAL_FACE category permit the indexing of crystal faces using the higher-dimensional Miller indices introduced for aperiodic structures.

3.4.3.2. Analysis

The categories related to refinement that have been extended in this dictionary are as follows:

Refinement techniques and results (§3.4.3.2.1)
REFINE ¶
The reflections used in the refinement (§3.4.3.2.2)
REFLN ¶
REFLNS ¶

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

3.4.3.2.1. *Refinement techniques and results*

New data items in this category are as follows:

REFINE

_refine_ls_mod_func_description
_refine_ls_mod_hydrogen_treatment
_refine_ls_mod_overall_phason_coeff
_refine_ls_mod_overall_phason_formula

During the early stages of the development of the msCIF dictionary, several sets of data items were defined to accommodate the need to specify residual *R* factors for the different sets of main reflections and satellite reflections. It was then recognized that the binning of reflection classes had more general application, and these new data items were transferred to the core CIF dictionary, where, of course, they are still available for use in an msCIF.

The new items in the REFINE category in the msCIF dictionary are specific to the refinement of modulated structures. **_refine_ls_mod_func_description** allows a free-text description of the types of modulation present in the structural model and how they are handled. The treatment of hydrogen-atom modulation parameters is specified by **_refine_ls_mod_hydrogen_treatment**. Information on an overall phason correction (the use of which should in general be discouraged) may be given using the **_refine_ls_mod_overall_phason_*** items.

3.4.3.2.2. *The reflections used in the refinement*

New data items in these categories are as follows:

(*a*) REFLN

_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

(*b*) REFLNS

_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

As with the **_diffrn_refln_*** and **_diffrn_reflns_*** items (Section 3.4.3.1.2), these data names extend the corresponding core data items into the higher-dimensional space used in the treatment of modulated structures and composites. They apply to the list of reflections used in the refinement, as distinct from the experimentally collected set of intensities described by the **_diffrn_*** data items.

3.4.3.3. Atomicity, chemistry and structure

The categories relevant to the description of the structural model are as follows:

ATOM group
Atom sites (§3.4.3.3.1)
ATOM_SITE ¶
ATOM_SITE_PHASON
Modulation functions as Fourier series (§3.4.3.3.2)
ATOM_SITE_DISPLACE_FOURIER
ATOM_SITE_DISPLACE_FOURIER_PARAM
ATOM_SITE_FOURIER_WAVE_VECTOR
ATOM_SITE_OCC_FOURIER
ATOM_SITE_OCC_FOURIER_PARAM
ATOM_SITE_ROT_FOURIER
ATOM_SITE_ROT_FOURIER_PARAM
ATOM_SITE_U_FOURIER
ATOM_SITE_U_FOURIER_PARAM
ATOM_SITES_DISPLACE_FOURIER
ATOM_SITES_MODULATION
ATOM_SITES_ROT_FOURIER
Special modulation functions (§3.4.3.3.3)
ATOM_SITE_DISPLACE_SPECIAL_FUNC
ATOM_SITE_OCC_SPECIAL_FUNC
Molecular or packing geometry (§3.4.3.3.4)
GEOM group
GEOM_ANGLE ¶
GEOM_BOND ¶
GEOM_CONTACT ¶
GEOM_TORSION ¶
Symmetry information (§3.4.3.3.5)
SYMMETRY group
SPACE_GROUP ¶
SPACE_GROUP_SYMOP ¶

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

Most of the new categories introduced to the msCIF dictionary appear here, since their function is to describe in great detail the

modulation of the atom-site properties. They fall naturally into families describing the modulation of atomic displacement, of site occupation or of thermal parameters.

New data items are added to several categories in the core CIF dictionary that describe molecular or packing geometry. There are also new data items to describe superspace-group symmetry.

3.4.3.3.1. *Atom sites*

Data items in these categories are as follows:

(*a*) ATOM_SITE

```
  _atom_site_displace_modulation_flag
  _atom_site_occ_modulation_flag
  _atom_site_subsystem_code
        → _cell_subsystem_code
  _atom_site_U_modulation_flag
```

(*b*) ATOM_SITE_PHASON

```
• _atom_site_phason_atom_site_label
        → _atom_site_label
  _atom_site_phason_coeff
  _atom_site_phason_formula
```

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

The ATOM_SITE category is extended in the msCIF dictionary by the addition of a small number of items that may appear in the main looped list of atom-site information (see Section 3.2.4.1.1). The `*_flag` items indicate whether each individual atom site has been modelled through modulation of atomic displacement, site occupation or thermal parameters. In each case, the default value of the item is `no`, so that any or all of the flags may be omitted when that particular type of modulation has not been applied to the structural model.

