This is version 1.0.1 of the powder CIF dictionary (pdCIF). The data names defined in this dictionary complement those in the core dictionary (Chapter 4.1) and should be used to describe the results of powder diffraction studies. The organization of powder data sets, especially for studies of multiphase samples and for studies referring to external calibration standards, is discussed in Chapter 3.3.

The pdCIF data structure departs from the rigorous relational nature of the core dictionary in that it does not adhere fully to the close coupling of data names and associated category names. The dictionary is therefore presented here strictly alphabetically by data name. Not all pdCIF categories are described in this dictionary. Further, the pdCIF dictionary defines items that belong to categories in the core CIF dictionary. Care must therefore be taken in checking the category membership of each data name; this is particularly important to ensure that items in the same category are presented together in the same looped lists. See Chapters 3.1 and 3.3 for a more complete discussion.

### pdCIF category definitions

#### PD_BLOCK

(pd_block_id) is used to assign a unique ID code to a data block. This code is then used for references between different blocks (see pd_block_diffractogram_id, pd_calib_std_external_block_id and pd_phase_block_id). Note that a data block may contain only a single diffraction data set or information about a single crystalline phase. However, a single diffraction measurement may yield structural information on more than one phase, or a single structure determination may use more than one data set. Alternatively, results from a single data set, such as calibration parameters from measurements of a standard, may be used for many subsequent analyses. Through use of the ID code, a reference made between data sets may be preserved when the file is exported from the laboratory from which the CIF originated. The ID code assigned to each data block should be unique with respect to an ID code assigned for any other data block in the world. The naming scheme chosen for the block-ID format is also possible to use the Internet name or address for the instrument as possible) for the data-collection instrument, preferably containing the instrument serial number for commercial instruments. It is also possible to use the Internet name or address for the instrument computer as a unique name.

As blocks are created in a CIF, the original sample identifier (i.e. (creator_name) should be retained, but the (creator_name) may be changed and the (date-time) will always change. The (date-time) will usually match either the pd_meas_datetime_initiated or the pd_proc_info_datetime entry.

Within each section of the code, the following characters may be used:

- `A-Za-z-0-9` and _ `+`.
- `-` _ `*` _ `/` _ `( )` _ `{ }`
- `*` may substitute the URL for the file containing the appropriate program such as LAZY/PULVERIX or the computed intensities from a Rietveld refinement.

The sections are separated with vertical rules `|` which are not allowed within the sections. Blank spaces may also not be used. Capitalization may be used within the ID code but should not be considered significant – searches for data-set ID names should be case-insensitive.

Date-time entries are in the standard CIF format `yyyymm-ddThh:mm:ssZ`. Use of seconds and a time zone is optional, but use of hours and minutes is strongly encouraged as this will help to ensure that the code is unique.

An archive site that wishes to make CIFs available via the web may substitute the URL for the file containing the appropriate block for the final two sections of the ID (`creator_name`) and `instr_name`). Note that this should not be done unless the archive site is prepared to keep the file available online indefinitely.

May appear in list.


#### pd_block_diffractogram_id

(pd_block_diffractogram_id) A block ID code (see pd_block_id) that identifies diffraction data contained in a data block other than the current block. This will occur most frequently when more than one set of diffraction data is used for a structure determination. The data block containing the diffraction data will contain a pd_block_id code matching the code in pd_block_diffractogram_id.
**PD_CALIB**

This section defines the parameters used for the calibration of the instrument that are used directly or indirectly in the interpretation of this data set. The information in this section of the CIF should generally be written when the intensities are first measured, but from then on should remain unchanged. Loops may be used for calibration information that differs by detector channel. The pd_calibration_items, however, are never looped.

