Chapter 3.7. Classification and use of image data
(H. J. Bernstein)

Chapter 4.6. Image dictionary (imgCIF)
(A. P. Hammersley, H. J. Bernstein and J. D. Westbrook)

Volume G describes the standard data exchange and archival file format (CIF) used throughout crystallography. It provides in-depth information vital for small-molecule, inorganic and macromolecular crystallographers, mineralogists, chemists, materials scientists, solid-state physicists and others who wish to record or use the results of a single-crystal or powder diffraction experiment. The volume also provides the detailed data ontology necessary for programmers and database managers to design interoperable computer applications. The accompanying CD-ROM contains the CIF dictionaries in machine-readable form and a collection of libraries and utility programs.

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3.7. Classification and use of image data

BY H. J. BERNSTEIN

3.7.1. Introduction
This chapter describes the categories and organization of data items defined in the CBF/IMG/CIF dictionary. The classification of image data applies to both Crystallographic Binary File (CBF) and Image-Supporting Crystallographic Information File (IMG/CIF) representations. An introduction to CBF data and construction is given in Chapter 2.3. Full details of the CBF/IMG/CIF dictionary are given in Chapter 4.6.

The main reason for introducing the new items defined in the CBF/IMG/CIF dictionary was to extend the mmCIF dictionary (Chapter 3.6) to allow the storage of synchrotron diffraction images. However, these items are also important in other fields that use binary image data, including the publication of articles, the creation of web pages and the production of movies.

Data categories in the CBF/IMG/CIF dictionary can describe one-, two- and three-dimensional array detectors that output data organized by time and/or wavelength. The categories defined at present support modular data that can be extended for future applications without having to make fundamental structural changes. For example, it is anticipated that additional data items will be needed soon to allow higher-dimensional data representations and more complex data structures; these should be accommodated easily.

The CBF/IMG/CIF dictionary consists of three groups of categories: the ARRAY_DATA group, the AXIS group and the DIFFRN group (Table 3.7.1.1). All fall within the ‘Experimental measurements’ classification of Table 3.1.10.1. The DIFFRN group already exists in the mmCIF dictionary (Section 3.6.5.2; see also Section 3.2.2.2) and describes the diffraction data and their measurement. Definitions in the CBF/IMG/CIF dictionary extend and in some cases restate the definitions in the mmCIF dictionary.

The data categories defined in the CBF/IMG/CIF dictionary are described in this chapter. Table 3.7.1.1 lists the formal categories and groups declared in the dictionary and the sections of this chapter in which they are discussed. Each section is divided into subsections describing a single category or a small set of closely related categories. Within each subsection, the data names within the relevant categories are listed. Category keys, pointers to parent data items and aliases to data items in the mmCIF dictionary are indicated. The data collected in an experiment are organized into scans. Each scan consists of one or more frames. Each frame consists of one or more data arrays. The logical data in the data arrays need to be described in terms of physical arrays of image elements. The axes of the laboratory coordinate system needed to describe the physical positions of the image elements and the positioning of the specimen are given in the AXIS category. The axes used for the positioning systems for the specimen and the detector are constructed in the same laboratory coordinate system.

The DIFFRN_DETECTOR_AXIS category relates detector elements to axes. The DIFFRN_MEASUREMENT AXIS category relates goniometers to axes. The DIFFRN_SCAN_AXIS and DIFFRN_SCAN_FRAME_AXIS categories relate scans to overall axis settings and individual frames to frame-by-frame axis settings, respectively.

The organization of the data in the collected arrays of data is given in the ARRAY_STRUCTURE_LIST category and the physical settings of axes for the centres of pixels that correspond to data points are given in the ARRAY_STRUCTURE_LIST_AXIS category.

3.7.2. Binary image data
The six categories that collectively define the relationship between the sequences of octets in arrays of binary data and the information in the images those octets represent are as follows:

- ARRAY_DATA
- The image data (§3.7.2.1)
  - ARRAY_DATA
- Array elements (§3.7.2.2)
  - ARRAY_ELEMENT_SIZE
- Intensities (§3.7.2.3)
  - ARRAY_INTEncITIES
- Organization and encoding of data (§3.7.2.4)
  - ARRAY_STRUCTURE
  - ARRAY_STRUCTURE_LIST
  - ARRAY_STRUCTURE_LIST_AXIS

3.7.2.1. The image data
Data items in this category are as follows:

- ARRAY_DATA
  - __array_data.array_id
  - __array_data.binary_id
  - __array_data.data

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

Each value of the __array_data.data data item is a sequence of ocets representing a binary image. __array_data.array_id and __array_data.binary_id, taken together, uniquely identify each image. The value of __array_data.array_id is a pointer to __array_structure.id to provide the relationship between the sequence of octets and the logical structure of the image. Since multiple images may have the same logical structure, the purpose of __array_data.binary_id is to ensure that each image has a unique identifier.

Table 3.7.1.1. Category groups defined in the CBF/IMG/CIF dictionary

<table>
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<tr>
<th>Section</th>
<th>Category group</th>
<th>Subject covered</th>
</tr>
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<tr>
<td>Experimental measurements</td>
<td>ARRAY_DATA</td>
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<td>AXIS</td>
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3.7.2.2. Array elements

Data items in this category are as follows:

- **ARRAY_ELEMENT_SIZE**
  - _array_element_size.array_id
  - _array_element_size.index

- **_array_element_size.size**

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

The value of the _array_element_size.size data item is a size in metres of an image element (a pixel or voxel). The direction of the measurement is given in each dimension by _array_element_size.index. The array structure specifying the organization of the dimensions is referenced by the value of _array_element_size.array_id, which is a pointer to _array_structure.id. The value of _array_element_size.index is a pointer to _array_structure_list.id. For data organized into rectangular arrays of pixels or voxels, this gives the spatial dimensions of the individual image elements.

3.7.2.3. Intensities

Data items in this category are as follows:

- **ARRAY_INTENSITIES**
  - _array_intensities.array_id
  - _array_intensities.binary_id
  - _array_intensities.gain
  - _array_intensities.linear
  - _array_intensities.offset
  - _array_intensities.scaling
  - _array_intensities.undef_value

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

The relationship between the data values for individual image elements and the number of incident photons can be complex. The data items in the ARRAY_INTENSITIES category provide information about this relationship. The value of _array_intensities.linear states the type of relationship, and the values of _array_intensities.array_id and _array_intensities.binary_id identify the array structure and the image being discussed. The other items are used in different ways depending on the relationship. If the value of _array_intensities.linear is raw, then the image elements hold uninterpreted raw data values from the detector, e.g., for calibration. If the value of _array_intensities.linear is linear, then the count in an image element is proportional to the incident number of photons by the value of _array_intensities.gain. The standard uncertainty (estimated standard deviation) of the gain may be given in _array_intensities.linear_e. The value used for this should be estimated from a good understanding of the physical characteristics of the experimental apparatus. If the value of _array_intensities.linear is offset, then the value of _array_intensities.offset should be added to the image element value. If the value of _array_intensities.linear is scaling, scaling_offset, sqrt_scaled or logarithmic_scaled, the necessary scaling factor is given by the value of _array_intensities.scaling. In all cases, the scaling factor is applied to the image element value before the other operations are applied. In the first case, only simple scaling is used. In the second case, the value of _array_intensities_offset is added after scaling. In the third case, the scaled value is squared. In the final case, 10 is taken to the power given by the scaled value.

3.7.2.4. Organization and encoding of array data

Data items in these categories are as follows:

(a) **ARRAY_STRUCTURE**
- _array_structure.id
- _array_structure.byte_order
- _array_structure.compression_type
- _array_structure.encoding_type

(b) **ARRAY_STRUCTURE_LIST**
- _array_structure_list.array_id
- _array_structure_list.index
- _array_structure_list_axis.axis_id
- _array_structure_list_axis.axis_set_id
- _array_structure_list_axis.dimension
- _array_structure_list_axis.precedence

(c) **ARRAY_STRUCTURE_LIST_AXIS**
- _array_structure_list_axis.axis_id
- _array_structure_list_axis.axis_set_id
- _array_structure_list_axis.dimension
- _array_structure_list_axis.angle_increment
- _array_structure_list_axis.angular_pitch
- _array_structure_list_axis.displacement_increment
- _array_structure_list_axis.radial_pitch

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

The data items in the ARRAY_STRUCTURE category show how the stream of octets in a binary image is to be reorganized into words of an appropriate size. Each possible encoding is identified by a value of _array_structure.id. In most cases, large images will have been compressed. The type of compression used is given by _array_structure.compression_type. Once a stream of octets has been decompressed, it can be organized into words. The type of each word is given by the value of _array_structure.encoding_type and the order of mapping octets onto words, most significant octet first ('big-endian') or least significant octet first ('little-endian'), is given by the value of _array_structure.byte_order.

