For a polychromatic beam, the other data items in the DIFFRN_RADIATION_WAVELENGTH category allow different wavelength components and an associated weighting factor for each component to be listed. In the list of experimental intensity measurements from a polychromatic beam (the DIFFRN_REFLN category, discussed below), each reflection has an associated **_diffrn_refln_wavelength_id** that must match the corresponding **_diffrn_radiation_wavelength_id** in this list.

The DIFFRN_SOURCE category specifies the characteristics of the radiation source in the experiment and is closely related to the DIFFRN_RADIATION category, which is concerned with the handling of the radiation beam before it reaches the specimen. (The now-deprecated data name **_diffrn_radiation_source** shows that there was no formal separation of the descriptions of the radiation generator and the radiation in the first release of the core dictionary.)

The general class of radiation is specified by the data name **_diffrn_source**, which is a free-text field. Typical entries would be 'sealed X-ray tube', 'nuclear reactor', 'synchrotron', 'spallation source', 'rotating-anode X-ray tube' or 'electron microscope'. It is clear that the category could describe non-X-ray experiments, but several of the data names within the category (*e.g.* **_diffrn_source_target**) have meanings that are specific to an X-ray experiment. New data names might be introduced if experiments using other radiation types become more common. For now, details that a user wishes to record that are not properly described by the existing data names may be stored in the **_diffrn_source_details** field.

3.2.2.2.3. *Apparatus and instrumentation at the crystal*

The data items in these categories are as follows:

(*a*) DIFFRN_MEASUREMENT
- **_diffrn_measurement_details**
- **_diffrn_measurement_device**
- **_diffrn_measurement_device_details**
- **_diffrn_measurement_device_type**
- **_diffrn_measurement_method**
- **_diffrn_measurement_specimen_support**

(*b*) DIFFRN_ORIENT_MATRIX
- **_diffrn_orient_matrix_type**
- **_diffrn_orient_matrix_UB_11**
- **_diffrn_orient_matrix_UB_12**
- **_diffrn_orient_matrix_UB_13**
- **_diffrn_orient_matrix_UB_21**
- **_diffrn_orient_matrix_UB_22**
- **_diffrn_orient_matrix_UB_23**
- **_diffrn_orient_matrix_UB_31**
- **_diffrn_orient_matrix_UB_32**
- **_diffrn_orient_matrix_UB_33**

(*c*) DIFFRN_ORIENT_REFLN
- • **_diffrn_orient_refln_index_h**
- • **_diffrn_orient_refln_index_k**
- • **_diffrn_orient_refln_index_l**
- **_diffrn_orient_refln_angle_chi**
- **_diffrn_orient_refln_angle_kappa**
- **_diffrn_orient_refln_angle_omega**
- **_diffrn_orient_refln_angle_phi**
- **_diffrn_orient_refln_angle_psi**
- **_diffrn_orient_refln_angle_theta**

The bullet (•) indicates a category key. Where multiple items within a category are marked with a bullet, they must be taken together to form a compound key.

The DIFFRN_MEASUREMENT category currently concerns specifically the mounting of the crystal and the details of the goniometer or other device on which it is mounted, with the exception of **_diffrn_measurement_method**, which is defined simply as the 'method used to measure intensities'. In practice, for a typical single-crystal diffractometer setup this field is generally used to specify the scan type, as in Example 3.2.2.2, where the CIF code for the Greek character θ, \q, is used to indicate $\theta/2\theta$ scans.

Example 3.2.2.2. *An indication of the scan type of a diffractometer-based experiment.*

```
_diffrn_measurement_method
    'profile data from \q/2\q scans'
```

The orientation matrix gives the transformation between coordinates in a crystal-centric reference frame and those referred to the diffractometer axes. The data items defined in the DIFFRN_ORIENT_MATRIX category can be used to store the values in the matrix as recorded on an individual diffractometer and a reference to the convention used (in **_diffrn_orient_matrix_type**). However, the reference is not by itself sufficient to understand the transformation without additional external knowledge of the convention. Authors are encouraged to provide a full description of the convention in the text field **_diffrn_orient_matrix_type**.

The terminology UB refers to the conventional designation of the matrix relating reciprocal space and the reference frame of a diffractometer, calculated as the product of the orientation matrix **U** and the material matrix **B** by the method of Busing & Levy (1967).

The reflections used to determine the orientation matrix can be listed in the category DIFFRN_ORIENT_REFLN. As discussed above, this list is useful for analysing the results on a diffractometer of known type, but is not useful if the convention for establishing the individual terms of the orientation matrix is not known.

3.2.2.2.4. *Apparatus and instrumentation after the crystal*

The data items in this category are as follows:

DIFFRN_DETECTOR
- **_diffrn_detector**
- **_diffrn_detector_area_resol_mean**
- **_diffrn_detector_details**
- **_diffrn_detector_dtime**
- **_diffrn_detector_type**
- † **_diffrn_radiation_detector**
- † **_diffrn_radiation_detector_dtime**

The dagger (†) indicates a deprecated item, which should not be used in the creation of new CIFs.

The DIFFRN_DETECTOR category is intended to describe the detector used to measure the scattered radiation, including any analyser and post-sample collimation. There are not many data names in this category, as it is not often necessary to know a lot about the detector beyond its make, model or name if it is made by a well known manufacturer. A record of the detector deadtime (**_diffrn_detector_dtime**) and the resolution of an area detector (**_diffrn_detector_area_resol_mean**) are useful details worth recording explicitly; other unusual or noteworthy details may be recorded in **_diffrn_detector_details**.

The deprecated items (retained for compatibility with the original release version) have been replaced by **_diffrn_detector** and **_diffrn_detector_dtime** to produce names better matched to the formal category assignment.

3.2.2.2.5. *Intensity measurements*

The data items in these categories are as follows:

(*a*) DIFFRN_REFLN
- • **_diffrn_refln_index_h**
- • **_diffrn_refln_index_k**
- • **_diffrn_refln_index_l**