**Example 1.**

```plaintext
 pd_calib_std_external_block_id
 QuartzPlate|D500|236-978 [B.Toby:91-15-09] 14:02
 pd_calib_std_external_name
 'Arkansas Stone quartz plate'
```

**Example 2.**

\[
2	heta_{\text{actual}} = 2	heta_{\text{setting}} + \arctan\left(\frac{\cos(P_0)}{\sin(P_0)\left(1/\left(\left(CC - CH_0 - P_0^2 CC^2\right) - \sin(P_0)\right)\right)}\right).
\]

This allows for the calibration of 2\(\theta\) for a linear position-sensitive detector (PSD) where the PSD has been set such that the 'centre channel' (CH\_0) is located at 2\(\theta\)setting as a function of the channel number (CC). In addition to CH\_0, variables P\_0, P\_1 and P\_2 are calibration constants, where P\_0 is the width of a PSD channel in degrees, P\_1 is the angle of the PSD with respect to the perpendicular and P\_2 is a quadratic term for nonlinearity in the detector.

**pd_calibration_conversion_eqn**

A code which identifies the detector or channel number in a position-sensitive, energy-dispersive or other multiple-detector instrument. Note that this code should match the code name used for pd_meas_detector_id. Appears in list as essential element of loop structure. May match child data name(s):

**Example:**

```plaintext
; 2\(\theta\)_{actual} = 2\(\theta\)_{setting} + \arctan\left(\frac{\cos(P_1)}{\sin(P_0)\left(1/\left(\left(CC - CH_0 - P_0^2 CC^2\right) - \sin(P_0)\right)\right)}\) + \arctan\left(\frac{\cos(P_1)}{\sin(P_0)\left(1/\left(\left(CC - CH_0 - P_0^2 CC^2\right) - \sin(P_0)\right)\right)}\right)
```

4.2. POWDER DICTIONARY (pdCIF)
**_pd_calibration_special_details_**

**_pd_calibration_special_details_** *(char)*

Description of how the instrument was calibrated, particularly for instruments where calibration information is used to make hardware settings that would otherwise be invisible once data collection is completed. Do not use this item to specify information that can be specified using other _pd_calib_ items.

[PD_CALIBRATION]

**_pd_char_atten_coef_mu_obs_** *(namb)*

The observed and calculated attenuation coefficient, \( \mu \), in units of inverse millimetres. Note that this quantity is sometimes referred to as the mass absorption coefficient; however, this term accounts for other potentially significant losses of incident radiation, for example incoherent scattering of neutrons. The calculated \( \mu \) will be obtained from the atomic content of the cell, the average density (allowing for specimen packing) and the radiation wavelength. The observed \( \mu \) will be determined by a transmission measurement. Note that _pd_char_atten_coef_mu_calc_ will differ from _extvl_absorpt_coeficient_mu_ if the packing density is not unity.

The permitted range is \( 0 \rightarrow \infty \).

[PD_CHAR]

**_pd_char_colour_** *(char)*

The colour of the material used for the measurement. To facilitate more standardized use of names, the following guidelines for colour naming developed by Peter Bayliss for the International Centre for Diffraction Data (ICDD) should be followed. Note that combinations of descriptors are separated by an underscore. Allowed colours are: colourless, white, black, gray, brown, red, pink, orange, yellow, green, blue, violet. Colours may be modified using prefixes of: light, dark, whitish, blackish, grayish, brownish, reddish, pinkish, orangish, yellowish, greenish, bluish. Intermediate hues may be indicated with two colours: e.g. blue_green or bluish_green. For metallic materials, the term metallic may be added: e.g. reddish_orange_metallic for copper. The ICDD standard allows commas to be used for minerals that occur with ranges of colours; however this usage is not appropriate for the description of a single sample.


[PD_CHAR]

**_pd_char_particle_morphology_** *(char)*

A description of the sample morphology and estimates for particle sizes (before grinding/sieving, if noted by _pd_spec_preparation_). Include the method used for these estimates (SEM, visual estimate etc.).

[PD_CHAR]

**_pd_char_special_details_** *(char)*

Additional characterization information relevant to the sample or documentation of non-routine processing steps used for characterization.

[PD_CHAR]

**_pd_data_point_id_** *(char)*

Arbitrary label identifying an entry in the table of diffractogram intensity values.