The data items in the ARRAY_STRUCTURE_LIST category show how the list of words defined by the ARRAY_STRUCTURE category should be organized into image arrays. The value of _array_structure_list.array_id is a pointer to _array_structure.id. Each dimension (row, column, sheet etc.) of the image is identified by an index, counting from 1, given by _array_structure_list.index. The order of nesting of the indices is given by the values of _array_structure_list.precedence, with the index of precedence 1 varying most rapidly (i.e., having values stored sequentially). The direction of index change for increasing memory location is given by the value of _array_structure_list.dimension. For a given index, the number of image elements in that dimension is given by the value of _array_structure_list.dimension.

Data items in the ARRAY_STRUCTURE_LIST_AXIS category describe the physical settings of sets of axes for the centres of pixels that correspond to data points described in the ARRAY_STRUCTURE_LIST category.

In the simplest cases, the physical increments of a single axis correspond to the increments of a single array index. More complex organizations (e.g., spiral scans) may require coupled motions along multiple axes.
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Note that a spiral scan uses two coupled axes, one for the angular direction and one for the radial direction. This differs from a cylindrical scan for which the two axes are not coupled into one set.

Multiple related axes are gathered together into sets. Each set is identified by the value of the axis set identifier, _array_structure_list_axis.axis_set_id, and each axis within a set is identified by the value of _array_structure_list_axis.axis_id. Each set given by a value of _array_structure_list_axis.axis_set_id is linked to a corresponding value for _array_structure_list_axis.axis_set_id to relate settings of the axes in the axis set to particular image elements in ARRAY_STRUCTURE_LIST.

If axes are all independent, no value need be given for _array_structure_list_axis.axis_set_id, which is then implicitly given the corresponding value of _array_structure_list_axis.axis_id. Each axis given by a value of _array_structure_list_axis.axis_set_id is linked to a corresponding value for _array_structure_list_axis.axis_id to provide a physical description of the axis, _array_structure_list_axis.axis_id and _array_structure_list_axis.axis_set_id together uniquely identifying a row of data in an ARRAY_STRUCTURE_LIST_AXIS table.

For the remaining data items, there are two important cases to consider: axes that step by Euclidean distance and axes that step by angle. Fig. 3.7.2.1 shows a portion of an array of image elements laid out on a rectangular grid. The starting point of an axis is specified in millimetres by the value of _array_structure_list_axis.displacement and the centre-to-centre distance between pixels is specified in millimetres by the value of _array_structure_list_axis.displacement_increment.

Fig. 3.7.2.2 shows a portion of an array of image elements laid out in concentric cylinders. The starting point of the angular axis is specified in degrees by the value of _array_structure_list_axis.angle and the centre-to-centre angular distance between pixels is specified in degrees by the value of _array_structure_list_axis.angle_increment. The starting point of the radial axis is specified by the value of _array_structure_list_axis.displacement and the radial distance between cylinders of pixels is specified in millimetres by the value of _array_structure_list_axis.radial_pitch. Note that the image elements further from the centre are larger than the image elements closer to the centre.

Fig. 3.7.2.3 shows a portion of a spiral scan array in which the angular and radial axes are coupled. This example represents a 'constant-velocity' scan, in which the size of the image elements does not depend on the distance from the centre. The starting point of the angular axis is again specified in degrees by the value of _array_structure_list_axis.angle, but the centre-to-centre distance between pixels is specified in millimetres by the value of _array_structure_list_axis.angular_pitch. The coupled radial axis is handled in much the same way as for the uncoupled radial axis in the cylindrical array.

These examples show some of the more common two-dimensional data structures. By coupling an additional axis not in the plane of the first two, regular three-dimensional arrays of data can be represented without additional tags. The categories in the DIFFRN group allow arrays of data to be associated with frames and thereby with time and/or wavelength. More general data structures, for example ones based on dope vectors or hash tables, would require the definition of additional tags, but any data structure (see Aho et al., 1987) that can be handled by a modern computer should be manageable within this framework.

3.7.3. Axes

The category describing the axes required to specify the data collection is as follows:

AXIS group

AXIS
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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 originates 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 used in the laboratory, and not in 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 (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 DECTOR 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 _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 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_DECT OR
DIFFRN_DECT OR_AXIS
DIFFRN_DECT OR_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/imagCIF 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_DECT OR, 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/imagCIF extensions.
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3.7.4.1. Frames of data

Data items in this category are as follows:

DIFFRN_DATA_FRAME
- _diffn_detector_frame.detector_element_id
- _diffn_detector_frame.detector_id
- _diffn_detector_frame.array_id
  - _array_structure.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 _diffn_detector_frame.id. The detector elements used are specified by values of _diffn_detector_element_id, which forms the category key together with _diffn_detector_frame.id. _diffn_detector_element_id is a pointer to _diffn_detector_element_id in the DIFFRN_DETECTOR_ELEMENT category. The structure of the data in the frame is completed by giving values for _diffn_detector_frame.array_id (a pointer to _array_structure.id). The particular blocks of data in the frame are specified by giving values of _diffn_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
- _diffn_detector.diffrn_id
  - _diffrn.id
- _diffn_detector.id
- _diffn_detector.details
- _diffn_detector.detector
  - _detector.id
- _diffn_detector.detector.dtime
  - _dtime
- _diffn_detector.number_of_axes
  - _number_of_axes
- _diffn_detector.type
  - _type

(b) DIFFRN_DETECTOR_AXIS
- _diffn_detector_axis.axis_id
  - _axis.id
- _diffn_detector_axis.detector_id
  - _detector.id

(c) DIFFRN_DETECTOR_ELEMENT
- _diffn_detector_element.id
- _diffn_detector_element.detector_id
- _diffn_detector_element_detector_id
  - _detector.id
- _diffn_detector_element.detector_element_center[1]
- _diffn_detector_element.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 _diffn_detector.id to uniquely identify each detector. If there is only one detector, _diffn_detector.id need not be specified, and it will implicitly default to the value of _diffn_detector.diffrn_id (a pointer to _diffrn in the DIFFRN category in the mmCIF dictionary). The general class of detector is given by the value of _diffn_detector.detector with the make and model given by the value of _diffn_detector.type. Any special aspects of the detector not covered elsewhere are given by the value of _diffn_detector.details. As in mmCIF, the value of _diffn_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 _diffn_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 _diffn_detector_axis.detector_id (a pointer to _diffn_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 _diffn_detector_element_id and the detector of which it is an element is identified by the value of _diffn_detector_element.detector_id (a pointer to _diffn_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
- _diffn_measurement.diffrn_id
  - _diffrn.id
- _diffn_measurement.device
  - _device
- _diffn_measurement.details
  - _details
- _diffn_measurement.device_type
  - _type
- _diffn_measurement.method
  - _method
- _diffn_measurement.number_of_axes
  - _number_of_axes
- _diffn_measurement.specimen_support
  - _specimen_support

