

## 3. CIF DATA DEFINITION AND CLASSIFICATION

Data items in the DIFFRN\_MEASUREMENT\_AXIS category associate axes with goniometers, just as data items in the DIFFRN\_DETECTOR\_AXIS category associate axes with detectors.

## 3.7.4.4. The radiation source

Data items in this category are as follows:

DIFFRN\_RADIATION

- *\_diffrn\_radiation.diffrn\_id*  
→ *\_diffrn.id*
- \_diffrn\_radiation.collimation*
- \_diffrn\_radiation.div\_x\_source*
- \_diffrn\_radiation.div\_y\_source*
- \_diffrn\_radiation.div\_x\_y\_source*
- \_diffrn\_radiation.filter\_edge*
- \_diffrn\_radiation.inhomogeneity*
- \_diffrn\_radiation.monochromator*
- \_diffrn\_radiation.polarisn\_norm*
- \_diffrn\_radiation.polarisn\_ratio*
- \_diffrn\_radiation.polarizn\_source\_norm*
- \_diffrn\_radiation.polarizn\_source\_ratio*
- \_diffrn\_radiation.probe*
- \_diffrn\_radiation.type*
- \_diffrn\_radiation.wavelength\_id*  
→ *\_diffrn\_radiation.wavelength.id*
- \_diffrn\_radiation.xray\_symbol*

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

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

## 3.7.4.5. Intensity measurements

Data items in this category are as follows:

DIFFRN\_REFLN

- *\_diffrn\_refl.n.frame\_id*  
→ *\_diffrn\_data\_frame.id*
- *\_diffrn\_refl.id*
- *\_diffrn\_refl.diffrn\_id*
- \_diffrn\_refl.angle\_chi*
- \_diffrn\_refl.angle\_kappa*
- \_diffrn\_refl.angle\_omega*
- \_diffrn\_refl.angle\_phi*
- \_diffrn\_refl.angle\_psi*
- \_diffrn\_refl.angle\_theta*

- \_diffrn\_refl.attenuator\_code*
- \_diffrn\_refl.counts\_bg\_1*
- \_diffrn\_refl.counts\_bg\_2*
- \_diffrn\_refl.counts\_net*
- \_diffrn\_refl.counts\_peak*
- \_diffrn\_refl.counts\_total*
- \_diffrn\_refl.detect\_slit\_horiz*
- \_diffrn\_refl.detect\_slit\_vert*
- \_diffrn\_refl.elapsed\_time*
- \_diffrn\_refl.index\_h*
- \_diffrn\_refl.index\_k*
- \_diffrn\_refl.index\_l*
- \_diffrn\_refl.intensity\_net*
- \_diffrn\_refl.intensity\_sigma*
- \_diffrn\_refl.scale\_group\_code*
- \_diffrn\_refl.scan\_mode*
- \_diffrn\_refl.scan\_mode\_backgd*
- \_diffrn\_refl.scan\_rate*
- \_diffrn\_refl.scan\_time\_backgd*
- \_diffrn\_refl.scan\_width*
- \_diffrn\_refl.sint\_over\_lambda*
- \_diffrn\_refl.standard\_code*
- \_diffrn\_refl.wavelength*
- \_diffrn\_refl.wavelength\_id*

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

The DIFFRN\_REFLN category is defined in the mmCIF dictionary (Section 3.6.5.2; see the detailed discussion in Section 3.2.2.2.2). Data items in the DIFFRN\_REFLN category record details of the intensities measured in the diffraction data set identified by *\_diffrn\_refl.diffrn\_id*. The CBF/imgCIF dictionary extends the key with *\_diffrn\_refl.frame\_id* (a pointer to *\_diffrn\_data\_frame.id*), so that multiple data sets may be recorded.

## 3.7.4.6. Diffraction scans

Data items in these categories are as follows:

(a) DIFFRN\_SCAN

- *\_diffrn\_scan.id*
- \_diffrn\_scan.date\_end*
- \_diffrn\_scan.date\_start*
- \_diffrn\_scan.frame\_id\_start*  
→ *\_diffrn\_data\_frame.id*
- \_diffrn\_scan.frame\_id\_end*  
→ *\_diffrn\_data\_frame.id*
- \_diffrn\_scan.frames*
- \_diffrn\_scan.integration\_time*

(b) DIFFRN\_SCAN\_AXIS

- *\_diffrn\_scan\_axis.axis\_id*  
→ *\_axis.id*
- *\_diffrn\_scan\_axis.scan\_id*  
→ *\_diffrn\_scan.id*
- \_diffrn\_scan\_axis.angle\_start*
- \_diffrn\_scan\_axis.angle\_range*
- \_diffrn\_scan\_axis.angle\_increment*
- \_diffrn\_scan\_axis.angle\_rstrt\_incr*
- \_diffrn\_scan\_axis.displacement\_start*
- \_diffrn\_scan\_axis.displacement\_range*
- \_diffrn\_scan\_axis.displacement\_increment*
- \_diffrn\_scan\_axis.displacement\_rstrt\_incr*

(c) DIFFRN\_SCAN\_FRAME

- \_diffrn\_scan\_frame.date*
- *\_diffrn\_scan\_frame.frame\_id*  
→ *\_diffrn\_data\_frame.id*
- *\_diffrn\_scan\_frame.scan\_id*  
→ *\_diffrn\_scan.id*
- \_diffrn\_scan\_frame.frame\_number*
- \_diffrn\_scan\_frame.integration\_time*

(d) DIFFRN\_SCAN\_FRAME\_AXIS

- *\_diffrn\_scan\_frame\_axis.axis\_id*  
→ *\_axis.id*
- *\_diffrn\_scan\_frame\_axis.frame\_id*  
→ *\_diffrn\_data\_frame.id*
- \_diffrn\_scan\_frame\_axis.angle*