International Tables for Crystallography (2006). Vol. G, Section 3.2.2.2.5, pp. 95–97.

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
```

```
  _diffrn_refln_angle_chi
  _diffrn_refln_angle_kappa
  _diffrn_refln_angle_omega
  _diffrn_refln_angle_phi
  _diffrn_refln_angle_psi
  _diffrn_refln_angle_theta
  _diffrn_refln_attenuator_code
       → _diffrn_attenuator_code
  _diffrn_refln_class_code
       → _diffrn_reflns_class_code
  _diffrn_refln_counts_bg_1
  _diffrn_refln_counts_bg_2
  _diffrn_refln_counts_net
  _diffrn_refln_counts_peak
  _diffrn_refln_counts_total
  _diffrn_refln_crystal_id
       → _exptl_crystal_id
  _diffrn_refln_detect_slit_horiz
  _diffrn_refln_detect_slit_vert
  _diffrn_refln_elapsed_time
  _diffrn_refln_intensity_net
† _diffrn_refln_intensity_sigma
  _diffrn_refln_intensity_u
  _diffrn_refln_scale_group_code
       → _diffrn_scale_group_code
  _diffrn_refln_scan_mode
  _diffrn_refln_scan_mode_backgd
  _diffrn_refln_scan_rate
  _diffrn_refln_scan_time_backgd
  _diffrn_refln_scan_width
  _diffrn_refln_sint/lambda
  _diffrn_refln_standard_code
       → _diffrn_standard_refln_code
  _diffrn_refln_wavelength
  _diffrn_refln_wavelength_id
       → _diffrn_radiation_wavelength_id
```

(*b*) DIFFRN_REFLNS

```
  _diffrn_reflns_av_R_equivalents
† _diffrn_reflns_av_sigmaI/netI
  _diffrn_reflns_av_unetI/netI
  _diffrn_reflns_limit_h_max
  _diffrn_reflns_limit_h_min
  _diffrn_reflns_limit_k_max
  _diffrn_reflns_limit_k_min
  _diffrn_reflns_limit_l_max
  _diffrn_reflns_limit_l_min
  _diffrn_reflns_number
  _diffrn_reflns_reduction_process
  _diffrn_reflns_resolution_full
  _diffrn_reflns_resolution_max
  _diffrn_reflns_theta_full
  _diffrn_reflns_theta_max
  _diffrn_reflns_theta_min
  _diffrn_reflns_transf_matrix_11
  _diffrn_reflns_transf_matrix_12
  _diffrn_reflns_transf_matrix_13
  _diffrn_reflns_transf_matrix_21
  _diffrn_reflns_transf_matrix_22
  _diffrn_reflns_transf_matrix_23
  _diffrn_reflns_transf_matrix_31
  _diffrn_reflns_transf_matrix_32
  _diffrn_reflns_transf_matrix_33
```

(*c*) DIFFRN_REFLNS_CLASS

```
• _diffrn_reflns_class_code
  _diffrn_reflns_class_av_R_eq
† _diffrn_reflns_class_av_sgI/I
  _diffrn_reflns_class_av_uI/I
  _diffrn_reflns_class_d_res_high
  _diffrn_reflns_class_d_res_low
  _diffrn_reflns_class_description
  _diffrn_reflns_class_number
```

(*d*) DIFFRN_SCALE_GROUP

```
• _diffrn_scale_group_code
  _diffrn_scale_group_I_net
```

(*e*) DIFFRN_STANDARD_REFLN

```
• _diffrn_standard_refln_index_h
• _diffrn_standard_refln_index_k
• _diffrn_standard_refln_index_l
  _diffrn_standard_refln_code
```

(*f*) DIFFRN_STANDARDS

