Table 3.6.4.1. *Major category groups defined in the mmCIF dictionary*

The groups are listed in the order in which they are described in this chapter. There is also an INCLUSIVE category group, which serves as a formal higher-order container group to which all other category groups belong.

Section	Category group	Subject covered
(*a*) Experimental measurements		
3.6.5.1	CELL	Unit cell
3.6.5.2	DIFFRN	Diffraction experiment
3.6.5.3	EXPTL	Experimental conditions
(*b*) Analysis		
3.6.6.1	PHASING	Phasing techniques
3.6.6.2	REFINE	Refinement procedures
3.6.6.3	REFLN	Reflection measurements
(*c*) Atomicity, chemistry and structure		
3.6.7.1	ATOM	Atom sites
3.6.7.2	CHEMICAL	Chemical properties and nomenclature
3.6.7.3	ENTITY	Chemical entities
3.6.7.4	GEOM	Geometry of atom sites
3.6.7.5	STRUCT	Crystallographic structure
3.6.7.6	SYMMETRY	Symmetry information
3.6.7.7	VALENCE	Bond-valence information
(*d*) Publication		
3.6.8.1	CITATION	Bibliographic references
3.6.8.2	COMPUTING	Computational details of the experiment
3.6.8.3	DATABASE	Database information
3.6.8.4	IUCR	Journal housekeeping and the contents of a published article
(*e*) File metadata		
3.6.9.1	AUDIT	Dictionary maintenance and identification
3.6.9.2	ENTRY	Links between data blocks
3.6.9.3	COMPLIANCE	Compliance with previous dictionaries

attribute `_type_conditions_esd` and allows the standard uncertainty of the value to be placed in parentheses after the numerical value, as in

```
_cell_length_a      58.39(5)
```

This is also permitted in mmCIF, but it is preferable to use a separate data item to record the standard uncertainty, as in

```
_cell.length_a        58.39
_cell.length_a_esd     0.05
```

There are many of these kinds of data names in the mmCIF dictionary. The name of each is derived by adding `_esd` to the data name for the value. They are indicated by a + symbol in the category summaries in this chapter.

3.6.5. Experimental measurements

The CELL, DIFFRN and EXPTL category groups are used to describe the crystallographic experiment. The data items used for this purpose in mmCIF are for the most part identical to those in the core CIF dictionary. A complete discussion of the data names in each category may be found in Section 3.2.2.

mmCIF also contains the new categories EXPTL_CRYSTAL_GROW and EXPTL_CRYSTAL_GROW_COMP (Section 3.6.5.3.2), which are used to provide a more structured description of crystallization than is available in the core CIF dictionary.

3.6.5.1. Crystal cell parameters and measurement conditions

The categories describing the crystal unit cell and its determination are as follows:

CELL group
- CELL
- CELL_MEASUREMENT
- CELL_MEASUREMENT_REFLN

The mmCIF dictionary differs from the core CIF dictionary in assigning separate categories to data names that define the crystal unit-cell parameters and to data names relating to the experimental determination of the unit cell. Details of the unit-cell parameters are given in the CELL category and data items in the distinct CELL_MEASUREMENT category are used to describe how the unit-cell parameters were measured. The category CELL_MEASUREMENT_REFLN, which is used to list the reflections used in the unit-cell determination, is common to the core and mmCIF dictionaries.

The data items in these categories are as follows:

(*a*) CELL

```
• _cell.entry_id
        → _entry.id
+ _cell.angle_alpha
+ _cell.angle_beta
+ _cell.angle_gamma
  _cell.details (~ _cell_special_details)
  _cell.formula_units_Z
+ _cell.length_a
+ _cell.length_b
+ _cell.length_c
+ _cell.reciprocal_angle_alpha
+ _cell.reciprocal_angle_beta
+ _cell.reciprocal_angle_gamma
+ _cell.reciprocal_length_a
+ _cell.reciprocal_length_b
+ _cell.reciprocal_length_c
+ _cell.volume
  _cell.Z_PDB
```

