

3. CIF DATA DEFINITION AND CLASSIFICATION

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.id*
- *_diffrn_refl.diffrn_id*
- _diffrn_refl.angle_chi*
- _diffrn_refl.angle_kappa*
- _diffrn_refl.angle_omega*
- _diffrn_refl.angle_phi*
- _diffrn_refl.angle_psi*
- _diffrn_refl.angle_theta*

- _diffrn_refl.attenuator_code*
- _diffrn_refl.counts_bg_1*
- _diffrn_refl.counts_bg_2*
- _diffrn_refl.counts_net*
- _diffrn_refl.counts_peak*
- _diffrn_refl.counts_total*
- _diffrn_refl.detect_slit_horiz*
- _diffrn_refl.detect_slit_vert*
- _diffrn_refl.elapsed_time*
- _diffrn_refl.index_h*
- _diffrn_refl.index_k*
- _diffrn_refl.index_l*
- _diffrn_refl.intensity_net*
- _diffrn_refl.intensity_sigma*
- _diffrn_refl.scale_group_code*
- _diffrn_refl.scan_mode*
- _diffrn_refl.scan_mode_backgd*
- _diffrn_refl.scan_rate*
- _diffrn_refl.scan_time_backgd*
- _diffrn_refl.scan_width*
- _diffrn_refl.sint_over_lambda*
- _diffrn_refl.standard_code*
- _diffrn_refl.wavelength*
- _diffrn_refl.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.diffrn_id*. The CBF/imgCIF dictionary extends the key with *_diffrn_refl.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_rstrt_incr*
 - _diffrn_scan_axis.displacement_start*
 - _diffrn_scan_axis.displacement_range*
 - _diffrn_scan_axis.displacement_increment*
 - _diffrn_scan_axis.displacement_rstrt_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*