```
  _diffrn_standards_decay_%
  _diffrn_standards_interval_count
  _diffrn_standards_interval_time
  _diffrn_standards_number
† _diffrn_standards_scale_sigma
  _diffrn_standards_scale_u
```

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 arrow (→) is a reference to a parent data item. The dagger (†) indicates a deprecated item, which should not be used in the creation of new CIFs.

The DIFFRN_REFLN category describes the measured reflections in a diffraction experiment. Example 3.2.2.3 shows a listing from a CAD-4 single-crystal diffractometer.

Note that the data in this list refer to the raw measurements as acquired at the time of data collection. This is in contrast to the data in the REFLN list, which refer to the reflections after merging and scaling.

The meanings of most of the data names can be deduced by inspection of this example. Full definitions are given in the dictionary.

However, the category also contains a number of data items which are used to group blocks of reflections with additional properties described by data items in other categories. For example, a number of reflections in the list might share a common value of `_diffrn_refln_scale_group_code`; this value would link to a description in the DIFFRN_SCALE_GROUP category of the scaling factor that needs to be applied to this group of reflections to bring all intensities in the list on to a common scale. (For example, intensities might be obtained from individual films in a multi-film data set or from a number of separate crystals.)

Likewise, individual reflections might be marked to indicate that they were monitored as standards during the course of the

Example 3.2.2.3. *Listing of experimental diffraction intensities.*

```
loop_
     _diffrn_refln_index_h
     _diffrn_refln_index_k
     _diffrn_refln_index_l
     _diffrn_refln_angle_chi
     _diffrn_refln_scan_rate
     _diffrn_refln_counts_bg_1
     _diffrn_refln_counts_total
     _diffrn_refln_counts_bg_2
     _diffrn_refln_angle_theta
     _diffrn_refln_angle_phi
     _diffrn_refln_angle_omega
     _diffrn_refln_angle_kappa
     _diffrn_refln_scan_width
     _diffrn_refln_elapsed_time
0  0 -16  0. 4.12  28 127  36  33.157  -75.846
         16.404   50.170  1.516 19.43
0  0 -15  0. 4.12  38 143  28  30.847  -75.846
         14.094   50.170  1.516 19.82
0  0 -14  0. 1.03 142 742 130  28.592  -75.846
         11.839   50.170  1.516 21.32
0  0 -13  0. 4.12  26 120  37  26.384  -75.846
          9.631   50.170  1.450 21.68
0  0 -12  0. 0.97 129 618 153  24.218  -75.846
          7.464   50.170  1.450 23.20
0  0 -11  0. 4.12  33 107  38  22.087  -75.846
          5.334   50.170  1.384 23.55
0  0 -10  0. 4.12  37 146  33  19.989  -75.846
          3.235   50.170  1.384 23.90
   # - - - - abbreviated - - - -
3  4  -4  0. 1.03  69 459  73  30.726  -53.744
         46.543  -47.552  1.516 2082.58
3  4  -5  0. 1.03  91 465  75  31.407  -54.811
         45.519  -42.705  1.516 2084.07
3 14  -6  0. 1.03  84 560  79  32.228  -55.841
         44.745  -38.092  1.516 2085.57
   # - - - - abbreviated - - - -
```

experiment, using the data name `_diffrn_refln_standard_code`. These standard reflections may be listed separately in the DIFFRN_STANDARD_REFLN category, in which case they are labelled by `_diffrn_standard_refln_code`, which must have values matching those assigned in the main list of intensities.

Apart from these specific classes of reflections, the intensity data may be binned according to different criteria (*e.g.* for modulated structures the intensities are often partitioned into classes with the same value of $m = \sum |m_i|$, where the m_i are the integer coefficients indexing diffraction vectors in an n-dimensional representation). The data name `_diffrn_refln_class_code` is provided as a link to the different classes of reflections defined in the DIFFRN_REFLNS_CLASS category.

The DIFFRN_REFLNS category describes collective properties of the set of experimental intensity measurements and follows the convention (common elsewhere in the dictionary) of having a name very similar to the related DIFFRN_REFLN category, but using a plural form of the relevant term in the composite name. While the individual DIFFRN_REFLN entries appear in a looped list, the items in the DIFFRN_REFLNS category are not looped.

This category describes properties of the *complete* measurement set; descriptions of specific portions of the complete set are handled by the DIFFRN_REFLNS_CLASS category.

Several of the items that appear in this category can be derived from the contents of the DIFFRN_REFLN lists, but it is often convenient to list them separately for ease of access and as a consistency check.

Note the definition of `_diffrn_reflns_number` as the total number of measured intensities *excluding* those classed as 'systematically absent' (reflections whose intensities are null as a consequence of crystallographic symmetry). There is no data item to specifically flag systematic absences (although one could assign a distinct `_diffrn_refln_class_code` value and define the relevant DIFFRN_REFLNS_CLASS). Because the measured diffraction data may (and often do) include reduced measurements and symmetry-equivalent reflection intensities, there is no formal way to check the value of `_diffrn_reflns_number` with dictionary-driven validation software. (Note that systematic absences *are* flagged in the structure-factor listing of the REFLN category.)

The data items in the DIFFRN_REFLNS_CLASS category record details about classes of reflections measured in the diffraction experiment. The user is free to assign classes according to arbitrary criteria; two specific cases, the marking of standard reflections and the clustering of intensities that need to be scaled by a common factor, have their own specific data items and associated categories, as discussed above. The example given in the dictionary (Example 3.2.2.4) describes a one-dimensional incommensurately modulated structure, where each reflection class is defined by the number $m = \sum |m_i|$, where the m_i are the integer coefficients that, in addition to h, k, l, index the corresponding diffraction vector in the basis defined for the reciprocal lattice.

The DIFFRN_SCALE_GROUP category records scaling factors which must be applied to specific intensities in the DIFFRN_REFLN list to bring all the measurements on to a common scale (Example 3.2.2.5). The scale factor `_diffrn_scale_group_I_net` is the factor by which the relevant net values in the intensities list must be multiplied. The intensities to which it must be applied are those in the intensities list marked with a `_diffrn_refln_scale_group_code` that matches the corresponding `_diffrn_scale_group_code` in this category.

The DIFFRN_STANDARD_REFLN category allows a separate tabulation of the reflections used as standards. Note that the actual *measurements* on these reflections are stored alongside all the other measurements in the DIFFRN_REFLN list. The results of the analysis of the standard reflections are described by the DIFFRN_STANDARDS category.

Example 3.2.2.4. *Use of the DIFFRN_REFLNS_CLASS category to specify the main and satellite reflections collected for a modulated incommensurate structure*

