

3. CIF DATA DEFINITION AND CLASSIFICATION

Table 3.3.3.1. Category groups defined in the powder CIF dictionary

The groups are listed in the order in which they are described in this chapter.

Section	Category group	Subject covered
<i>(a) Experimental measurements</i>		
3.3.4.1	PD_CHAR	Characterization of a sample
3.3.4.1	PD_PREP	Preparation of a sample
3.3.4.2	PD_SPEC	Specimen used in an experiment
3.3.4.3	PD_CALIB	Calibration information
3.3.4.3	PD_INSTR	The experimental instrument
3.3.4.4	PD_MEAS	Raw measurements and instrumental settings
<i>(b) Analysis</i>		
3.3.5.1	PD_PROC	Processed settings
3.3.5.2	PD_CALC	Simulated settings
3.3.5.3	PD_PEAK	Diffraction peak table
3.3.5.4	REFLN	Reflection assignments and intensities
<i>(c) Atomicity, chemistry and structure</i>		
3.3.6.1	PD_PHASE	Phases present
<i>(d) File metadata</i>		
3.3.7.1	PD_BLOCK	Relationships between data blocks
3.3.4.3, 3.3.4.4, 3.3.5.1, 3.3.5.2	PD_DATA	Measured and simulated intensities

separate loops, for example, if the increment between data points differs.

This need to contain diverse items in a common 'looped' list has led the pdCIF dictionary to use category names in a different way from the other CIF dictionaries, in which CIF data items are usually named according to their category. In the pdCIF dictionary, data items that might appear in the loop for diffraction intensities are assigned to the category PD_DATA. Only one data item is named using this category as prefix, `_pd_data_point_id`. Another departure from the convention used in other dictionaries is that several `_pd_refl*_` data names are assigned to the category REFLN so that these items may be included in a loop with `_refln_*` items defined in the core CIF dictionary.

Table 3.3.3.1 summarizes the category groups in the pdCIF dictionary; the individual categories are listed alphabetically in Appendix 3.3.1. The appendix also lists for each category the section of this chapter in which the category is described.

The order in which the categories are discussed follows the scheme of Table 3.1.10.1, so that the contents of the dictionary are summarized under the headings *Experimental measurements* (Section 3.3.4), *Analysis* (Section 3.3.5), *Atomicity, chemistry and structure* (Section 3.3.6) and *File metadata* (Section 3.3.7). The pdCIF dictionary does not contribute any new data items relevant to publication beyond those already in the core CIF dictionary.

The data items in each category are listed below. Category keys, if specified, are listed first and are marked by a bullet (●); the remaining data items in each category are listed alphabetically. Note that the category PD_DATA is discussed in several different sections.

3.3.4. Experimental measurements

The categories in the powder CIF dictionary relating to the crystallographic experiment are as follows:

Characterization and preparation of the sample (§3.3.4.1)

PD_CHAR group
 PD_CHAR
 PD_PREP group
 PD_PREP

Description of the specimen (§3.3.4.2)

PD_SPEC group
 PD_SPEC

Instrument calibration and design (§3.3.4.3)

PD_CALIB group
 PD_CALIB
 PD_CALIBRATION
 PD_INSTR group
 PD_INSTR

Observations and measurement conditions (§3.3.4.4)

PD_DATA group
 PD_DATA (items beginning with `_pd_meas_*`)
 PD_MEAS group
 PD_MEAS_INFO
 PD_MEAS_METHOD

The pdCIF dictionary differentiates between the terms *sample* and *specimen*. The terms are often treated as interchangeable, but they have quite distinct meanings. The term *sample* refers to a batch of material, while the term *specimen* refers to the particular portion of the sample that was used for a measurement. In some cases, the specimen is modified before it is used for data collection. For example, it may be mixed with an internal standard, dried, hydrated or pressed into a pellet.

3.3.4.1. Characterization and preparation of the sample

The data items in these categories are as follows:

- (a) PD_CHAR
 ● `_pd_char_atten_coef_mu_calc`
 ● `_pd_char_atten_coef_mu_obs`
 ● `_pd_char_colour`
 ● `_pd_char_particle_morphology`
 ● `_pd_char_special_details`
- (b) PD_PREP
 ● `_pd_prep_conditions`
 ● `_pd_prep_cool_rate`
 ● `_pd_prep_pressure`
 ● `_pd_prep_temperature`

The PD_CHAR data items describe information known about the sample from observation and chemical analysis. For example, a description of the sample morphology can be specified using `_pd_char_particle_morphology`. Note that there are data items in the core dictionary that are appropriate for use with powder diffraction. For example, `_atom_type_analytical_mass_%` can be used for chemical analysis results and `_chemical_melting_point` for the melting point. Several similar data items occur in the pdCIF and core dictionaries. `_expt1_crystal_colour` and `_pd_char_colour` both describe the sample colour, but `_pd_char_colour` is more systematic. Also, `_pd_char_atten_coef_mu_calc` and `_expt1_absorpt_coefficient_mu` describe similar properties, but `_pd_char_atten_coef_mu_calc` is adjusted for the sample packing fraction, so it can be compared with the experimental value, `_pd_char_atten_coef_mu_obs`, when a direct measurement is made.

The PD_PREP data items describe how the sample was collected or prepared. For example, `_pd_prep_pressure` and `_pd_prep_temperature` describe the pressure and temperature used to prepare the sample. Note that these will probably differ from the pressure and temperature conditions at which diffraction measurements are made. Measurement conditions are recorded in `_diffrn_ambient_pressure` and `_diffrn_ambient_temperature`.