(b) DIFFRN_MEASUREMENT_AXIS
- _diffn_measurement_axis.axis_id
  - _axis.id
- _diffn_measurement_axis.measurement_device
  - _device
- _diffn_measurement_axis.measurement_id
  - _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, _diffn_measurement.id has been added to the category key. The number of axes is given by the value of _diffn_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
  • _diffn_radiation.diffrn_id
    → _diffrn.id
    _diffrn_radiation.collision
    _diffrn_radiation.dif_x_source
    _diffrn_radiation.dif_y_source
    _diffrn_radiation.dif_x_y_source
    _diffrn_radiation.filter_edge
    _diffrn_radiation.inhomogeneity
    _diffrn_radiation.monochromator
    _diffrn_radiation.polarization_ratio
    _diffrn_radiation.polarization_source_norm
    _diffrn_radiation.polarization_source_ratio
    _diffrn_radiation.probe
    _diffrn_radiation.type
    _diffrn_radiation.wavelength
    _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/mmCIF dictionary adds the items _diffrn_radiation.dif_x_source, _diffrn_radiation.dif_y_source and _diffrn_radiation.dif_x_y_source to specify beam crossfire, and the items _diffrn_radiation.polarization_source_norm and _diffrn_radiation.polarization_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.dif_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.dif_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.dif_x_y_source is the correlation of the X and Y components. The value of the normal component of the polarization _diffrn_radiation.polarization_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.polarization_ratio is the ratio \((l_p - l_h) / (l_p + l_h)\), where \(l_i\) is the intensity (amplitude squared) of the electric vector of the illumination of the sample normal to the polarization and \(l_p\) 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_refln.frame_id
    → _diffrn_data_frame.id
  • _diffrn_refln.id
  • _diffrn_refln.diffrn_id
    → _diffrn_data_frame.id
    _diffrn_refln.chem
    _diffrn_refln.angle_chisq
    _diffrn_refln.angle_sumsq
    _diffrn_refln.angle_sumsq

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_refln.diffrn_id. The CBF/mmCIF dictionary extends the key with _diffrn_refln.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_data_frame.id
    _diffrn_scan.date
    _diffrn_scan.start
    _diffrn_scan.frame_id
    → _diffrn_data_frame.id
    _diffrn_scan.end
    _diffrn_scan.frame_id
    → _diffrn_data_frame.id
    _diffrn_scan.x
    _diffrn_scan.y
    _diffrn_scan.z
    _diffrn_scan.scan_style
    _diffrn_scan.scan_mode
    _diffrn_scan.angle_range
    _diffrn_scan.angle_increment
    _diffrn_scan.angle_increment
    _diffrn_scan.angle_increment
    _diffrn_scan.angle_increment
    _diffrn_scan.angle_increment
    _diffrn_scan.angle_increment

(b) DIFFRN_SCAN_AXIS
  • _diffrn_scan_axis.id
    → _diffrn_data_frame.id
    _diffrn_scan_axis.scan_id
    → _diffrn_scan.id
    _diffrn_scan_axis.angle
    _diffrn_scan_axis.angle_increment
    _diffrn_scan_axis.angle_increment
    _diffrn_scan_axis.angle_increment
    _diffrn_scan_axis.angle_increment
    _diffrn_scan_axis.angle_increment

(c) DIFFRN_SCAN_FRAME
  • _diffrn_scan_frame.id
    → _diffrn_data_frame.id
    _diffrn_scan_frame.data
    _diffrn_scan_frame.scan_id
    → _diffrn_scan.id
    _diffrn_scan_frame.frame_id
    _diffrn_scan_frame.integration_time

(d) DIFFRN_SCAN_FRAME_AXIS
  • _diffrn_scan_frame_axis.id
    → _diffrn_data_frame.id
    _diffrn_scan_frame_axis.id
    → _diffrn_data_frame.id
    _diffrn_scan_frame_axis.angle

3.7. CLASSIFICATION AND USE OF IMAGE DATA

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.data_start and _diffrn.data_end give the starting and ending time for a scan. The original definition of the yyyy-mm-dd date type, which includes date and time, has been extended in the CBF/igmCIF 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 _diffrn.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.data.frame.id) identifies the scan and the values of _diffrn.scan_axis.axis_id (a pointer to _axis.axis_id) associate particular axes with that scan. The steps of each axis are specified by _start, _range, _increment and _retrt_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 _retrt_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.data 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/igmCIF dictionary |
| Array elements refer to the section of this chapter in which each category is described in detail. |
| ARRAY.data_group | DIFFRN.detector.axis |
| ARRAY.data | DIFFRN.detector.axis | (3.7.4.20d) |
| ARRAY.element | DIFFRN.detector.axis | (3.7.4.20c) |
| ARRAY.intensities | DIFFRN.measurement | (3.7.4.36) |
| ARRAY.structure | DIFFRN.measurement | (3.7.4.36) |
| ARRAY.structure.list | DIFFRN.measurement | (3.7.4.36) |
| AXIS.group | DIFFRN.radiation | (3.7.4.4) |
| AXIS | DIFFRN.refln | (3.7.4.5) |
| DIFFRN.group | DIFFRN.scan | (3.7.4.56a) |
| DIFFRN.data.frame | DIFFRN.scan | (3.7.4.56a) |
| DIFFRN.detector | DIFFRN.scan | (3.7.4.56a) |

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 nonzero 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 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.axis_id). Together _diffrn.scan.frame.axis.frame_id and _axis.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_incr. and _angle_retrt_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_incr. and _displacement_retrt_incr. The integration begins at the setting given by the value of _diffrn.scan.frame.axis.angle or of _displacement. The _angle_incr 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 _angle_retrt_incr.

Appendix 3.7.1
Category structure of the CBF/igmCIF dictionary

Table A3.7.1.1 provides an overview of the structure of the CBF/igmCIF 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.

References

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This is version 1.3.2 of the image CIF dictionary (imgCIF) and crystallographic binary file dictionary (CBF) extending the macromolecular CIF dictionary (Chapter 4.5). Use of the dictionary is described in Chapter 3.7. See also Chapter 2.3 for a description of the CBF format and Chapter 5.6 for discussion of a software library for manipulating image data.

There are three category groups in this dictionary: array.data.array contains categories that describe array data; axis.group contains categories that describe axes; and diffraction.group contains categories that describe details of the diffraction experiment.

### ARRAY DATA

Data items in the ARRAY DATA category are the containers for the array data items described in the category ARRAY_STRUCTURE.

#### Category group(s):
- inclusive_group
- array.data.array_group
- array.data.array.id

#### Category key(s):
- array.data.array_id
- array.data.array.id

#### Example 1.

This example shows two binary data blocks. The first one was compressed by the CBF.CANONICAL compression algorithm and is presented as hexadecimal data. The first character ‘H’ on the data lines means hexadecimal. It could have been ‘O’ for octal or ‘D’ for decimal. The second character on the line shows the number of bytes in each word (in this case ‘2’), which then requires eight hexadecimal digits per word. The third character gives the order of octets within a word, in this case ‘>’ for the ordering 4321 (i.e. ‘big-endian’). Alternatively, the character ‘<’ could have been used for the ordering 1234 (i.e. ‘little-endian’). The block has a message digest to check the integrity of the data. The second block is similar, but uses CBF.PACKED compression and BASE64 encoding. Note that the size and the digest are different.

```plaintext
loop
  _array.data.array.id
  _array.data.array.id
  _array.data.array
  image_1

  --CIF-BINARY-FORMAT-SECTION--
  Content-Type: application/octet-stream;
  conversions="x-CBF-PACKED"
  Content-Transfer-Encoding: BASE64
  X-Binary-Size: 3745758
  X-Binary-ID: 2
  Content-MD5: 1aa33d606118b124+QbXw=

  .....
  --CIF-BINARY-FORMAT-SECTION---
```

#### `array.data.array_id` (code)

This item is a pointer to _array.structure.id in the ARRAY_STRUCTURE category.

```plaintext
[array_data]
```

(*) `array.data.binary_id` (int)

This item is an integer identifier which, along with `array.data.array_id`, should uniquely identify the particular block of array data. If `array.data.binary_id` is not explicitly given, it defaults to 1. The value of `array.data.binary_id` distinguishes among multiple sets of data with the same array structure. If the MIME header of the data array specifies a value for X-Binary-ID, the value of `array.data.array_id` should be equal to the value given for X-Binary-ID.

