3.4. CLASSIFICATION AND USE OF MODULATED AND COMPOSITE STRUCTURES DATA

3.4.3.1. Experimental measurements

The categories relevant to a structure determination experiment are in the CELL, DIFFRN and EXPTL groups. Most of the items extend the existing core CIF categories, but the categories describing cell subsystems are new.

3.4.3.1.1. *Cell and modulation wave vectors*

The categories describing the unit cell (or cells for composite structures), the wave vectors of the modulations and, for composites, the cell subsystems are as follows:

CELL group
    CELL ¶
    CELL_SUBSYSTEM
    CELL_SUBSYSTEMS
    CELL_WAVE_VECTOR
    CELL_WAVE_VECTORS

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

The data items in these categories are as follows:

(*a*) CELL
```
_cell_modulation_dimension
_cell_reciprocal_basis_description
```

(*b*) CELL_SUBSYSTEM
```
_cell_subsystem_code
_cell_subsystem_description
_cell_subsystem_matrix_W_1_1
          ⋮
```
(and `_cell_subsystem_matrix_W_`*m*`_`*n* for all combinations $1 \le m, n \le 11$)
```
          ⋮
_cell_subsystem_matrix_W_11_11
```

(*c*) CELL_SUBSYSTEMS
```
_cell_subsystems_number
```

(*d*) CELL_WAVE_VECTOR
```
_cell_wave_vector_seq_id
_cell_wave_vector_x
_cell_wave_vector_y
_cell_wave_vector_z
```

(*e*) CELL_WAVE_VECTORS
```
_cell_wave_vectors_meas_details
_cell_wave_vectors_pressure_max
_cell_wave_vectors_pressure_min
_cell_wave_vectors_temp_max
_cell_wave_vectors_temp_min
_cell_wave_vectors_variation
```

As explained in Section 3.4.2, the msCIF dictionary arbitrarily allows an upper limit of 11 for the dimension of superspace for which data names are defined. `_cell_modulation_dimension` specifies the number of additional reciprocal vectors needed to index the whole diffraction pattern and has values *d* ranging from 1 to 8 to express the dimensionality $(3 + d)$ of the superspace. `_cell_reciprocal_basis_description` is a text field allowing a free description of the higher-dimensional basis chosen.

For a composite structure, different cell subsystems may be specified. Each such subsystem is identified and characterized by the data items in the CELL_SUBSYSTEM category (see Section 3.4.4.1). `_cell_subsystems_number` gives the number of such subsystems as an independent check of the completeness of the description.

Data items in the CELL_WAVE_VECTOR category specify the wave vectors of the modulation (see Section 3.4.4.1). In accordance with the limits on dimensionality of the current version of the msCIF dictionary, no more than eight additional modulation wave vectors may be specified. The number used must agree with the value of `_cell_modulation_dimension`.

The data items in the CELL_WAVE_VECTORS category describe the experimental conditions during the determination of the independent modulation wave vectors.

3.4.3.1.2. *Data collection*

The categories describing data collection are as follows:

DIFFRN group
    DIFFRN_REFLN ¶
    DIFFRN_REFLNS ¶
    DIFFRN_STANDARD_REFLN ¶

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

New data items in these categories are as follows:

(*a*) DIFFRN_REFLN
```
_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
```

(*b*) DIFFRN_REFLNS
```
_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
_diffrn_reflns_satellite_order_max
```

(*c*) DIFFRN_STANDARD_REFLN
```
_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
```

The data items in these categories are straightforward extensions of the core CIF dictionary definitions to the indexing of diffraction intensities by higher-dimensional components. The `_diffrn_refln_index_m_`* items are the additional Miller indices m_i indexing the modulation wave vectors $\mathbf{q}_i$ when the diffraction wave vector is written as $\mathbf{H} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^* + \sum_i m_i \mathbf{q}_i$.

The upper limit of 8 was chosen arbitrarily to limit the number of data items defined in the msCIF dictionary.

`_diffrn_reflns_limit_index_m_`* items provide independent checks on the range of values recorded for each of the additional Miller indices m_i. `_diffrn_standard_refln_index_m_`* items allow the higher-dimensional Miller indices of standard reflections to be recorded.

3.4.3.1.3. *Experimental measurements on the crystal*

The categories describing measurements on the crystal or crystals used in the experiment are as follows:

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

references