`_atom_site_subsystem_code` identifies the cell subsystem to which the atom site must be assigned in the description of composite structures. Each value of `_atom_site_subsystem_code` must match one of the values of `_cell_subsystem_code` in the overall description of the subsystems defined for a composite.

The ATOM_SITE_PHASON category allow details of an atom-dependent phason correction, as implemented in *JANA2000*, to be given. The use of these phason corrections is discouraged.

3.4.3.3.2. *Modulation functions as Fourier series*

Data items in these categories are as follows:

(*a*) ATOM_SITE_DISPLACE_FOURIER

```
• _atom_site_displace_Fourier_id
  _atom_site_displace_Fourier_atom_site_label
        → _atom_site_label
  _atom_site_displace_Fourier_axis
  _atom_site_displace_Fourier_wave_vector_seq_id
        → _atom_site_Fourier_wave_vector_seq_id
```

(*b*) ATOM_SITE_DISPLACE_FOURIER_PARAM

```
• _atom_site_displace_Fourier_param_id
        → _atom_site_displace_Fourier_id
  _atom_site_displace_Fourier_param_cos
  _atom_site_displace_Fourier_param_modulus
  _atom_site_displace_Fourier_param_phase
  _atom_site_displace_Fourier_param_sin
```

(*c*) ATOM_SITE_FOURIER_WAVE_VECTOR

```
  _atom_site_Fourier_wave_vector_description
  _atom_site_Fourier_wave_vector_seq_id
  _atom_site_Fourier_wave_vector_x
  _atom_site_Fourier_wave_vector_y
  _atom_site_Fourier_wave_vector_z
```

(*d*) ATOM_SITE_OCC_FOURIER

```
• _atom_site_occ_Fourier_id
  _atom_site_occ_Fourier_atom_site_label
        → _atom_site_label
  _atom_site_occ_Fourier_wave_vector_seq_id
        → _atom_site_Fourier_wave_vector_seq_id
```

(*e*) ATOM_SITE_OCC_FOURIER_PARAM

```
• _atom_site_occ_Fourier_param_id
        → _atom_site_occ_Fourier_id
  _atom_site_occ_Fourier_param_cos
  _atom_site_occ_Fourier_param_modulus
  _atom_site_occ_Fourier_param_phase
  _atom_site_occ_Fourier_param_sin
```

(*f*) ATOM_SITE_ROT_FOURIER

```
• _atom_site_rot_Fourier_id
  _atom_site_rot_Fourier_atom_site_label
        → _atom_site_label
  _atom_site_rot_Fourier_axis
  _atom_site_rot_Fourier_wave_vector_seq_id
        → _atom_site_Fourier_wave_vector_seq_id
```

(*g*) ATOM_SITE_ROT_FOURIER_PARAM

```
• _atom_site_rot_Fourier_param_id
        → _atom_site_rot_Fourier_id
  _atom_site_rot_Fourier_param_cos
  _atom_site_rot_Fourier_param_modulus
  _atom_site_rot_Fourier_param_phase
  _atom_site_rot_Fourier_param_sin
```

(*h*) ATOM_SITE_U_FOURIER

```
• _atom_site_U_Fourier_id
  _atom_site_U_Fourier_atom_site_label
        → _atom_site_label
  _atom_site_U_Fourier_tens_elem
  _atom_site_U_Fourier_wave_vector_seq_id
        → _atom_site_Fourier_wave_vector_seq_id
```

(*i*) ATOM_SITE_U_FOURIER_PARAM

```
• _atom_site_U_Fourier_param_id
        → _atom_site_U_Fourier_id
  _atom_site_U_Fourier_param_cos
  _atom_site_U_Fourier_param_modulus
  _atom_site_U_Fourier_param_phase
  _atom_site_U_Fourier_param_sin
```

(*j*) ATOM_SITES_DISPLACE_FOURIER

```
  _atom_sites_displace_Fourier_axes_description
```

(*k*) ATOM_SITES_MODULATION

```
  _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
```

(*l*) ATOM_SITES_ROT_FOURIER

```
  _atom_sites_rot_Fourier_axes_description
```

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

It is common to represent a modulated structure using a reference periodic structure on which are superimposed atomic modulation functions expanded as Fourier series. (A full discussion of this is given in Section 3.4.4.3.) The msCIF dictionary provides separate categories for listing the modulated parameters that apply to atom positions, site occupancies and thermal parameters. The structuring of the data items within each of these categories follows a similar pattern.

For example, consider the modulation of the atomic displacements. The ATOM_SITE_DISPLACE_FOURIER category allows a listing of the axis along which the displacement occurs (`*_axis`) and the wave vectors contributing to that displacement component (`*_wave_vector_seq_id`) for each relevant atom site (labelled by `_atom_site_displace_Fourier_atom_site_label`).

_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.