The following item(s) have an equivalent role in their respective categories:

```plaintext
  _diffraction.frame.binary_id
  _array.intensities.binary_id

  The permitted range is [1, \infty). Where no value is given, the assumed value is 1.'
```

(*) `array.data.data` (binary)

The value of `array.data.data` contains the array data encapsulated in a STAR string. The representation used is a variant on the Multipurpose Internet Mail Extensions (MIME) specified in RFC 2045-2049 by N. Freed et al. The boundary delimiter used in writing an imgCIF or CBF is `--CIF-BINARY-FORMAT-SECTION--` (including the required initial `--`). The Content-Type may be any of the discrete types permitted in RFC 2045; ‘application/octet-stream’ is recommended. If an octet stream was compressed, the compression should be specified by the parameter `conversions="x-CBF_PACKED"` or the parameter `conversions="x-CBF_CANONICAL"`. The Content-Transfer-Encoding may be ‘BASE64’, ‘Quoted-Printable’, ‘X-BASE8’, ‘X-BASE10’ or ‘X-BASE16’ for an imgCIF or ‘BINARY’ for a CBF. The octal, decimal and hexadecimal transfer encodings are for convenience and are not recommended for archiving and data interchange. In an imgCIF file, the encoded binary data begin after the empty line terminating the header. In a CBF, the raw binary data begin after an empty line terminating the header and after the sequence

### Octet Hexadecimal Decimal Purpose

<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0C</td>
<td>12</td>
<td>Ctrl-L: page break</td>
</tr>
<tr>
<td>1</td>
<td>1A</td>
<td>26</td>
<td>Ctrl-Z: stop listings, MS-DOS</td>
</tr>
<tr>
<td>2</td>
<td>04</td>
<td>04</td>
<td>Ctrl-D: stop listings, UNIX</td>
</tr>
<tr>
<td>3</td>
<td>03</td>
<td>213</td>
<td>binary section begins</td>
</tr>
</tbody>
</table>

None of these octets are included in the calculation of the message size or in the calculation of the message digest. The X-Binary-Size
header specifies the size of the equivalent binary data in octets. If compression was used, this size is the size after compression, including any book-keeping fields. An adjustment is made for the deprecated binary formats in which eight bytes of binary header are used for the compression type. In this case, the eight bytes used for the compression type are subtracted from the size, so that the same size will be reported if the compression type is supplied in the MIME header. Use of the MIME header is the recommended way to supply the compression type. In general, no portion of the binary header is included in the calculation of the size. The X-Binary-Element-Type header specifies the type of binary data in the octets, using the same descriptive phrases as in _array_structure.encoding_type_. The default value is 'unsigned 32-bit integer'. An MD5 message digest may, optionally, be used. The RSA Data Security, Inc. MDS Message-Digest Algorithm should be used. No portion of the header is included in the calculation of the message digest. If the Transfer Encoding is 'X-BASE8', 'X-BASE16' or 'X-BASE16', the data are presented as octal, decimal or hexadecimal data organized into lines or words. Each word is created by composing octets of data in fixed groups of 2, 3, 4, 6 or 8 octets, even in the order ..., 4321, 1234... ("big-endian") or 1234... ("little-endian"). If there are fewer than the specified number of octets to fill the last word, then the missing octets are presented as '*-' for each missing octet. Exactly two equal signs are used for each missing octet even for octal and decimal encoding. The format of lines is

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**ARRAY_INTENSITIES**

The estimated standard deviation in detector ‘gain’. The permitted range is [0.0, ∞).

Related item: _array_intensities.gain (associated esd)

**array_intensities.linearity**

The intensity linearity scaling method used to convert from the raw intensity to the stored element value. ‘linear’ is linear. ‘offset’ means that the value defined by _array_intensities.offset should be added to each element value. ‘scaling’ means that the value defined by _array_intensities.scaling should be multiplied with each element value. ‘scaling-offset’ is the combination of the two previous cases, with the scale factor applied before the offset value. ‘sqrt.scaled’ means that the square root of raw intensities multiplied by _array_intensities.scaling is calculated and stored, perhaps rounded to the nearest integer. Thus, linearization involves dividing the stored values by _array_intensities.scaling and squaring the result. ‘logarithmic.scaled’ means that the logarithm base 10 of raw intensities multiplied by _array_intensities.scaling is calculated and stored, perhaps rounded to the nearest integer. Thus, linearization involves dividing the stored values by _array_intensities.scaling and squaring the result.

**array_intensities.offset**

The value defined by _array_intensities.offset should be added to each element value.

**array_intensities.scaling**

The value defined by _array_intensities.scaling should be multiplied with each element value.

**array_intensities.scaling.offset**

The combination of scaling and offset with the scale factor applied before the offset value.

**sqrt.scaled**

The square root of raw intensities multiplied by _array_intensities.scaling is calculated and stored, perhaps rounded to the nearest integer. Thus, linearization involves dividing the stored values by _array_intensities.scaling and squaring the result.

**logarithmic.scaled**

The logarithm base 10 of raw intensities multiplied by _array_intensities.scaling is calculated and stored, perhaps rounded to the nearest integer. Thus, linearization involves dividing the stored values by _array_intensities.scaling and squaring 10 to the power of this number.

**raw**

The array consists of raw values to which no corrections have been applied. While the handling of the data is similar to that given for ‘linear’ data with no offset, the meaning of the data differs in that the number of incident photons is not necessarily linearly related to the number of counts reported. This value is intended for use either in calibration experiments or to allow for handling more complex data-fitting algorithms than are allowed for by this data item.

**array_intensities.offset**

Offset value to add to array element values in the manner described by the item _array_intensities.linearity.

**array_intensities.overload**

The saturation intensity level for this data array.

**array_intensities.scaling**

Multiplicative scaling value to be applied to array data in the manner described by item _array_intensities.linearity.

**array_intensities.undefined_value**

A value to be substituted for undefined values in the data array.

**array_structure**

Data items in the ARRAY_STRUCTURE category record the organization and encoding of array data in the ARRAY_DATA category.

<table>
<thead>
<tr>
<th>Category group(s)</th>
<th>inclusive group</th>
<th>array_data_group</th>
</tr>
</thead>
<tbody>
<tr>
<td>array_structure.id</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**array_structure.byte_order**

The order of bytes for integer values which require more than 1 byte. (IBM PCs and compatibles, and DEC VAXs use low-byte-first ordered integers, whereas Hewlett Packard 700 series, Sun-4 and Silicon Graphics use high-byte-first ordered integers. Dec Alphas can produce/use either depending on a compiler switch.)

<table>
<thead>
<tr>
<th>Data value must be one of the following:</th>
</tr>
</thead>
<tbody>
<tr>
<td>big_endian</td>
</tr>
<tr>
<td>little_endian</td>
</tr>
</tbody>
</table>

**array_structure.compression_type**

Type of data-compression method used to compress the array data.

<table>
<thead>
<tr>
<th>Data value must be one of the following:</th>
</tr>
</thead>
<tbody>
<tr>
<td>none</td>
</tr>
<tr>
<td>packed</td>
</tr>
<tr>
<td>canonical</td>
</tr>
</tbody>
</table>

Where no value is given, the assumed value is ‘none’.

**array_structure.encoding_type**

Data encoding of a single element of array data. In several cases, the IEEE format is referenced. See IEEE Standard 754-1985 (IEEE, 1985).


The data value must be one of the following:

<table>
<thead>
<tr>
<th>Data value must be one of the following:</th>
</tr>
</thead>
<tbody>
<tr>
<td>‘signed 8-bit integer’</td>
</tr>
<tr>
<td>‘signed 16-bit integer’</td>
</tr>
<tr>
<td>‘signed 32-bit integer’</td>
</tr>
<tr>
<td>‘signed 32-bit integer’</td>
</tr>
<tr>
<td>‘signed 32-bit real IEEE’</td>
</tr>
<tr>
<td>‘signed 64-bit real IEEE’</td>
</tr>
<tr>
<td>‘signed 32-bit complex IEEE’</td>
</tr>
</tbody>
</table>

**array_structure.id**

The value of _array_structure.id must uniquely identify each item of array data.