(*b*) CELL_MEASUREMENT

```
• _cell_measurement.entry_id
        → _entry.id
+ _cell_measurement.pressure
  _cell_measurement.radiation
  _cell_measurement.reflns_used
+ _cell_measurement.temp
        (~ _cell_measurement_temperature)
  _cell_measurement.theta_max
  _cell_measurement.theta_min
  _cell_measurement.wavelength
```

(*c*) CELL_MEASUREMENT_REFLN

```
• _cell_measurement_refln.index_h
• _cell_measurement_refln.index_k
• _cell_measurement_refln.index_l
  _cell_measurement_refln.theta
```

The bullet (•) indicates a category key. Where multiple items within a category are marked with a bullet, they must be taken together to form a compound key. Items in italics have aliases in the core CIF dictionary formed by changing the full stop (.) to an underscore (_) except where indicated by the ~ symbol. Data items marked with a plus (+) have companion data names for the standard uncertainty in the reported value, formed by appending the string `_esd` to the data name listed.

The summary above includes the formal category keys that have been introduced in mmCIF because the corresponding core categories do not expect looped data, and therefore do not require the specification of a unique identifier. In the relational model of DDL2, all categories are considered to be tables and therefore each category must have a unique identifier. Where core CIF categories have one or more data names that fulfil the role of table-row identifiers, these have generally been carried over as category keys in the mmCIF dictionary (for example, the data items that correspond to the *h*, *k*, and *l* Miller indices of a reflection in the CELL_MEASUREMENT_REFLN category).

Example 3.6.5.1. *Cell constants and their measurement for an HIV-1 protease crystal (PDB 5HVP) described with data items in the* CELL *and* CELL_MEASUREMENT *categories (Fitzgerald et al., 1990).*

```
_cell.entry_id                          '5HVP'
_cell.length_a                          58.39
_cell.length_a_esd                       0.05
_cell.length_b                          86.70
_cell.length_b_esd                       0.12
_cell.length_c                          46.27
_cell.length_c_esd                       0.06
_cell.angle_alpha                       90.00
_cell.angle_beta                        90.00
_cell.angle_gamma                       90.00
_cell.volume                           234237
_cell.details
; The cell parameters were refined every twenty
  frames during data integration. The cell lengths
  given are the mean of 55 such refinements; the
  esds given are the root-mean-square deviations
  of these 55 observations from that mean.
;
_cell_measurement.entry_id              '5HVP'
_cell_measurement.temp                    293
_cell_measurement.temp_esd                  3
_cell_measurement.theta_min                11
_cell_measurement.theta_max                31
_cell_measurement.wavelength             1.54
```

Example 3.6.5.1 shows how data items from these categories are used in practice and shows the use of separate data items to record standard uncertainties of measurable quantities.

3.6.5.2. Data collection

The categories describing data collection are as follows:

DIFFRN group
- DIFFRN
- DIFFRN_ATTENUATOR
- DIFFRN_DETECTOR
- DIFFRN_MEASUREMENT
- DIFFRN_ORIENT_MATRIX
- DIFFRN_ORIENT_REFLN
- DIFFRN_RADIATION
- DIFFRN_RADIATION_WAVELENGTH
- DIFFRN_REFLN
- DIFFRN_REFLNS
- DIFFRN_REFLNS_CLASS
- DIFFRN_SCALE
- DIFFRN_SOURCE
- DIFFRN_STANDARD_REFLN
- DIFFRN_STANDARDS

The categories in the DIFFRN category group describe the diffraction experiment. Data items in the DIFFRN category itself can be used to give overall information about the experiment, such as the temperature and pressure. Examples of the other categories are DIFFRN_DETECTOR, which is used for describing the detector used for data collection, and DIFFRN_SOURCE, which is used to give details of the source of the radiation used in the experiment. Data items in the DIFFRN_REFLN category can be used to give information about the raw data and data items in the DIFFRN_REFLNS category can be used to give information about all the reflection data collectively.

