

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.

Data items in the DIFFRN_MEASUREMENT_AXIS category associate axes with goniometers, just as data items in the DIFFRN_DETECTOR_AXIS category associate axes with detectors.

3.7.4.4. The radiation source

Data items in this category are as follows:

```
DIFFRN_RADIATION
• _diffrn_radiation.diffrn_id
  → _diffrn.id
  _diffrn_radiation.collimation
  _diffrn_radiation.div_x_source
  _diffrn_radiation.div_y_source
  _diffrn_radiation.div_x_y_source
  _diffrn_radiation.filter_edge
  _diffrn_radiation.inhomogeneity
  _diffrn_radiation.monochromator
  _diffrn_radiation.polarisn_norm
  _diffrn_radiation.polarisn_ratio
  _diffrn_radiation.polarizn_source_norm
  _diffrn_radiation.polarizn_source_ratio
  _diffrn_radiation.probe
  _diffrn_radiation.type
  _diffrn_radiation.wavelength_id
  → _diffrn_radiation.wavelength.id
  _diffrn_radiation.xray_symbol
```

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_RADIATION category is defined in the mmCIF dictionary (Section 3.6.5.2; see the detailed discussion in Section 3.2.2.2.2). The CBF/imgCIF dictionary adds the items *_diffrn_radiation.div_x_source*, **.div_y_source* and **.div_x_y_source* to specify beam crossfire, and the items *_diffrn_radiation.polarizn_source_norm* and **.polarizn_source_ratio* to provide a definition of polarization relative to the laboratory coordinate system rather than relative to the diffraction plane. The value of the beam crossfire component *_diffrn_radiation.div_x_source* is the mean deviation in degrees of the X-ray beam from being parallel to the X axis as it illuminates the sample. The value of the beam crossfire component *_diffrn_radiation.div_y_source* is the mean deviation in degrees of the X-ray beam from being parallel to the Y axis as it illuminates the sample. The value of the beam crossfire component *_diffrn_radiation.div_x_y_source* is the correlation of the X and Y components. The value of the normal component of the polarization *_diffrn_radiation.polarizn_source_norm* is the angle in degrees, as viewed from the specimen, between the normal to the polarization plane and the laboratory Y axis as defined in the AXIS category. The dimensionless value of *_diffrn_radiation.polarisn_ratio* is the ratio $(I_p - I_n)/(I_p + I_n)$, where I_n is the intensity (amplitude squared) of the electric vector of the illumination of the sample normal to the polarization and I_p is the intensity of the electric vector of the illumination of the sample in the plane of polarization. With suitable choices of laboratory axes, the definitions conform to synchrotron conventions. See Chapter 4.6 for a detailed description of these items.

3.7.4.5. Intensity measurements

Data items in this category are as follows:

```
DIFFRN_REFLN
• _diffrn_refl.n.frame_id
  → _diffrn_data_frame.id
• _diffrn_refl.n.id
• _diffrn_refl.n.diffrn_id
  _diffrn_refl.n.angle_chi
  _diffrn_refl.n.angle_kappa
  _diffrn_refl.n.angle_omega
  _diffrn_refl.n.angle_phi
  _diffrn_refl.n.angle_psi
  _diffrn_refl.n.angle_theta
```

```
_diffrn_refl.n.attenuator_code
_diffrn_refl.n.counts_bg_1
_diffrn_refl.n.counts_bg_2
_diffrn_refl.n.counts_net
_diffrn_refl.n.counts_peak
_diffrn_refl.n.counts_total
_diffrn_refl.n.detect_slit_horiz
_diffrn_refl.n.detect_slit_vert
_diffrn_refl.n.elapsed_time
_diffrn_refl.n.index_h
_diffrn_refl.n.index_k
_diffrn_refl.n.index_l
_diffrn_refl.n.intensity_net
_diffrn_refl.n.intensity_sigma
_diffrn_refl.n.scale_group_code
_diffrn_refl.n.scan_mode
_diffrn_refl.n.scan_mode_backgd
_diffrn_refl.n.scan_rate
_diffrn_refl.n.scan_time_backgd
_diffrn_refl.n.scan_width
_diffrn_refl.n.sint_over_lambda
_diffrn_refl.n.standard_code
_diffrn_refl.n.wavelength
_diffrn_refl.n.wavelength_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_REFLN category is defined in the mmCIF dictionary (Section 3.6.5.2; see the detailed discussion in Section 3.2.2.2.2). Data items in the DIFFRN_REFLN category record details of the intensities measured in the diffraction data set identified by *_diffrn_refl.n.diffrn_id*. The CBF/imgCIF dictionary extends the key with *_diffrn_refl.n.frame_id* (a pointer to *_diffrn_data_frame.id*), so that multiple data sets may be recorded.

3.7.4.6. Diffraction scans

Data items in these categories are as follows:

- (a) DIFFRN_SCAN
- *_diffrn_scan.id*
 - _diffrn_scan.date_end*
 - _diffrn_scan.date_start*
 - _diffrn_scan.frame_id_start*
 - *_diffrn_data_frame.id*
 - _diffrn_scan.frame_id_end*
 - *_diffrn_data_frame.id*
 - _diffrn_scan.frames*
 - _diffrn_scan.integration_time*
- (b) DIFFRN_SCAN_AXIS
- *_diffrn_scan_axis.axis_id*
 - *_axis.id*
 - *_diffrn_scan_axis.scan_id*
 - *_diffrn_scan.id*
 - _diffrn_scan_axis.angle_start*
 - _diffrn_scan_axis.angle_range*
 - _diffrn_scan_axis.angle_increment*
 - _diffrn_scan_axis.angle_rstrtd_incr*
 - _diffrn_scan_axis.displacement_start*
 - _diffrn_scan_axis.displacement_range*
 - _diffrn_scan_axis.displacement_increment*
 - _diffrn_scan_axis.displacement_rstrtd_incr*
- (c) DIFFRN_SCAN_FRAME
- _diffrn_scan_frame.date*
 - *_diffrn_scan_frame.frame_id*
 - *_diffrn_data_frame.id*
 - *_diffrn_scan_frame.scan_id*
 - *_diffrn_scan.id*
 - _diffrn_scan_frame.frame_number*
 - _diffrn_scan_frame.integration_time*
- (d) DIFFRN_SCAN_FRAME_AXIS
- *_diffrn_scan_frame_axis.axis_id*
 - *_axis.id*
 - *_diffrn_scan_frame_axis.frame_id*
 - *_diffrn_data_frame.id*
 - _diffrn_scan_frame_axis.angle*