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