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_diffrn_scan_frame_axis.angle_increment
_diffrn_scan_frame_axis.angle_rstrt_incr
_diffrn_scan_frame_axis.displacement
_diffrn_scan_frame_axis.displacement_increment
_diffrn_scan_frame_axis.displacement_rstrt_incr
```

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

Data items in the DIFFRN_SCAN category describe the parameters of one or more scans, relating axis positions to frames. Each scan is uniquely identified by the value of `_diffrn_scan.id`. The data items in this category give overall information for the scan. The detailed frame-by-frame data are given in DIFFRN_SCAN_FRAME and DIFFRN_SCAN_FRAME_AXIS. The values of `_diffrn_scan.date_start` and `*.date_end` give the starting and ending time for a scan. The original definition of the `yyyy-mm-dd` data type, which includes date and time, has been extended in the CBF/imgCIF dictionary. This allows the seconds part of the time to include an optional decimal fraction. The approximate average integration time for each step of the scan is given by the value of `_diffrn_scan.integration_time`. The scan is tied to individual frame IDs by the values of `_diffrn_scan.frame_id_start` and `*.frame_id_end`. The number of frames in the scan is given by the value of `_diffrn_scan.frames`.

Data items in the DIFFRN_SCAN_AXIS category describe the settings of axes for particular scans. Unspecified axes are assumed to be at their zero points. The vector of each axis is not given here, because it is provided in the AXIS category. By making `_diffrn_scan_axis.scan_id` and `_diffrn_scan_axis.axis_id` keys of the DIFFRN_SCAN_AXIS category, an arbitrary number of scanning and fixed axes can be specified for a scan. The value of `_diffrn_scan_axis.scan_id` (a pointer to `_diffrn_scan.id`) identifies the scan and the values of `_diffrn_scan_axis.axis_id` (a pointer to `_axis.id`) associate particular axes with that scan. The steps of each axis are specified by `*_start`, `*_range`, `*_increment` and `*_rstrt_incr` values for angles or for displacements. The `*_start` value is the setting of the relevant axis at the start of the scan. The `*_range` value is the total change in the axis setting through the scan. The `*_increment` value is the increment in the axis setting for each step of the scan. The `*_rstrt_incr` value is the increment in the axis setting after each step of the scan.

Data items in the DIFFRN_SCAN_FRAME category describe the relationship of particular frames to scans. The value of `_diffrn_scan_frame.frame_id` (a pointer to `_diffrn_data_frame.id`) identifies the frame. The value of `_diffrn_scan_frame.scan_id` (a pointer to `_diffrn_scan.id`) identifies the scan of which the frame is a part. Together `_diffrn_scan_frame.frame_id` and `*.scan_id` form the category key. The value of `_diffrn_scan_frame.date` gives the date and time of the start of the data collection for the frame. The value of `_diffrn_scan_frame.frame_number` gives the number of the frame (starting with 1). The value of `_diffrn_scan_frame.integration_time` gives the precise time in seconds to integrate this step of the scan.

Table A3.7.1.1. Categories in the CBF/imgCIF dictionary

Numbers in parentheses refer to the section of this chapter in which each category is described in detail.

ARRAY_DATA group (§3.7.2)	DIFFRN_DETECTOR_AXIS (§3.7.4.2(b))
ARRAY_DATA (§3.7.2.1)	DIFFRN_DETECTOR_ELEMENT (§3.7.4.2(c))
ARRAY_ELEMENT_SIZE (§3.7.2.2)	DIFFRN_MEASUREMENT (§3.7.4.3(a))
ARRAY_INTENSITIES (§3.7.2.3)	DIFFRN_MEASUREMENT_AXIS (§3.7.4.3(b))
ARRAY_STRUCTURE (§3.7.2.4(a))	DIFFRN_RADIATION (§3.7.4.4)
ARRAY_STRUCTURE_LIST (§3.7.2.4(b))	DIFFRN_REFLN (§3.7.4.5)
ARRAY_STRUCTURE_LIST_AXIS (§3.7.2.4(c))	DIFFRN_SCAN (§3.7.4.6(a))
AXIS group (§3.7.3)	DIFFRN_SCAN_AXIS (§3.7.4.6(b))
AXIS (§3.7.3)	DIFFRN_SCAN_FRAME (§3.7.4.6(c))
DIFFRN group (§3.7.4)	DIFFRN_SCAN_FRAME_AXIS (§3.7.4.6(d))
DIFFRN_DATA_FRAME (§3.7.4.1)	
DIFFRN_DETECTOR (§3.7.4.2(a))	

Data items in the DIFFRN_SCAN_FRAME_AXIS category describe the settings of axes for particular frames. Unspecified axes are assumed to be at their zero points. If for any given frame non-zero values apply for any of the data items in this category, those values should be given explicitly in this category and not simply inferred from values in DIFFRN_SCAN_AXIS. Since the collection for a given frame may involve multiple axes, the frame involved is identified by the value of `_diffrn_scan_frame_axis.frame_id` (a pointer to `_diffrn_data_frame.id`) and each axis is identified by the value of `_diffrn_scan_frame_axis.axis_id` (a pointer to `_axis.id`). Together `_diffrn_scan_frame_axis.frame_id` and `*.axis_id` form the category key. If the axis is an axis of rotation, the axis settings for the frame are given by the values of `_diffrn_scan_frame_axis.angle`, `*.angle_increment` and `*.angle_rstrt_incr`. If the axis is a translation axis, the axis settings for the frame are given by the values of `_diffrn_scan_frame_axis.displacement`, `*.displacement_increment` and `*.displacement_rstrt_incr`. The integration begins at the setting given by the value of `_diffrn_scan_frame_axis.angle` or of `*.displacement`. The `*_increment` value gives the change of axis setting during the scan. At the end of the integration, the axis may need to be repositioned by an additional amount. That amount is given by `*_rstrt_incr`.

Appendix 3.7.1

Category structure of the CBF/imgCIF dictionary

Table A3.7.1.1 provides an overview of the structure of the CBF/imgCIF dictionary by category group and member categories.

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References

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