The following item(s) have an equivalent role in their respective categories:

<table>
<thead>
<tr>
<th>Category group(s)</th>
<th>inclusive group</th>
<th>array_data_group</th>
</tr>
</thead>
<tbody>
<tr>
<td>_array_data.array_id</td>
<td></td>
<td></td>
</tr>
<tr>
<td>_array_structure_list.array_id</td>
<td></td>
<td></td>
</tr>
<tr>
<td>_array_intensities.array_id</td>
<td></td>
<td></td>
</tr>
<tr>
<td>_diffmainframe.array_id</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

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**ARRAY_STRUCTURE_LIST**

Data items in the **ARRAY_STRUCTURE_LIST** category record the size and organization of each array dimension. The relationship to physical axes may be given.

- **Category group(s):** inclusive_group
- **Category key(s):** array_structure_list.array_id

*array_structure_list.axis_set_id*  
This is a descriptor for the physical axis or set of axes corresponding to an array index. This data item is related to the axes of the detector itself given in **DIFFRN_DETECTOR_AXIS**, but usually differs in that the axes in this category are the axes of the coordinate system of reported data points, while the axes in **DIFFRN_DETECTOR_AXIS** are the physical axes of the detector describing the 'poise' of the detector as an overall physical object. If there is only one axis in the set, the identifier of that axis should be used as the identifier of the set.

The following items have an equivalent role in their respective categories:
- **array_structure_list.axis_set_id**: [array_structure_list]
  
*array_structure_list.dimension*  
The number of elements stored in the array structure in this dimension.

The permitted range is [1, ∞).  
[array_structure_list]

*array_structure_list.direction*  
Identifies the direction in which this array index changes.

The data value must be one of the following:
- **increasing**: Indicates the index changes from 1 to the maximum dimension.
- **decreasing**: Indicates the index changes from the maximum dimension to 1.  
[array_structure_list]

*array_structure_list.index*  
Identifies the one-based index of the row or column in the array structure.

The following items have an equivalent role in their respective categories:
- **element informatie**: [array_structure_list]

The permitted range is [1, ∞).  
[array_structure_list]

*array_structure_list.precedence*  
Identifies the rank order in which this array index changes with respect to other array indices. The precedence of 1 indicates the index which changes fastest.

The permitted range is [1, ∞).  
[array_structure_list]
When specifying detector axes, the axis is given to the beam centre. The location of the beam centre on the detector should be given in the DIFFR._DETECTOR category in distortion-corrected millimetres from the (0,0) corner of the detector. It should be noted that many different origins arise in the definition of an experiment. In particular, as noted above, it is necessary 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.


Example 1.
This example shows the axis specification of the axes of a kappa-geometry goniometer (see Stout, G. H. & Jensen, L. H. (1989). X-ray structure determination. A practical guide, 2nd ed. p. 134. New York: Wiley InterScience). There are three axes specified, and no offsets. The outermost axis, omega, is pointed along the X axis. The next innermost axis, kappa, is at a 50° angle to the X axis, pointed away from the source. The innermost axis, phi, aligns with the Y axis when omega and phi are at their zero points. If T00, T01, and T02 are the transformation matrices derived from the axis settings, the complete transformation would be S = T00 T01 T02.

```
loop
  _axis.id
  _axis.type
  _axis.equipment
  _axis.depends_on
  omega rotation goniometer . 1 0 0
  kappa rotation goniometer omega -.64279 0 -.76604
  phi rotation goniometer kappa 1 0 0
```

Example 2.
This example shows the axis specification of the axes of a detector, source and gravity. The order has been changed as a reminder that the ordering of presentation of tokens is not significant. The centre of rotation of the detector has been taken to be 68 mm in the direction away from the source.

```
loop
  _axis.id
  _axis.type
  _axis.equipment
  _axis.depends_on
  source . source . 0 0 1 . .
  gravity . gravity . 0 -1 0 .
  trans translation detector rots 0 0 1 0 0 -68
  twtheta rotation detector . 1 0 0 .
  roty rotation detector twtheta 0 1 0 0 0 -68
  rots rotation detector roty 0 1 0 0 0 -68
```

The value of _axis.depends_on specifies the next outermost axis upon which this axis depends. This item is a pointer to _axis.id in the same category.

```
_axis.equipment
```

The value of _axis.equipment specifies the type of equipment using the axis: 'goniometer', 'detector', 'gravity', 'source' or 'general'.

The data value must be one of the following:

- goniometer: equipment used to orient or position samples
- detector: equipment used to detect reflections
- general: equipment used for general purposes
- gravity: axis specifying the downward direction
- source: axis specifying the direction sample to source

Where no value is given, the assumed value is 'general'.

---

Axis 1 (X): The X axis is aligned to the mechanical axis pointing from the sample or specimen along the principal axis of the goniometer. Axis 2 (Y): The Y axis completes an orthogonal right-handed system defined by the X axis and the Z axis (see below). Axis 3 (Z): The Z axis is derived from the source axis which goes from the sample to the source. The Z axis is the component of the source axis in the direction of the source orthogonal to the X axis in the plane defined by the X axis and the source axis. 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 (Leslie & Powell, 2004). In MOSFLM, X is along the X-ray beam (the CBF/imgCIF 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 goniometer axis the direction of which 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.
**DIFFRN.DATASET**

