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

_diffrn_radiation.wavelength_id
→ _diffrn_radiation_wavelength.id
_diffrn_radiation.xray_symbol

(*h*) DIFFRN_RADIATION_WAVELENGTH
• _diffrn_radiation_wavelength.id
• _diffrn_radiation_wavelength.wavelength
(∼ _diffrn_radiation_wavelength.wavelength)
• _diffrn_radiation_wavelength.wt

(*i*) DIFFRN_REFLN
• _diffrn_refln.diffrn_id
→ _diffrn.id
• _diffrn_refln.id
_diffrn_refln.angle_chi
_diffrn_refln.angle_kappa
_diffrn_refln.angle_omega
_diffrn_refln.angle_phi
_diffrn_refln.angle_psi
_diffrn_refln.angle_theta
_diffrn_refln.attenuator_code
→ _diffrn_attenuator.code
_diffrn_refln.class_code
_diffrn_refln.counts_bg_1
_diffrn_refln.counts_bg_2
_diffrn_refln.counts_net
_diffrn_refln.counts_peak
_diffrn_refln.counts_total
_diffrn_refln.detect_slit_horiz
_diffrn_refln.detect_slit_vert
_diffrn_refln.elapsed_time
_diffrn_refln.index_h
_diffrn_refln.index_k
_diffrn_refln.index_l
_diffrn_refln.intensity_net
_diffrn_refln.intensity_sigma
_diffrn_refln.intensity_u
_diffrn_refln.scale_group_code
→ _diffrn_scale_group.code
_diffrn_refln.scan_mode
_diffrn_refln.scan_mode_backgd
_diffrn_refln.scan_rate
_diffrn_refln.scan_time_backgd
_diffrn_refln.scan_width
_diffrn_refln.sint_over_lambda
(∼ _diffrn_refln.sint/lambda)
_diffrn_refln.standard_code
→ _diffrn_standard_refln.code
_diffrn_refln.wavelength
_diffrn_refln.wavelength_id
→ _diffrn_radiation.wavelength_id

(*j*) DIFFRN_REFLNS
• _diffrn_reflns.diffrn_id
→ _diffrn.id
_diffrn_reflns.av_R_equivalents
_diffrn_reflns.av_sigmaI_over_netI
_diffrn_reflns.av_unetI/netI
_diffrn_reflns.limit_h_max
_diffrn_reflns.limit_h_min
_diffrn_reflns.limit_k_max
_diffrn_reflns.limit_k_min
_diffrn_reflns.limit_l_max
_diffrn_reflns.limit_l_min
_diffrn_reflns.number
_diffrn_reflns.reduction_process
_diffrn_reflns.theta_max
_diffrn_reflns.theta_min
_diffrn_reflns.transf_matrix[1][1]
(∼ _diffrn_reflns_transf_matrix_11)
_diffrn_reflns.transf_matrix[1][2]
(∼ _diffrn_reflns_transf_matrix_12)
_diffrn_reflns.transf_matrix[1][3]
(∼ _diffrn_reflns_transf_matrix_13)
_diffrn_reflns.transf_matrix[2][1]
(∼ _diffrn_reflns_transf_matrix_21)
_diffrn_reflns.transf_matrix[2][2]
(∼ _diffrn_reflns_transf_matrix_22)
_diffrn_reflns.transf_matrix[2][3]
(∼ _diffrn_reflns_transf_matrix_23)
_diffrn_reflns.transf_matrix[3][1]
(∼ _diffrn_reflns_transf_matrix_31)
_diffrn_reflns.transf_matrix[3][2]
(∼ _diffrn_reflns_transf_matrix_32)
_diffrn_reflns.transf_matrix[3][3]
(∼ _diffrn_reflns_transf_matrix_33)

(*k*) DIFFRN_REFLNS_CLASS
• _diffrn_reflns_class.code
_diffrn_reflns_class.av_R_eq
_diffrn_reflns_class.av_sgI/I
_diffrn_reflns_class.av_uI/I
_diffrn_reflns_class.d_res_high
_diffrn_reflns_class.d_res_low
_diffrn_reflns_class.description
_diffrn_reflns_class.number