[PD_DATA]

**_pd_data_set_id_** *(char)*

Arbitrary label identifying an entry in the table of diffractogram intensity values.

[PD_DATA]

**_pd_data_set_source_** *(char)*

Arbitrary label identifying an entry in the table of diffractogram intensity values.

[PD_DATA]

**_pd_exptl_absorpt_coefficient_mu_** *(namb)*

The observed and calculated linear absorption coefficient, \( \mu \), for metallic materials, the term metallic may be added: e.g. reddish_orange_metallic for copper. The ICDD standard allows commas to be used for minerals that occur with ranges of colours; however this usage is not appropriate for the description of a single sample.

[PD_DATA]

**_pd_loop_** *(char)*

A description of the sample morphology and estimates for particle sizes (before grinding/sieving, if noted by _pd_spec_preparation_). Include the method used for these estimates (SEM, visual estimate etc.).

[PD_LOOP]

**_pd_meas_2theta_corrected_** *(namb)*

The observed and calculated linear absorption coefficient, \( \mu \), for metallic materials, the term metallic may be added: e.g. reddish_orange_metallic for copper. The ICDD standard allows commas to be used for minerals that occur with ranges of colours; however this usage is not appropriate for the description of a single sample.

[PD_MEAS]

**_pd_meas_intensity_total_** *(namb)*

The observed and calculated linear absorption coefficient, \( \mu \), for metallic materials, the term metallic may be added: e.g. reddish_orange_metallic for copper. The ICDD standard allows commas to be used for minerals that occur with ranges of colours; however this usage is not appropriate for the description of a single sample.

[PD_MEAS]

**_pd_proc_2theta_corrected_** *(namb)*

The observed and calculated linear absorption coefficient, \( \mu \), for metallic materials, the term metallic may be added: e.g. reddish_orange_metallic for copper. The ICDD standard allows commas to be used for minerals that occur with ranges of colours; however this usage is not appropriate for the description of a single sample.

[PD_PROC]

**_pd_proc_2theta_scan_** *(namb)*

The observed and calculated linear absorption coefficient, \( \mu \), for metallic materials, the term metallic may be added: e.g. reddish_orange_metallic for copper. The ICDD standard allows commas to be used for minerals that occur with ranges of colours; however this usage is not appropriate for the description of a single sample.

[PD_PROC]

**_pd_proc_intensity_bkg_calc_** *(namb)*

The observed and calculated linear absorption coefficient, \( \mu \), for metallic materials, the term metallic may be added: e.g. reddish_orange_metallic for copper. The ICDD standard allows commas to be used for minerals that occur with ranges of colours; however this usage is not appropriate for the description of a single sample.

[PD_PROC]

**_pd_proc_intensity_bkg_meas_** *(namb)*

The observed and calculated linear absorption coefficient, \( \mu \), for metallic materials, the term metallic may be added: e.g. reddish_orange_metallic for copper. The ICDD standard allows commas to be used for minerals that occur with ranges of colours; however this usage is not appropriate for the description of a single sample.

[PD_PROC]

**_pd_proc_intensity_bkg_measured_** *(namb)*

The observed and calculated linear absorption coefficient, \( \mu \), for metallic materials, the term metallic may be added: e.g. reddish_orange_metallic for copper. The ICDD standard allows commas to be used for minerals that occur with ranges of colours; however this usage is not appropriate for the description of a single sample.

[PD_PROC]
This section contains information relevant to the instrument used for the diffraction measurement. For most laboratories, very little of this information will change, so a standard file may be prepared and included with each data set. Note that several definitions in the core CIF dictionary are relevant here. For example, use: _diffrn_radiation_wavelength for the source wavelength, _diffrn_radiation_type for the X-ray wavelength type, _diffrn_source for the radiation source, _diffrn_radiation_polarization_ratio for the source polarization, _diffrn_radiation_probe for the radiation type.