Data items in the `DIFFRN.DATASET` category describe the detector used to measure the scattered radiation, including any analyser and post-sample collimation. The following item(s) have an equivalent role in their respective categories:

```plaintext
*diffn_detector

**diffn_detector.detector_element_id**
**diffn_detector.detector_element_id**
  
*diffn_detector.detector_details
  (**text**)  
  *diffn_detector.details*(cif:core.dic 2.0.1)

Example 1 - based on PDB entry SHVP and laboratory records for the structure corresponding to PDB entry SHVP:

- `diffn_detector.detector_id`
- `diffn_detector.detector_id`
- `diffn_detector.type` 'Siemens'

A description of special aspects of the radiation detector.

Example: 'slow mode'.

**DIFFRN.DATASET**
4. DATA DICTIONARIES

**DIFFRN.DETECTOR**

*diffn_detector.detector* (text)

The general class of the radiation detector.

Example: 'photographic film', 'scintillation counter', 'CCD plate', 'BF-2 counter'.

*diffn_detector.diffn_detector* (code)

This data item is a pointer to *diffn_detector_id* in the DIFFRN category. The value of *diffn_detector_id* uniquely defines a set of diffraction data.

*diffn_detector.timer* (foot)

The deadtime in microseconds of the detector(s) used to measure the diffraction intensities. The permitted range is [0, ∞).

*diffn_detector.id* (code)

The value of *diffn_detector_id* must uniquely identify each detector used to collect each diffraction data set. If the value of *diffn_detector_id* is not given, it is implicitly equal to the value of _diffn_detector_diffn_detector_id_.

The following items have an equivalent role in their respective categories:

*diffn_detector_number_of_axes* (int)

The value of *diffn_detector_number_of_axes* gives the number of axes of the positioner for the detector identified by *diffn_detector_id*. The word 'positioner' is a general term used in instrumentation design for devices that are used to change the positions of portions of apparatus by linear translation, rotation, or combinations of such motions. Axes which are used to provide a coordinate system for the face of an area detector should not be counted for this data item. The description of each axis should be provided by entries in DIFFRN_D boxing.

The permitted range is [1, ∞).

*diffn_detector.type* (text)

The make, model or name of the detector device used.

**DIFFRN.DETECTOR_AXIS**

Data items in the DIFFRN_D category are associated with detectors.

Category groups: inclusive group

diffn_detector

Category key(s): _diffn_detector_axis.detector_id

*diffn_detector_axis.axis_id* (code)

This data item is a pointer to *axis_id* in the AXIS category.

*diffn_detector_axis.detector_id* (code)

This data item is a pointer to *detector_id* in the DIFFRN.DETECTOR category. This item was previously named _diffn_detector_axis.detector_id_, which is now deprecated. The old name is provided as an alias but should not be used for new work.

*diffn_detector_axis.id* (code)

This data item is a pointer to *detector_id* in the DIFFRN.DETECTOR category. Deprecated: do not use.

**DIFFRN.DETECTOR_ELEMENT**

Data items in the DIFFRN.DETECTOR_ELEMENT category record the details about spatial layout and other characteristics of each element of a detector which may have multiple elements. In most cases, giving more detailed information in ARRAY_STRUCTURE_LIST and ARRAY_STRUCTURE_LIST_AXIS is preferable to simply providing the centre of the detector element.

Category group(s): inclusive group

<table>
<thead>
<tr>
<th>Category key(s)</th>
<th>_diffn_detector_element.detector_id</th>
<th>_diffn_detector_element.detector_id</th>
</tr>
</thead>
</table>

Example 1

Detector 1 is composed of four CCD detector elements, each 200 by 200 mm, arranged in a square, in the pattern

1 2
3 4

Note that the beam centre is slightly displaced from each of the detector elements, just beyond the lower right corner of 1, the lower left corner of 2, the upper right corner of 3 and the upper left corner of 4.

loop

<table>
<thead>
<tr>
<th>_diffn_detector_element.detector_id</th>
<th>_diffn_detector_element.detector_id</th>
</tr>
</thead>
<tbody>
<tr>
<td>d1 d1 ccd_1 201.5 1.5</td>
<td></td>
</tr>
<tr>
<td>d1 d1 ccd_2 201.1 1.5</td>
<td></td>
</tr>
<tr>
<td>d1 d1 ccd_3 201.6 1.5</td>
<td></td>
</tr>
<tr>
<td>d1 d1 ccd_4 201.5 1.5</td>
<td></td>
</tr>
</tbody>
</table>

*diffn_detector_element.center[1]* (foot)

The value of _diffn_detector_element.center[1]_ is the X component of the distortion-corrected beam centre in millimetres from the (0, 0) (lower-left) corner of the detector element viewed from the sample side. The X and Y axes are the laboratory coordinate system coordinates defined in the AXIS category measured when all positioning axes for the detector are at their zero settings.

If the resulting X or Y axis is then orthogonal to the detector, the Z axis is used instead of the orthogonal axis.

Where no value is given, the assumed value is '0.0'.

*diffn_detector_element* (code)

*diffn_detector_element.center[2]* (foot)

The value of _diffn_detector_element.center[2]_ is the Y component of the distortion-corrected beam centre in millimetres from the (0, 0) (lower-left) corner of the detector element viewed from the sample side. The X and Y axes are the laboratory coordinate system coordinates defined in the AXIS category measured when all positioning axes for the detector are at their zero settings.

If the resulting X or Y axis is then orthogonal to the detector, the Z axis is used instead of the orthogonal axis.

Where no value is given, the assumed value is '0.0'.

*diffn_detector_element* (code)

*diffn_detector_element.detector_id* (code)

This data item is a pointer to _diffn_detector_id_ in the DIFFRN.DETECTOR category.

*diffn_detector_element* (code)

The value of _diffn_detector_element_id_ must uniquely identify each element of a detector.
DIFFRNX.FRAME.DATA

Data items in the DIFFRNX.FRAME.DATA category record the details about each frame of data. The items in this category are now in the DIFFRNX.FRAME_DATA category. The items in the DIFFRNX.FRAME_DATA category are now deprecated. The items from this category are provided as aliases in version 1.0 of the dictionary but should not be used for new work. The items from the old category are provided in this dictionary for completeness, but should not be used or cited. To avoid confusion, the example has been removed and the redundant parent-child links to other categories have been removed.

Category group(s): inclusive group
array_data_group
  category(key(s)): DIFFRNX.FRAME_DATA

THE DIFFRNX.FRAME.DATA category is deprecated and should not be used.

*/

* diffrnx_frame_data.array_id

This item is a pointer to _array_structure_id in the ARRAY_STRUCTURE category. Deprecated: do not use.

* diffrnx_frame_data.binary_id

This item is a pointer to _array_data.binary_id in the ARRAY_STRUCTURE category. Deprecated: do not use.

* diffrnx_frame_data.detector_element_id

This item is a pointer to _diffrnx_detector_element_id in the DIFFRNX_DETECTOR_ELEMENT category. Deprecated: do not use.

* diffrnx_frame_data.data_id

The value of _diffrnx_frame_data.data_id must uniquely identify each complete frame of data. Deprecated: do not use.

DIFFRNX.MEASUREMENT

Data items in the DIFFRNX.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.

Category group(s): inclusive group
diffrnx_group
category(key(s)): DIFFRNX.MEASUREMENT device

Example 1 - based on PDB entry 5HPV and laboratory records for the structure corresponding to PDB entry 5HPV

* diffrnx_measurement.diffrnx_id


*/

- diffrnx_measurement.data_id

The value of _diffrnx_measurement.data_id must uniquely identify the set of mechanical characteristics of the device used to orient and/or position the sample used during the collection of each diffraction data set. If the value of _diffrnx_measurement.data_id is not given, it is implicitly equal to the value of _diffrnx_measurement.diffrnx_id. Either _diffrnx_measurement.device or _diffrnx_measurement.id may be used to link to other categories. If the experimental setup admits multiple devices, then _diffrnx_measurement.id is used to provide a unique link.

The following item(s) have an equivalent role in their respective categories:

- _diffrnx_measurement.device

Method used to measure intensities.

Example: 'profile data from theta/2theta \(\langle q/2\rangle\) scans'.

*/

- diffrnx_measurement.number_of_axes

The value of _diffrnx_measurement.number_of_axes gives the number of axes of the positioner for the goniometer or other sample orientation or positioning device identified by _diffrnx_measurement.id. The description of the axes should be provided by entries in DIFFRNX.MEASUREMENT_AXIS.

The permitted range is \([1, \infty)\).

*/
**DIFFRN. MEASUREMENT**

Data items in the **DIFFRN. MEASUREMENT** category associate axes with axes devices.

**Category group(s):** inclusive group

**Category key(s):**

- `diffn_measurement specimen support`
- `diffn_measurement specimen support (cif.core.doc 2.0.1)`
- `DIFFRN MEASUREMENT AXIS`
- `DIFFRN.Radiation`

---

**DIFFRN. MEASUREMENT AXIS**

Data items in the **DIFFRN. MEASUREMENT AXIS** category associate axes with axes devices.

**Category group(s):** inclusive group

**Category key(s):**

- `diffn_measurement_axis axis id`
- `diffn_measurement_axis id`
- `diffn_measurement_axis measurement_device`
- `DIFFRN MEASUREMENT AXIS AXIS ID`
- `DIFFRN MEASUREMENT AXIS MEASUREMENT ID`
- `DIFFRN MEASUREMENT AXIS AXIS ID`

---

**DIFFRN.RADIATION**

Data items in the **DIFFRN. RADIATION** category describe the radiation used for measuring diffraction intensities, its collimation and monochromatization before the sample. Post-sample treatment of the beam is described by data items in the **DIFFRN. DETECTOR** category.

**Category group(s):** inclusive group

**Category key(s):**

- `diffn.radiation.diffn id`
- `diffn.radiation.collimation`
- `diffn.radiation.monochromator`
- `diffn.radiation.type`
- `diffn.radiation.wavelength id`
- `diffn.radiation.linear`
- `diffn.radiation.linear_type`
- `DIFFRN. RADIATION DIFFN ID`
- `DIFFRN. RADIATION COLLIMATION`
- `DIFFRN. RADIATION MONOCHROMATOR`
- `DIFFRN. RADIATION POLARISATION`
- `DIFFRN. RADIATION POLARISATION NORM`

---

**diffn.radiation.div_x_source**

Beam crossfire in degrees parallel to the laboratory X axis (see **AXIS** category). This is a characteristic of the X-ray beam as it illuminates the sample (or specimen) after all monochromation and collimation. This is the standard uncertainty (s.d.) of the directions of photons in the **XZ** plane around the mean source beam direction. Note that for some synchrotrons this value is specified in milli-radians, in which case a conversion is needed. To convert a value in milli-radians to a value in degrees, multiply by 0.180 and divide by π.

**diffn.radiation.div_y_source**

Beam crossfire in degrees parallel to the laboratory **Y** axis (see **AXIS** category). This is a characteristic of the X-ray beam as it illuminates the sample (or specimen) after all monochromation and collimation. This is the standard uncertainty (s.d.) of the directions of photons in the **YZ** plane around the mean source beam direction. Note that for some synchrotrons this value is specified in milli-radians, in which case a conversion is needed. To convert a value in milli-radians to a value in degrees, multiply by 0.180 and divide by π.

---

**diffn.radiation.filter_edge**

Absorption edge in ångströms of the radiation filter used.

**diffn.radiation.inhomogeneity**

Half-width in millimetres of the incident beam in the direction perpendicular to the diffraction plane.

**diffn.radiation.monochromator**

The method used to obtain monochromatic radiation. If a monochromator crystal is used, the material and the indices of the Bragg reflection are specified.

---

The physical device used to support the crystal during data collection.

Examples: 'glass capillary', 'quartz capillary', 'fiber', 'metal loop'.

This data item is a pointer to **axis.id** in the **AXIS** category.

This data item is a pointer to **diffn.measurement.id** in the **DIFFRN. MEASUREMENT** category. Deprecated: do not use.

This data item is a pointer to **diffn.measurement.device id** in the **DIFFRN. MEASUREMENT** category.
**diffrn_radiation.wavelength_id**

This data item is a pointer to **diffrn_radiation_wavelength_id** in the **DIFFRN_RADIATION_WAVELENGTH** category.

**diffrn_radiation.xray_symbol**

The IUPAC symbol for the X-ray wavelength for the probe radiation.

The data value must be one of the following:
- K-<i>L</i>"<sup>1</sup>
- K-<i>L</i>"<sup>2</sup>
- K-<i>M</i>"<sup>3</sup>

where K-<i>L</i> is used where K-<i>L</i> and K-<i>L</i>-2 are not resolved.

**DIFFRN.REFLN**

This category redefinition has been added to extend the key of the standard **DIFFRN.REFLN** category.

**DIFFRN_SCAN**

Data items in the **DIFFRN_SCAN** category describe the parameters of one or more scans, relating axis positions to frames.

**Example 1 – derived from a suggestion by R. M. Sweet.**

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. In this example, three rotation axes and one translation axis at nonzero values are specified, with one axis stepping. There is no reason why more axes could not have been specified to step. Range information has been specified, but note that it can be calculated from the number of frames and the increment, so the data item **diffrn_scan_axis.angle_range** could be dropped. Both the sweep data and the data for a single frame are specified. Note that the information on how the axes are stepped is given twice, once in terms of the overall averages in the value of **diffrn_scan.integration_time** and the values for **DIFFRN_SCAN.AXIS**. If dose-related adjustments are made to scan times and nonlinear stepping is done, these values may differ. Therefore, in interpreting the data for a particular frame it is important to use the frame-specific data.
Example 2 — a more extensive example (R. M. Sweet, P. J. Ellis & H. J. Bernstein).
A detector is placed 240 mm along the Z axis from the goniometer. This leads to a choice: either the axes of the detector are defined at the origin, and then a Z setting of −240 is entered, or the axes are defined with the necessary Z offset. In this case, the setting is used and the offset is left as zero. This axis is called DETECTOR.Z. The axis for positioning the detector in the Y direction depends on the detector Z axis. This axis is called DETECTOR.Y. The axis for positioning the detector in the X direction depends on the detector Y axis (and therefore on the detector Z axis). This axis is called DETECTOR.X. The detector may be rotated around the Y axis. This rotation axis depends on the three translation axes. It is called DETECTOR.PITCH. A coordinate system is defined on the face of the detector in terms of 1100.0100 mm pixels in each direction. The ELEMENT.X axis is used to index the first array index of the data array and the ELEMENT.Y axis is used to index the second array index. Because the pixels are 0.150 x 0.150 mm, the centre of the first pixel is at (0.075, 0.075) in this coordinate system.