(*l*) DIFFRN_SCALE_GROUP
• _diffrn_scale_group.code
_diffrn_scale_group.I_net

(*m*) DIFFRN_SOURCE
• _diffrn_source.diffrn_id
→ _diffrn.id
_diffrn_source.current
_diffrn_source.details
_diffrn_source.power
_diffrn_source.size
_diffrn_source.source (∼ _diffrn_source)
_diffrn_source.take-off_angle
_diffrn_source.target
_diffrn_source.type
_diffrn_source.voltage

(*n*) DIFFRN_STANDARD_REFLN
• _diffrn_standard_refln.code
• _diffrn_standard_refln.diffrn_id
→ _diffrn.id
_diffrn_standard_refln.index_h
_diffrn_standard_refln.index_k
_diffrn_standard_refln.index_l

(*o*) DIFFRN_STANDARDS
• _diffrn_standards.diffrn_id
→ _diffrn.id
_diffrn_standards.decay_%
_diffrn_standards.interval_count
_diffrn_standards.interval_time
_diffrn_standards.number
_diffrn_standards.scale_sigma
_diffrn_standards.scale_u

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. The arrow* (→) *is a reference to a parent data item. 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.*

To a very great extent, data items in the DIFFRN category group are used in the same way in the mmCIF and core CIF dictionaries, and Section 3.2.2.2 can be consulted for details. Example 3.6.5.2 shows how these categories are used to describe the data collection for a macromolecule.

There is, however, one important difference. An mmCIF may describe several separate diffraction experiments that were conducted with a common purpose; each such experiment would be given a unique value of _diffrn.id, the key for the DIFFRN category. Descriptions of features of that experiment in related categories would be given a matching identifier with the same value (*e.g.* _diffrn_detector.diffrn_id). The use of the suffix *.diffrn_id for the key data names in each related category emphasizes the connection to the parent experiment.

As a consequence, there are differences between the mmCIF and core CIF dictionaries in the definition of the category keys for

Example 3.6.5.2. *Data collection for an HIV-1 protease crystal (PDB 5HVP) described with data items in the* DIFFRN *and related categories.*

```
_diffrn.id                              'set1'
_diffrn.crystal_id                       1
_diffrn.ambient_temp                     293(3)
_diffrn.ambient_environment
; Mother liquor from the reservoir of the vapor
  diffusion experiment, mounted in room air
;
_diffrn.crystal_support
;  0.7 mm glass capillary, sealed with dental wax
;
_diffrn.crystal_treatment
; Equilibrated in rotating anode radiation enclosure
  for 18 hours prior to beginning of data collection.
;
_diffrn_detector.diffrn_id               'set1'
_diffrn_detector.detector                'multiwire'
_diffrn_detector.type                    'Siemens'

_diffrn_measurement.diffrn_id            'd1'
_diffrn_measurement.device          '3-circle camera'
_diffrn_measurement.device_type      'Supper model x'
_diffrn_measurement.device_details       'none'
_diffrn_measurement.method               'omega scan'
_diffrn_measurement.details
; 440 frames, 0.20 degrees, 150 sec, detector
  distance 12 cm, detector angle 22.5 degrees
;
_diffrn_radiation.diffrn_id               'set1'
_diffrn_radiation.collimation
                                 '0.3 mm double pinhole'
_diffrn_radiation.monochromator           'graphite'
_diffrn_radiation.type                    'Cu Kalpha'
_diffrn_radiation.wavelength_id            1
_diffrn_radiation_wavelength.id            1
_diffrn_radiation_wavelength.wavelength   1.54
_diffrn_radiation_wavelength.wt            1.0
_diffrn_source.diffrn_id                'set1'
_diffrn_source.source                   'rotating anode'
_diffrn_source.type                     'Rigaku RU-200'
_diffrn_source.power                     50
_diffrn_source.current                   180
_diffrn_source.target       '8mm x 0.4 mm broad-focus'
```

the DIFFRN categories. These differences were introduced in order to accommodate data from more than one experiment in the same table. For example, in the core CIF dictionary, the Miller indices `_diffrn_refln_index_h`, `*_k` and `*_l` play the role of the category key for the DIFFRN_REFLN category. In the mmCIF dictionary, the category key is formed by the data items `_diffrn_refln.id` and `_diffrn_refln.diffrn_id`.

3.6.5.3. Growth, description and analysis of the crystal

The categories describing the crystal properties and growth are as follows:

EXPTL group

Crystal properties (§3.6.5.3.1)

EXPTL

EXPTL_CRYSTAL

EXPTL_CRYSTAL_FACE

Crystal growth (§3.6.5.3.2)

EXPTL_CRYSTAL_GROW

EXPTL_CRYSTAL_GROW_COMP

Categories in the EXPTL category group are used to describe experimental measurements on the crystal (*e.g.* of its shape, size and density) and the growth of the crystal. Data items in the EXPTL category are used to describe the gross properties of the crystal or crystals used in the experiment. Data items in the EXPTL_CRYSTAL category are used to describe the crystal properties in detail and allow for cases where multiple crystals are used. The data items in the EXPTL_CRYSTAL_FACE category are used to describe the crystal faces.

Data items for describing crystal growth are given in two categories that are not found in the current version of the core CIF dictionary. Data items in the EXPTL_CRYSTAL_GROW category are used to describe the conditions and methods used to grow the crystals, and data items in the EXPTL_CRYSTAL_GROW_COMP category can be used to list the components of the solutions in which the crystals were grown.

3.6.5.3.1. *Crystal properties*

The data items in these categories are as follows:

(*a*) EXPTL

- `_exptl.entry_id`
  → `_entry.id`

  `_exptl.absorpt_coefficient_mu`
  `_exptl.absorpt_correction_T_max`
  `_exptl.absorpt_correction_T_min`
  `_exptl.absorpt_correction_type`
  `_exptl.absorpt_process_details`
  `_exptl.crystals_number`
  `_exptl.details` (∼ `_exptl_special_details`)
  `_exptl.method`
  `_exptl.method_details`

(*b*) EXPTL_CRYSTAL

- `_exptl_crystal.id`

  `_exptl_crystal.colour`
  `_exptl_crystal.colour_lustre`
  `_exptl_crystal.colour_modifier`
  `_exptl_crystal.colour_primary`
  `_exptl_crystal.density_diffrn`
  `_exptl_crystal.density_Matthews`
+ `_exptl_crystal.density_meas`
  `_exptl_crystal.density_meas_gt`
  `_exptl_crystal.density_meas_lt`
+ `_exptl_crystal.density_meas_temp`
  `_exptl_crystal.density_meas_temp_gt`
  `_exptl_crystal.density_meas_temp_lt`
  `_exptl_crystal.density_method`
  `_exptl_crystal.density_percent_sol`
  `_exptl_crystal.description`
  `_exptl_crystal.F_000`
  `_exptl_crystal.preparation`
  `_exptl_crystal.size_max`
  `_exptl_crystal.size_mid`
  `_exptl_crystal.size_min`
  `_exptl_crystal.size_rad`

(*c*) EXPTL_CRYSTAL_FACE

- `_exptl_crystal_face.crystal_id`
  → `_exptl_crystal.id`
- `_exptl_crystal_face.index_h`
- `_exptl_crystal_face.index_k`
- `_exptl_crystal_face.index_l`

  `_exptl_crystal_face.diffr_chi`
  `_exptl_crystal_face.diffr_kappa`
  `_exptl_crystal_face.diffr_phi`
  `_exptl_crystal_face.diffr_psi`
  `_exptl_crystal_face.perp_dist`

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. The arrow* (→) *is a reference to a parent data item. 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.*

Data items in these categories are used in the same way in the mmCIF and core CIF dictionaries, and Section 3.2.2.3 can be consulted for details (see Example 3.6.5.3). Identifiers have been introduced to the categories to provide the formal category keys required by the DDL2 data model.