For data sets measured with partially monochromatized radiation, for example, where both K01 and K02 are present, it is important that all wavelengths present are included in a loop using _diffrn_radiation_wavelength to define the wavelength and _diffrn_radiation_wavelength wt to define the relative intensity of that wavelength. It is required that _diffrn_radiation_wavelength id also be present in the wavelength loop. It may also be useful to create a 'dummy' ID to use for labelling peaks/ reflections where the K01 and K02 wavelengths are not resolved. Set _diffrn_radiation_wavelength wt to be 0 for such a dummy ID. In the _pd_instr definitions, the term monochromator refers to a primary beam (pre-specimen) monochromator and the term analyser refers to post-diffraction (post-specimen) monochromator. The analyser may be fixed for a specific wavelength or may be capable of being scanned. For multiple-detector instruments it may be necessary to loop the * anal/detc or * spec/detc values (for _pd_instr_dist, _pd_instr_divg, _pd_instr_slit, and _pd_instr_soller) with the detector IDs (*_pd_calib_detector_id). It is strongly recommended that the core dictionary term _diffrn_radiation_probe (specifying the nature of the radiation used) is employed for all data sets.

Example 1.

_pd_instr_slit_eq_src/spec 1.
_pd_instr_slit_eq_anal/detc 0.2
_pd_instr_geometry Bragg-Brentano
_pd_instr_monochr_post_spec 'graphite (0001)'
_pd_instr_cons_illum_flag no

_pd_instr_beam_size_ax
_pd_instr_beam_size_eq (numb)

Axial and equatorial dimensions of the radiation beam at the specimen position (in millimetres). The perpendicular to the plane containing the incident and scattered beam is the axial (*_ax) direction.

The permitted range is 0.0 → ∞.

_pd_instr_cons_illum_flag (char)

Use 'yes' for instruments where the divergence slit is θ-compensated to yield a constant illumination length (also see _pd_instr_cons_illum_len). For other flat-plate instruments, where the illumination length changes with 2θ, specify 'no'. Note that if the length is known, it may be specified using _pd_instr_var_illum_len. The data value must be one of the following:

yes
no

_pd_instr_cons_illum_len (numb)

Length of the specimen that is illuminated by the radiation source (in millimetres). Use _pd_instr_cons_illum_len for instruments where the illumination length does not vary with 2θ, by adjustment of the divergence slits (sometimes known as θ-compensated slits).

Use _pd_instr_var_illum_len for instruments where the illuminated length of the specimen has been characterized as a function of 2θ, most commonly true with a fixed divergence slit.

The permitted range is 0.0 → ∞.

_pd_instr_dist_src/mono
_pd_instr_dist_mono/spec
_pd_instr_dist_mono/mono
_pd_instr_dist_spec/anal
_pd_instr_dist_anal/detc
_pd_instr_dist_spec/detc

Specifies distances in millimetres for the instrument geometry: * src/mono, the distance from the radiation source to the monochromator; * mono/spec, the distance from the monochromator to the specimen; * src/spec, the distance from the radiation source to the specimen; * spec/anal, the distance from the specimen to the analyser; * anal/detc, the distance from the analyser to the detector; * spec/detc, the distance from the specimen to the detector. Note that * src/spec is used in place of * src/mono and * mono/spec if there is no monochromator in use, and * spec/detc is used in place of * spec/anal and * anal/detc if there is no analyser in use.

May appear in list.

The permitted range is 0.0 → ∞.

_pdinstr_divg_ax_src/mono
_pdinstr_divg_ax_mono/spec
_pdinstr_divg_ax_src/spec
_pdinstr_divg_ax_monochromator
_pdinstr_divg_ax_anal/detc
_pdinstr_divg_ax_spec/detc

(numb)

Describes collimation in the axial direction (perpendicular to the plane containing the incident and diffracted beams) for the instrument. Values are the maximum divergence angles in degrees, as limited by slits or beamline optics other than Soller slits (see _pd_instr_soller_ax): * src/mono, collimation between the radiation source and the monochromator; * mono/spec, collimation between the monochromator and the specimen; * src/spec, collimation between the radiation source and the specimen; * spec/anal, collimation between the specimen and the analyser; * anal/detc, collimation between the analyser and the detector; * spec/detc, collimation between the specimen and the detector. Note that * src/spec is used in place of * src/mono and * mono/spec if there is no monochromator in use, and * spec/detc is used in place of * spec/anal and * anal/detc if there is no analyser in use.