The data items in the categories in the DIFFRN group are as follows:

(*a*) DIFFRN
- **_diffrn.id**

  _diffrn.ambient_environment
+ **_diffrn.ambient_pressure**

  _diffrn.ambient_pressure_gt

  _diffrn.ambient_pressure_lt
+ **_diffrn.ambient_temp** (~ **_diffrn_ambient_temperature**)

  _diffrn.ambient_temp_details

  _diffrn.ambient_temp_gt

  _diffrn.ambient_temp_lt

  _diffrn.crystal_id (~ **_diffrn_refln_crystal_id**)

  _diffrn.crystal_support

  _diffrn.crystal_treatment

  _diffrn.details (~ **_diffrn_special_details**)

(*b*) DIFFRN_ATTENUATOR
- **_diffrn_attenuator.code**

  _diffrn_attenuator.material

  _diffrn_attenuator.scale

(*c*) DIFFRN_DETECTOR
- **_diffrn_detector.diffrn_id**
  → **_diffrn.id**

  _diffrn_detector.area_resol_mean

  _diffrn_detector.details

  _diffrn_detector.detector (~ **_diffrn_detector**)

  _diffrn_detector.dtime

  _diffrn_detector.type

(*d*) DIFFRN_MEASUREMENT
- **_diffrn_measurement.diffrn_id**
  → **_diffrn.id**

  _diffrn_measurement.details

  _diffrn_measurement.device

  _diffrn_measurement.device_details

  _diffrn_measurement.device_type

  _diffrn_measurement.method

  _diffrn_measurement.specimen_support

(*e*) DIFFRN_ORIENT_MATRIX
- **_diffrn_orient_matrix.diffrn_id**
  → **_diffrn.id**

  _diffrn_orient_matrix.type

  _diffrn_orient_matrix.UB[1][1]
  (~ **_diffrn_orient_matrix_UB_11**)

  _diffrn_orient_matrix.UB[1][2]
  (~ **_diffrn_orient_matrix_UB_12**)

  _diffrn_orient_matrix.UB[1][3]
  (~ **_diffrn_orient_matrix_UB_13**)

  _diffrn_orient_matrix.UB[2][1]
  (~ **_diffrn_orient_matrix_UB_21**)

  _diffrn_orient_matrix.UB[2][2]
  (~ **_diffrn_orient_matrix_UB_22**)

  _diffrn_orient_matrix.UB[2][3]
  (~ **_diffrn_orient_matrix_UB_23**)

  _diffrn_orient_matrix.UB[3][1]
  (~ **_diffrn_orient_matrix_UB_31**)

  _diffrn_orient_matrix.UB[3][2]
  (~ **_diffrn_orient_matrix_UB_32**)

  _diffrn_orient_matrix.UB[3][3]
  (~ **_diffrn_orient_matrix_UB_33**)

(*f*) DIFFRN_ORIENT_REFLN
- **_diffrn_orient_refln.diffrn_id**
  → **_diffrn.id**
- **_diffrn_orient_refln.index_h**
- **_diffrn_orient_refln.index_k**
- **_diffrn_orient_refln.index_l**

  _diffrn_orient_refln.angle_chi

  _diffrn_orient_refln.angle_kappa

  _diffrn_orient_refln.angle_omega

  _diffrn_orient_refln.angle_phi

  _diffrn_orient_refln.angle_psi

  _diffrn_orient_refln.angle_theta

(*g*) DIFFRN_RADIATION
- **_diffrn_radiation.diffrn_id**
  → **_diffrn.id**

  _diffrn_radiation.collimation

  _diffrn_radiation.filter_edge

  _diffrn_radiation.inhomogeneity

  _diffrn_radiation.monochromator

  _diffrn_radiation.polarisn_norm

  _diffrn_radiation.polarisn_ratio

  _diffrn_radiation.probe

  _diffrn_radiation.type