```plaintext
# category DIFFRN_DATAFRAME
loop_
  .diffn_dataframe.datafile_id
  .diffn_dataframe.datafile_id
  .diffn_dataframe.datafile_id
  .diffn_dataframe.datafile_id

# category DIFFRN_SOURCE
loop_
  .diffn_source.id
  .diffn_source.id
  .diffn_source.id
  .diffn_source.id

# category DIFFRN_RADIATION
loop_
  .diffn_radiation.detector_id
  .diffn_radiation.detector_id
  .diffn_radiation.detector_id
  .diffn_radiation.detector_id

# category DIFFRN_OUTER
loop_
  .diffn_outer.detector_id
  .diffn_outer.detector_id
  .diffn_outer.detector_id
  .diffn_outer.detector_id

# category DIFFRN_POWDER
loop_
  .diffn_powder.detector_id
  .diffn_powder.detector_id
  .diffn_powder.detector_id
  .diffn_powder.detector_id

# category DIFFRN_POINT
loop_
  .diffn_point.detector_id
  .diffn_point.detector_id
  .diffn_point.detector_id
  .diffn_point.detector_id
```

```
# category DIFFRN_TEMPERATURE
loop_
  .diffn_temperature.detector_id
  .diffn_temperature.detector_id
  .diffn_temperature.detector_id
  .diffn_temperature.detector_id

# category DIFFRN_FRAME
loop_
  .diffn_frame.detector_id
  .diffn_frame.detector_id
  .diffn_frame.detector_id
  .diffn_frame.detector_id
```

```
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```
Example 3—Example 2 revised for a spiral scan (R. M. Sweet, P. J. Ellis & H. J. Hermuth).
A detector is placed 240 mm along the Z-axis from the goniometer, as in Example 2 above, but in this example the image plane is scanned in a spiral pattern from the outside in. The axis for positioning the detector in the Y direction depends on the detector Z-axis. This axis is called detector Y. The axis for positioning the detector in the X direction depends on the detector Y-axis and (therefore on the detector Z-axis). This axis is called detector X. This detector may be raised around the Y-axis. This rotation axis depends on the three translation axes. It is called detector PITCH. A coordinate system is defined on the face of the detector in terms of a coupled rotation axis and radial scan axis to form a spiral scan. The rotation axis is called ELEMENT, ROT and the radial axis is called ELEMENT, RAD.

A 150 μm radial pitch and a 75 μm 'constant velocity' angular pitch are assumed. Indexing is carried out first on the rotation axis and the radial axis is made to be dependent on it. The two axes are coupled to form an axis set ELEMENT, SPIRAL.

---

# CIF: VERSION 1.1

data_image_1

# category DIFFRN
._diffn.id: PHFB
._diffn.crystal_id: PHFB_CRYSTAL7

# category DIFFRN_SOURCE
.loop
._diffn_source.diffn_id
._diffn_source.source
._diffn_source.type

# category DIFFRN_RADIATION
.loop
._diffn_radiation.diffn_id
._diffn_radiation.wavelength_id

# category DIFFRN_RADIATION_WAVELENGTH
.loop
._diffn_radiation.wavelength_id

# category DIFFRN_DETECTOR
.loop
._diffn_detector.diffn_id
._diffn_detector.type
._diffn_detector.number_of_axes

# category DIFFRN_DETECTOR_AXIS
.loop
._diffn_detector_axis.diffn_id
._diffn_detector_axis.axis_id

# category DIFFRN_DETECTOR_ELEMENT
.loop
._diffn_detector_element.diffn_id

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# category DIFFRN_DATA_FRAME

# category DIFFRN_MEASUREMENT

# category DIFFRN_MEASUREMENT_AXIS

# category DIFFRN_SCAN

# category DIFFRN_SCAN_AXIS

# category DIFFRN_SCAN_FRAME

# category AXIS

# category ARRAY_STRUCTURE_LIST

# category ARRAY_STRUCTURE_LIST_AXIS

# category ARRAY_ELEMENT_SIZE

# category ARRAY_INTENSITIES

# category ARRAY_STRUCTURE

# category ARRAY_DATA

# --CIF-BINARY-FORMAT-SECTION--

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X-Binary-Element-Type: "signed 32-bit integer"

X-Binary-Size: 000100

X-Binary-Endian: "little endian"
4.6. IMAGE DICTIONARY (imgCIF)

DIFFRN.SCAN.AXIS

- **diffn_scan.date_end** (yyy-mm-dd)
The date and time of the end of the scan. Note that this may be an estimate generated during the scan, before the precise time of the end of the scan is known.

- **diffn_scan.date_start** (yyy-mm-dd)
The date and time of the start of the scan.

- **diffn_scan.frame_id_end** (code)
The value of this data item is the identifier of the last frame in the scan. This item is a pointer to `diffn_data_frame.id` in the DIFFRN_DATA_FRAME category.