May appear in list.

The permitted range is 0.0 → ∞.

_pdinstr_divg_eq_src/mono
_pdinstr_divg_eq_mono/spec
_pdinstr_divg_eq_mono/mono
_pdinstr_divg_eq_spec/anal
_pdinstr_divg_eq_anal/detc
_pdinstr_divg_eq_spec/detc

(numb)

Describes collimation in the equatorial plane (the plane containing the incident and diffracted beams) for the instrument. Values are the maximum divergence angles in degrees, as limited by slits or beamline optics other than Soller slits (see _pdinstr_soller_eq): * src/mono, collimation between the radiation source and the monochromator; * mono/spec, collimation between the monochromator and the specimen; * src/spec, collimation between the radiation source and the specimen; * spec/anal, collimation between the specimen and the analyser; * anal/detc, collimation between the analyser and the detector; * spec/detc, collimation between the specimen and the detector. Note that * src/spec is used in place of * src/mono and * mono/spec if there is no monochromator in use,
Describes collimation in the equatorial plane (the plane containing the incident and diffracted beams) for the instrument as a slit width (as opposed to a divergence angle). Values are the width of the slit (in millimetres) defining: * src/mono, collimation between the radiation source and the monochromator; * mono/spec, collimation between the monochromator and the specimen; * src/spec, collimation between the radiation source and the specimen; * spec/anal, collimation between the specimen and the analyser; * anal/detc, collimation between the analyser and the detector; * spec/detc, collimation between the specimen and the detector. Note that * src/mono is used in place of * src/mono and * mono/spec if there is no monochromator in use, and * spec/detc is used in place of * spec/anal and * anal/detc if there is no analyser in use.

May appear in list. The permitted range is 0.0 → ∞.

4. DATA DICTIONARIES

Describes collimation in the equatorial plane (the plane containing the incident and diffracted beams) for the instrument as a slit width (as opposed to a divergence angle). Values are the width of the slit (in millimetres) defining: * src/mono, collimation between the radiation source and the monochromator; * mono/spec, collimation between the monochromator and the specimen; * src/spec, collimation between the radiation source and the specimen; * spec/anal, collimation between the specimen and the analyser; * anal/detc, collimation between the analyser and the detector; * spec/detc, collimation between the specimen and the detector. Note that * src/mono is used in place of * src/mono and * mono/spec if there is no monochromator in use, and * spec/detc is used in place of * spec/anal and * anal/detc if there is no analyser in use.

May appear in list. The permitted range is 0.0 → ∞.

Describes collimation in the axrual plane (perpendicular to the plane containing the incident and diffracted beams) for the instrument. Values are the maximum divergence angles in degrees, as limited by Soller slits located thus: * src/mono, collimation between the radiation source and the monochromator; * mono/spec, collimation between the monochromator and the specimen; * src/spec, collimation between the radiation source and the specimen; * spec/anal, collimation between the specimen and the analyser; * anal/detc, collimation between the analyser and the detector; * spec/detc, collimation between the specimen and the detector. Note that * src/mono is used in place of * src/mono and * mono/spec if there is no monochromator in use, and * spec/detc is used in place of * spec/anal and * anal/detc if there is no analyser in use.

May appear in list. The permitted range is 0.0 → ∞.
The permitted range is 0 → ∞.

_Axis and equatorial intrinsic dimensions of the radiation source (in millimetres). The perpendicular to the plane containing the incident and scattered beam is the axial (*_ax_) direction.

The permitted range is 0 → ∞.

_A brief description of the instrument giving details that cannot be given in other _pd_instr_entries_.

The permitted range is −180.0 → 180.0.

_The length of the specimen that is illuminated by the radiation source (in millimetres) for instruments where the illumination length varies with 2θ (fixed divergence slits). The _pd_instr_var_illum_len values should be included in the same loop as the intensity measurements (_pd_meas_). See _pd_instr_cons_illum_len for instruments where the divergence slit is θ-compensated to yield a constant illumination length.

Appears in list.

The permitted range is 0 → ∞.

_The date and time of the data-set measurement. Entries follow the standard CIF format ‘yyyy-mm-ddThh:mm:ss’. Use of seconds and a time zone is optional, but use of hours and minutes is strongly encouraged. Where possible, give the time when the measurement was started rather than when it was completed.


_A code or number which identifies the measuring detector or multiple detector instrument. Calibration information, such as angle offsets or a calibration function to convert channel numbers to Q, energy, wavelength, angle etc. should be described with _pd_calib_values. If _pd_calibration_conversion_eqn is used, the detector IDs should be the number to be used in the equation.

Appears in list. Must match parent data name _pd_calib_detector_id [pd_data]

_The address of the person who measured the data set. If there is more than one person, this will be looped with _pd_meas_info_author_address [pd_info]

The e-mail address of the person who measured the data set. If there is more than one person, this will be looped with _pd_meas_info_author_email [pd_info]

| _pd_meas_info_author_name | ‘Cranswick, Lachlan’ |
| _pd_meas_info_author_email | lachlan@dmp.csiro.au |
| _pd_meas_info_author_address | ? |
| _pd_meas_datetime_initiated | 1992-03-23T17:20 |
| _pd_meas_method | step |
| _pd_meas_2theta_range_min | 6.0 |
| _pd_meas_2theta_range_max | 164.0 |
| _pd_meas_2theta_range_inc | 0.025 |
| _pd_meas_step_count_time | 2.0 |
### 4. DATA DICTIONARIES

**_pd_meas_info_author_fax_**

The fax number of the person who measured the data set. If there is more than one person, this will be looped with _pd_meas_info_author_name_. The recommended style is the international dialing prefix, followed by the area code in parentheses, followed by the local number with no spaces.

May appear in list containing _pd_meas_info_author_name_. [pd_meas_info]

**_pd_meas_info_author_name_**

The name of the person who measured the data set. The family name(s), followed by a comma and including any dynastic components, precedes the first name(s) or initial(s). For more than one person use a loop to specify multiple values.

May appear in list. [pd_meas_info]

**_pd_meas_info_author_phone_**

The telephone number of the person who measured the data set. If there is more than one person, this will be looped with _pd_meas_info_author_name_. The recommended style is the international dialing prefix, followed by the area code in parentheses, followed by the local number with no spaces.

May appear in list containing _pd_meas_info_author_name_. [pd_meas_info]

**_pd_meas_intensity_total_**

**_pd_meas_intensity_background_**

**_pd_meas_intensity_container_**

**_pd_meas_intensity_monitor_**

Intensity measurements at the measurement point (see the definition of _pd_meas_2theta_). The defined fields are: _pd_meas_intensity_total_, scattering from the specimen (with background, specimen mounting or container scattering included); _pd_meas_intensity_background_, scattering measured without a specimen, specimen mounting etc., often referred to as the instrument background; _pd_meas_intensity_container_, the specimen container or mounting without a specimen, includes background; _pd_meas_intensity_monitor_, intensity measured by an incident-beam monitor to calibrate the flux on the specimen. Use these entries for measurements where intensity values are not counts (use _pd_meas_counts_ for event-counting measurements where the standard uncertainty is estimated as the square root of the number of counts). Corrections for background, detector deadtime etc., should not have been made to these values. Instead use _pd_proc_intensity_ for corrected diffractograms. _pd_meas_units_of_intensity_ should be used to specify the units of the intensity measurements.

Appears in list. [pd_data]

**_pd_meas_number_of_points_**

The total number of points in the measured diffractogram.

The permitted range is $1 \rightarrow \infty$. [pd_meas_method]

**_pd_meas_point_id_**

Arbitrary label identifying a measured data point. Used to identify a specific entry in a list of measured intensities. The role of this identifier may be adopted by _pd_data_point_id_ if measured, processed and calculated intensity values are combined in a single list.

Related item: _pd_data_point_id_ (alternate). [pd_data]

**_pd_meas_position_**

A linear distance in millimetres corresponding to the location where an intensity measurement is made. Used for detectors where a distance measurement is made as a direct observable, such as from a microdensitometer trace from film or a strip chart recorder. This is an alternative to _pd_meas_2theta_scan, which should only be used for instruments that record intensities directly against 2\(\theta\). For instruments where the position scale is nonlinear, the data item _pd_meas_detector_id_ should be used to record positions. Calibration information, such as angle offsets or a function to convert this distance to a 2\(\theta\) angle or d-space, should be supplied with the _pd_calib_ values. Do not confuse this with the instrument geometry descriptions given by _pd_instr_dist_. Appears in list. [pd_data]

**_pd_meas_rocking_angle_**

The angular range in degrees through which a sample is rotated or oscillated during a measurement step (see _pd_meas_rocking_axis_).

May appear in list.

The permitted range is $0 \rightarrow 360.0$. [pd_data]

**_pd_meas_rocking_axis_**

Description of the axis (or axes) used to rotate or rock the specimen for better randomization of crystallites (see _pd_meas_rocking_angle_).

The data value must be one of the following:

- chi
- omega
- phi

[pd_meas_method]

**_pd_meas_scan_method_**

Code identifying the method for scanning reciprocal space. The designation ‘fixed’ should be used for measurements where film, a stationary position-sensitive or area detector or other non-moving detection mechanism is used to measure diffraction intensities.

The data value must be one of the following:

- step
- step scan
- cont
- continuous scan
- tof
- time of flight
- disp
- energy dispersive
- fixed
- stationary detector

[pd_meas_method]

**_pd_meas_special_details_**

Special details of the diffraction measurement process. Include information about source instability, degradation etc. However, this item should not be used to record information that can be specified in other _pd_meas_ entries.

[pd_meas_method]

**_pd_meas_step_count_time_**

The count time in seconds for each intensity measurement. If this value varies for different intensity measurements, then this item will be placed in the loop with the diffraction measurements. If a single fixed value is used, it may be recorded outside the loop.

May appear in list.

The permitted range is $0.0 \rightarrow \infty$. [pd_data]

**_pd_meas_2theta_fixed_**

The 2\(\theta\) diffraction angle in degrees for measurements in a white-beam fixed-angle experiment. For measurements where 2\(\theta\) is scanned, see _pd_meas_2theta_scan_ or _pd_meas_2theta_range_.

The permitted range is $-180.0 \rightarrow 360.0$. [pd_meas_method]
**PD_PEAK**

This section contains peak information extracted from the measured or, if present, the processed diffractogram. Each peak in this table will have a unique label (see _pd_peak_id_). The reflections and phases associated with each peak will be specified in other sections (see the _pd_refln_ and _pd_phase_ sections). Note that peak positions are customarily determined from the processed diffractogram and thus corrections for position and intensity will have been previously applied.

### _pd_peak_d_spacing_ (numb, su)

Peak position as a d-spacing in ångströms.

The permitted range is 0.0 → ∞.

### _pd_peak_id_ (char)

An arbitrary code is assigned to each peak. Used to link with _pd_refln_peak_id_ so that multiple hkl and/or phase identifications can be assigned to a single peak. Each peak will have a unique code. In cases where two peaks are severely overlapped, it may be desirable to list them as a single peak. A peak ID must be included for every peak.

Appears in list as essential element of loop structure. May match child data name(s): _pd_refln_peak_id_.

### _pd_peak_pk_height_ (numb, su)

The maximum intensity of the peak, either extrapolated or the highest observed intensity value. The same scaling is used for the _pd_proc_intensity_ values. It is good practice to include s.u.'s for these values.

Appears in list containing _pd_peak_id_.

### _pd_peak_special_details_ (char)

Detailed description of any non-routine processing steps used for peak determination or other comments related to the peak table that cannot be given elsewhere.

Appears in list containing _pd_peak_id_.

