

3. CIF DATA DEFINITION AND CLASSIFICATION

Data items in this category are as follows:

```

AXIS
• _axis.equipment
• _axis.id
  _axis.depends_on
    → _axis.id
  _axis.offset [1]
  _axis.offset [2]
  _axis.offset [3]
  _axis.type
  _axis.vector [1]
  _axis.vector [2]
  _axis.vector [3]

```

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

Data items in the `AXIS` category record the information required to describe the goniometer, detector, source and other axes needed to specify a data collection. The location of each axis is specified by two vectors: the axis itself, given as a unit vector, and an offset to the base of the unit vector. These vectors are referenced to a right-handed laboratory coordinate system with its origin in the specimen, as shown in Fig. 3.7.3.1.

The `X` axis is aligned to the mechanical axis pointing from the specimen along the principal axis of the goniometer.

The `Z` axis is defined next. The `Z` axis is derived from the source axis (the axis running from the sample to the source). If the source axis is orthogonal to the `X` axis, the source axis is the `Z` axis. If the source axis is not orthogonal to the `X` axis, the `Z` axis is the component of the source axis orthogonal to the `X` axis. The direction is chosen to form an acute angle with the source axis.

The `Y` axis is defined last. The `Y` axis completes an orthogonal right-handed system defined by the `X` axis and the `Z` axis (see below).

These axes are based on the goniometer, not on the orientation of the detector, gravity *etc.* The vectors necessary to specify all other axes are given by sets of three components in the order (`X`, `Y`, `Z`). If the axis involved is a rotation axis, it is right-handed, *i.e.* as one views the object to be rotated from the origin (the tail) of the unit vector, the rotation is clockwise. If a translation axis is specified, the direction of the unit vector specifies the sense of positive translation.

Note: This choice of coordinate system is similar to but significantly different from the choice in *MOSFLM* (Lesley & Powell, 2003), in which `X` is along the X-ray beam (our `Z` axis) and `Z` is along the rotation axis.

All rotations are given in degrees and all translations are given in millimetres.

Axes may be dependent on one another. The `X` axis is the only axis that is strictly connected to the hardware. All other axes are specified by the positions they would assume when the axes upon which they depend are at their zero points.

When specifying detector axes, each axis is specified relative to the beam centre. The location of the beam centre on the detector should be given in the `DIFFRN_DETECTOR` category in millimetres from the (0, 0) corner of the detector and should be corrected for distortion.

It should be noted that many different origins arise in the definition of an experiment. In particular, as noted above, we need to specify the location of the beam centre on the detector in terms of the origin of the detector, which is, of course, not coincident with the centre of the sample.

Each axis is uniquely identified by the values of `_axis.id` and of `_axis.equipment`. An axis may be a translation axis, a rotation axis or an axis for which the mode of motion is not relevant. The

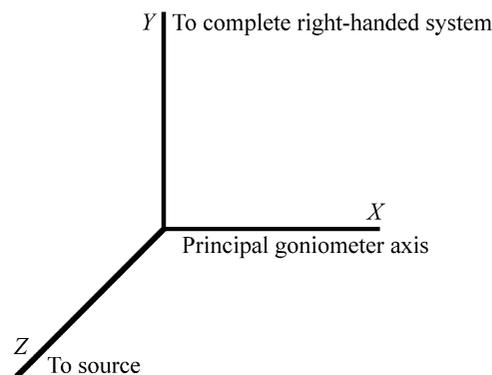


Fig. 3.7.3.1. `AXIS` laboratory coordinate system. The origin is centred in the specimen.

type of axis is specified by the value of `_axis.type`. The base of the axis is specified by the point in the laboratory coordinate system given by the values of `_axis.offset [1]`, `_axis.offset [2]` and `_axis.offset [3]`, and the direction of the axis from that base, as a dimensionless unit vector, is given by `_axis.vector [1]`, `_axis.vector [2]` and `_axis.vector [3]`.

3.7.4. The diffraction experiment

The categories relating to the diffraction experiment are as follows:

`DIFFRN` group

Frames of data (§3.7.4.1)

`DIFFRN_DATA_FRAME`

The detector apparatus (§3.7.4.2)

`DIFFRN_DETECTOR`

`DIFFRN_DETECTOR_AXIS`

`DIFFRN_DETECTOR_ELEMENT`

Apparatus and instrumentation at the crystal (§3.7.4.3)

`DIFFRN_MEASUREMENT`

`DIFFRN_MEASUREMENT_AXIS`

The radiation source (§3.7.4.4)

`DIFFRN_RADIATION`

Intensity measurements (§3.7.4.5)

`DIFFRN_REFLN`

Diffraction scans (§3.7.4.6)

`DIFFRN_SCAN`

`DIFFRN_SCAN_AXIS`

`DIFFRN_SCAN_FRAME`

`DIFFRN_SCAN_FRAME_AXIS`

The `CBF/imgCIF` dictionary extends the `mmCIF` categories in the `DIFFRN` group, which are very similar to their corresponding categories in the core CIF dictionary. The `DIFFRN` group is introduced in the description of the core CIF dictionary in Section 3.2.2.2. Its use in the `mmCIF` dictionary is described in Section 3.6.5.2, from which we quote: ‘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.’ In this chapter we focus on the `CBF/imgCIF` extensions.

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.

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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_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.

We are grateful to Frances C. Bernstein, Paula Fitzgerald and Bob Sweet for their helpful comments and suggestions.

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