- **diffn_scan.frame_id_start** (code)
The value of this data item is the identifier of the first frame in the scan. This item is a pointer to `diffn_data_frame.id` in the DIFFRN_DATA_FRAME category.

- **diffn_scan.frames** (int)
The value of this data item is the number of frames in the scan. The permitted range is $[1, \infty)$.

- **diffn.scan.id** (code)
The value of _diffn_scan.id uniquely identifies each scan. The identifier is used to tie together all the information about the scan.

The following item(s) have an equivalent role in their respective categories:
- _diffn_scan_axis.scan_id
- _diffn_scan_frame.scan_id

- **diffn_scan.integration_time** (float)
Approximate average time in seconds to integrate each step of the scan. The precise time for integration of each particular step must be provided in _diffn_scan_frame.integration_time, even if all steps have the same integration time. The permitted range is $[0.0, \infty)$.

DIFFRN.SCAN.AXIS

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.

- Category group: inclusive_group
  - **diffn.group**
  - Category key(s): _diffn_scan_axis.scan_id, _diffn_scan_axis.axis_id

- **diffn_scan_axis.angle_increment** (float)
The increment for each step for the specified axis in degrees. In general, this will agree with _diffn_scan_frame_axis.angle_increment. The sum of the values of _diffn_scan_frame_axis.angle and _diffn_scan_frame_axis.angle_increment is the angular setting of the axis at the end of the integration time for a given frame. If the individual frame values vary, then the value of _diffn_scan_axis.angle_increment will be representative of the ensemble of values of _diffn_scan_frame_axis.angle_increment (e.g. the mean).

  Where no value is given, the assumed value is '0.0'.

DIFFRN.SCAN.AXIS

- **diffn_scan_axis.angle_range** (float)
The range from the starting position for the specified axis in degrees.

  Where no value is given, the assumed value is '0.0'.

- **diffn_scan_axis.angle_rstrt_incr** (float)
The increment after each step for the specified axis in degrees. In general, this will agree with _diffn_scan_frame_axis.angle_rstrt_incr. The sum of the values of _diffn_scan_frame_axis.angle, _diffn_scan_frame_axis.angle_increment and _diffn_scan_frame_axis.angle_rstrt_incr is the angular setting of the axis at the start of the integration time for the next frame relative to a given frame and should equal _diffn_scan_frame_axis.angle for this next frame. If the individual frame values vary, then the value of _diffn_scan_axis.angle_rstrt_incr will be representative of the ensemble of values of _diffn_scan_frame_axis.angle_rstrt_incr (e.g. the mean).

  Where no value is given, the assumed value is '0.0'.

- **diffn_scan_axis.angle_start** (float)
The starting position for the specified axis in degrees.

  Where no value is given, the assumed value is '0.0'.

- **diffn_scan_axis.axis_id** (code)
The value of this data item is the identifier of one of the axes for the scan for which settings are being specified. Multiple axes may be specified for the same value of _diffn_scan.id. This item is a pointer to _axis_id in the AXIS category.

DIFFRN.SCAN.AXIS

- **diffn_scan_axis.displacement_increment** (float)
The increment for each step for the specified axis in millimetres. In general, this will agree with _diffn_scan_frame_axis.displacement_increment. The sum of the values of _diffn_scan_frame_axis.displacement and _diffn_scan_frame_axis.displacement_increment is the angular setting of the axis at the end of the integration time for a given frame. If the individual frame values vary, then the value of _diffn_scan_axis.displacement_increment will be representative of the ensemble of values of _diffn_scan_frame_axis.displacement_increment (e.g. the mean).

  Where no value is given, the assumed value is '0.0'.

- **diffn_scan_axis.displacement_range** (float)
The range from the starting position for the specified axis in millimetres.

  Where no value is given, the assumed value is '0.0'.

- **diffn_scan_axis.displacement_rstrt_incr** (float)
The increment for each step for the specified axis in millimetres. In general, this will agree with _diffn_scan_frame_axis.displacement_rstrt_incr. The sum of the values of _diffn_scan_frame_axis.displacement, _diffn_scan_frame_axis.displacement_increment and _diffn_scan_frame_axis.displacement_rstrt_incr is the angular setting of the axis at the start of the integration time for the next frame relative to a given frame and should equal _diffn_scan_frame_axis.displacement for this next frame. If the individual frame values vary, then the value of _diffn_scan_axis.displacement_rstrt_incr will be representative of the ensemble of values of _diffn_scan_frame_axis.displacement_rstrt_incr (e.g. the mean).

  Where no value is given, the assumed value is '0.0'.
DIFFRN_SCAN_AXIS

4. DATA DICTIONARIES

diffn_axis_start

The starting position for the specified axis in millimetres.
Where no value is given, the assumed value is 0.0.

* diffn_axis.scan_id

The value of this data item is the identifier of the scan for which axis settings are being specified. Multiple axes may be specified for the same value of diffn_axis.scan_id. This item is a pointer to _diffn_axis in the DIFFRN_SCAN category.

DIFFRN.Scan.FRAME

Data items in the DIFFRN_SCAN_FRAME category describe the relationships of particular frames to scans.
Category group: Inclusive_group
_diffn_frame
Category key: _diffn_frame.frame_id

_diffn_frame.date

The date and time of the start of the frame being scanned.

* diffn_frame.frame_id

The value of this data item is the identifier of the frame being examined. This item is a pointer to _diffn_data_frame.id in the DIFFRN_DATA_FRAME category.

_diffn_frame.frame_number

The value of this data item is the number of the frame within the scan, starting with 1. It is not necessarily the same as the value of _diffn_frame.frame_id, but it may be.
The permuted range is [0, oo).

* diffn_frame.integration_time

The time in seconds to integrate this step of the scan. This should be the precise time of integration of each particular frame. The value of this data item should be given explicitly for each frame and not inferred from the value of _diffn_scan.integration_time.
The permuted range is [0.0, oo).

* diffn_frame.scan_id

The value of _diffn_frame.scan_id identifies the scan containing this frame. This item is a pointer to _diffn_scan.frame_id in the DIFFRN_SCAN category.

DIFFRN.Scan.FRAME_AXIS

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, nonzero 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.
Category group: Inclusive_group
_diffn_axis
Category key: _diffn_axis.frame_id

_diffn_axis.axis

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The setting of the specified axis in degrees for this frame. This is the setting at the start of the integration time.
Where no value is given, the assumed value is 0.0.

* diffn_axis.angle

The increment for this frame for the angular setting of the specified axis in degrees. The sum of the values of _diffn_axis.angle and _diffn_axis.angle_increment is the angular setting of the axis at the start of the integration time for the next frame and should equal _diffn_axis.angle for this next frame.
Where no value is given, the assumed value is 0.0.

* diffn_axis.axis_id

The value of this data item is the identifier of one of the axes for the frame for which settings are being specified. Multiple axes may be specified for the same value of _diffn_axis.frame_id. This item is a pointer to _axis_id in the AXIS category.

* diffn_axis.displacement

The setting of the specified axis in millimetres for this frame. This is the setting at the start of the integration time.
Where no value is given, the assumed value is 0.0.

* diffn_axis.displacement_increment

The increment for this frame for the displacement setting of the specified axis in millimetres. The sum of the values of _diffn_axis.displacement and _diffn_axis.displacement_increment is the angular setting of the axis at the end of the integration time for this frame.
Where no value is given, the assumed value is 0.0.

* diffn_axis.displacement_rstrt_incr

The increment for this frame for the displacement setting of the specified axis in millimetres. The sum of the values of _diffn_axis.displacement, _diffn_axis.displacement_increment and _diffn_axis.displacement_rstrt_incr is the angular setting of the axis at the start of the integration time for the next frame and should equal _diffn_axis.displacement for this next frame.
Where no value is given, the assumed value is 0.0.

* diffn_axis.frame_id

The value of this data item is the identifier of the frame for which axis settings are being specified. Multiple axes may be specified for the same value of _diffn_scan.frame_id. This item is a pointer to _diffn_data_frame.id in the DIFFRN_DATA_FRAME category.