

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
 $1 \leq m, n \leq 11$)
 ⋮
 _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_refl_index_m_1
 _diffrn_refl_index_m_2
 _diffrn_refl_index_m_3
 _diffrn_refl_index_m_4
 _diffrn_refl_index_m_5
 _diffrn_refl_index_m_6
 _diffrn_refl_index_m_7
 _diffrn_refl_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_refl_index_m_1
 _diffrn_standard_refl_index_m_2
 _diffrn_standard_refl_index_m_3
 _diffrn_standard_refl_index_m_4
 _diffrn_standard_refl_index_m_5
 _diffrn_standard_refl_index_m_6
 _diffrn_standard_refl_index_m_7
 _diffrn_standard_refl_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_refl_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_refl_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: