3.7. CLASSIFICATION AND USE OF IMAGE DATA

3.7.4.1. Frames of data

Data items in this category are as follows:

DIFFRN_DATA_FRAME
- `_diffrn_data_frame.detector_element_id`
       → `_diffrn_detector_element.id`
- `_diffrn_data_frame.id`
  `_diffrn_data_frame.array_id`
       → `_array_structure.id`
  `_diffrn_data_frame.binary_id`
       → `_array_data.binary_id`

The bullet (●) indicates a category key. The arrow (→) is a reference to a parent data item.

Data items in the DIFFRN_DATA_FRAME category record details about each frame of data. An experiment may produce multiple frames of data and each frame may be constructed from data provided by multiple detector elements. Each complete frame of data is uniquely identified by the value of `_diffrn_data_frame.id`. The detector elements used are specified by values of `_diffrn_data_frame.detector_element_id`, which forms the category key together with `_diffrn_data_frame.id`. `_diffrn_data_frame.detector_element_id` is a pointer to `_diffrn_detector_element.id` in the DIFFRN_DETECTOR_ELEMENT category. The structure of the data in the frame is completed by giving values for `_diffrn_data_frame.array_id` (a pointer to `_array_structure.id`). The particular blocks of data in the frame are specified by giving values of `_diffrn_data_frame.binary_id` (a pointer to `_array_data.binary_id`).

3.7.4.2. The detector apparatus

Data items in these categories are as follows:

(*a*) DIFFRN_DETECTOR
- `_diffrn_detector.diffrn_id`
       → `_diffrn.id`
- `_diffrn_detector.id`
  `_diffrn_detector.details`
  `_diffrn_detector.detector`
  `_diffrn_detector.dtime`
  `_diffrn_detector.number_of_axes`
  `_diffrn_detector.type`

(*b*) DIFFRN_DETECTOR_AXIS
- `_diffrn_detector_axis.axis_id`
       → `_axis.id`
- `_diffrn_detector_axis.detector_id`
       → `_diffrn_detector.id`

(*c*) DIFFRN_DETECTOR_ELEMENT

- `_diffrn_detector_element.id`
- `_diffrn_detector_element.detector_id`
       → `_diffrn_detector.id`
  `_diffrn_detector_element.center[1]`
  `_diffrn_detector_element.center[2]`

The bullet (●) indicates a category key. The arrow (→) is a reference to a parent data item. Items in italics are defined in the mmCIF dictionary.

The DIFFRN_DETECTOR category is defined in the mmCIF dictionary (Section 3.6.5.2; see the detailed discussion in Section 3.2.2.2.4). The CBF/imgCIF dictionary restates the DIFFRN_DETECTOR category, adding new tags. Data items in the DIFFRN_DETECTOR category describe the detector used to measure the scattered radiation, including any analyser and post-sample collimation. In order to allow for multiple detectors, the category key has been extended to include `_diffrn_detector.id` to uniquely identify each detector. If there is only one detector, `_diffrn_detector.id` need not be specified, and it will implicitly default to the value of `_diffrn_detector.diffrn_id` (a pointer to `_diffrn.id` in the DIFFRN category in the mmCIF dictionary). The general class of detector is given by the value of `_diffrn_detector.detector` with the make and model given by the value of `_diffrn_detector.type`. Any special aspects of the detector not covered elsewhere are given by the value of `_diffrn_detector.details`. As in mmCIF, the value of `_diffrn_detector.dtime` gives the deadtime of the detector. Additional data items may need to be added in the future for complex inhomogeneous deadtime situations. In addition, the number of axes can be specified using `_diffrn_detector.number_of_axes`.

Data items in the DIFFRN_DETECTOR_AXIS category associate axes with detectors. Each axis is associated with a detector through the value of `_diffrn_detector_axis.detector_id` (a pointer to `_diffrn_detector.id`). The value of `*.axis_id` (a pointer to `_axis.id`) identifies an axis. Together `*.detector_id` and `*.axis_id` form the category key.

Data items in the DIFFRN_DETECTOR_ELEMENT category record details about the spatial layout and other characteristics of each element of a detector which may have multiple elements, giving the *X* and *Y* coordinates of the position of the beam centre relative to the lower left corner of each detector element. Each detector element is identified by the value of `_diffrn_detector_element.id` and the detector of which it is an element is identified by the value of `_diffrn_detector_element.detector_id` (a pointer to `_diffrn_detector.id`).

In most cases, it would be preferable to use the more detailed information provided in the ARRAY_STRUCTURE_LIST and ARRAY_STRUCTURE_LIST_AXIS categories rather than simply specifying the coordinates of the centre of the beam relative to the lower left corner of each detector element.

3.7.4.3. Apparatus and instrumentation at the crystal

Data items in these categories are as follows:

(*a*) DIFFRN_MEASUREMENT
- *`_diffrn_measurement.diffrn_id`*
       → `_diffrn.id`
- *`_diffrn_measurement.device`*
- `_diffrn_measurement.id`
  `_diffrn_measurement.details`
  `_diffrn_measurement.device_details`
  `_diffrn_measurement.device_type`
  `_diffrn_measurement.method`
  `_diffrn_measurement.number_of_axes`
  `_diffrn_measurement.specimen_support`

(*b*) DIFFRN_MEASUREMENT_AXIS
- `_diffrn_measurement_axis.axis_id`
       → `_axis.id`
- `_diffrn_measurement_axis.measurement_device`
       → `_diffrn_measurement.device`
- `_diffrn_measurement_axis.measurement_id`
       → `_diffrn_measurement.id`

The bullet (●) indicates a category key. The arrow (→) is a reference to a parent data item. Items in italics are defined in the mmCIF dictionary.

The DIFFRN_MEASUREMENT category is defined in the mmCIF dictionary (Section 3.6.5.2; see the detailed discussion in Section 3.2.2.2.3). The CBF/imgCIF dictionary restates the DIFFRN_MEASUREMENT category, adding new tags. Data items in the DIFFRN_MEASUREMENT category record details about the device used to orient and/or position the crystal during data measurement and the manner in which the diffraction data were measured. To allow for multiple measurement devices, `_diffrn_measurement.id` has been added to the category key. The number of axes is given by the value of `_diffrn_measurement.number_of_axes`. The axes should be described using entries in DIFFRN_MEASUREMENT_AXIS.

references