```
loop_
     _diffrn_reflns_class_number
     _diffrn_reflns_class_d_res_high
     _diffrn_reflns_class_d_res_low
     _diffrn_reflns_class_av_R_eq
     _diffrn_reflns_class_code
     _diffrn_reflns_class_description
       1580 0.551 6.136 0.015 'Main'
          'm=0; main reflections'
       1045 0.551 6.136 0.010 'Sat1'
          'm=1; first-order satellites'
```

Example 3.2.2.5. *Scaling factors for reflections listed by group.*

```
loop_
     _diffrn_scale_group_code
     _diffrn_scale_group_I_net
      1    .86473
      2   1.0654
```

The DIFFRN_STANDARDS category describes the interval between measurements of the standard reflections and their overall intensity change (usually a decay, so that the relevant data name is `_diffrn_standards_decay_%`; this data item has a negative value if the final measured intensities are greater than the initial ones). The items assume a constant time interval (or number of counts) between the measurement of each standard and a single global value for the overall intensity change. If required, detailed tracking of the intensity change of individual standard reflections can be extracted from the DIFFRN_REFLN list provided the elapsed time at each measurement has been recorded (`_diffrn_refln_elapsed_time`).

3.2.2.3. Experimental measurements on the crystal

The categories describing experimental conditions are as follows:

EXPTL group
- EXPTL
- EXPTL_CRYSTAL
- EXPTL_CRYSTAL_FACE

The data items in these categories are as follows:

(*a*) EXPTL

```
_exptl_absorpt_coefficient_mu
_exptl_absorpt_correction_T_max
_exptl_absorpt_correction_T_min
_exptl_absorpt_correction_type
_exptl_absorpt_process_details
_exptl_crystals_number
_exptl_special_details
```

(*b*) EXPTL_CRYSTAL

```
• _exptl_crystal_id
  _exptl_crystal_colour
  _exptl_crystal_colour_lustre
  _exptl_crystal_colour_modifier
  _exptl_crystal_colour_primary
  _exptl_crystal_density_diffrn
  _exptl_crystal_density_meas
  _exptl_crystal_density_meas_gt
  _exptl_crystal_density_meas_lt
  _exptl_crystal_density_meas_temp
  _exptl_crystal_density_meas_temp_gt
  _exptl_crystal_density_meas_temp_lt
  _exptl_crystal_density_method
```


references