### _pd_peak_wavelength_id_ (char)

Code identifying the wavelength appropriate for this peak from the wavelengths in the _diffrn_radiation_ list. (See _diffrn_radiation_wavelength_id_.)

For complex peak tables with multiple superimposed peaks, specify wavelengths in the reflection table using _pd_refln_wavelength_id_ rather than identifying peaks by wavelength.

Appears in list containing _pd_peak_id_. Must match parent data name _diffrn_radiation_wavelength_id_.

### _pd_peak_width_d_spacing_ (numb, su)

Peak width as full-width at half-maximum expressed as a d-spacing in ångströms.

Appears in list containing _pd_peak_id_.

### _pd_peak_width_2theta_ (numb, su)

Peak width as full-width at half-maximum expressed as a 2θ value in degrees.

Appears in list containing _pd_peak_id_.

**PD_PHASE**

This section contains a description of the crystalline phases contributing to the powder diffraction data set. Note that if multiple-phase Rietveld or other structural analysis is performed, the structural results will be placed in different data blocks, using CIF entries from the core CIF dictionary. The _pd_phase_block_id_ entry points to the CIF block with structural parameters for each crystalline phase. The _pd_phase_id_ serves to link to _pd_refln_phase_id_, which is used to label peaks by phase.
The permitted range is $0 \rightarrow \infty$.

Per cent composition of the specified crystal phase expressed as the total mass of the component with respect to the total mass of the specimen.

Appears in list containing _pd_phase_id

The name of the crystal phase identified by _pd_phase_id. It may be designated as unknown or by a structure type etc.

May appear in list containing _pd_phase_id

This section contains descriptive information about how the sample was prepared.

A description of how the material was prepared (reaction conditions etc.)

Cooling rate in kelvins per minute for samples prepared at high temperatures. If the cooling rate is not linear or is unknown (e.g., quenched samples), it should be described in _pd_prep_conditions instead.

The permitted range is $0 \rightarrow \infty$.

Preparation pressure of the sample in kilopascals. This is particularly important for materials which are metastable at the measurement pressure, diffrn_ambient_pressure.

The permitted range is $0 \rightarrow \infty$.

Preparation temperature of the sample in kelvins. This is particularly important for materials which are metastable at the measurement temperature, diffrn_ambient_temperature.

The permitted range is $0 \rightarrow \infty$.

This section contains the diffraction data set after processing and application of correction terms. If the data set is reprocessed, this section may be replaced (with the addition of a new _pd_block_id entry).

Incident energy in electronvolts of the source computed from secondary calibration information (time-of-flight and synchrotron data). Detection energy in electronvolts selected by the analyser, if not the same as the incident energy (triple-axis or energy-dispersive data). This may be a single value or may vary for each data point (triple-axis and time-of-flight data).

The permitted range is $0 \rightarrow \infty$.

The address of the person who processed the data. If there is more than one person, this will be looped with _pd_proc_info_author_name.

The telephone number of the person who processed the data. If there is more than one person, this will be looped with _pd_proc_info_author_phone.

The name of the person who processed the data, if different from the person(s) who measured the data set. The family name(s), followed by a comma and including any dynastic components, precedes the first name(s) or initial(s). For more than one person use a loop to specify multiple values.

The recommended style is the international dialing prefix, followed by the area code in parentheses, followed by the local number with no spaces.

The fax number of the person who processed the data. If there is more than one person, this will be looped with _pd_proc_info_author_fax.

The e-mail address of the person who processed the data. If there is more than one person, this will be looped with _pd_proc_info_author_email.

Date(s) and time(s) when the data set was processed. May be looped if multiple processing steps were used. Dates and times should be specified in the standard CIF format 'yyyy-mm-ddThh:mm:ss±zzz'. Use of seconds and a time zone is optional, but use of hours and minutes is strongly encouraged.

Example: '1990-07-13T14:40'.
4.2. POWDER DICTIONARY (pdCIF)

**_pd_proc_info_excluded_regions_** (char)
Description of regions in the diffractogram excluded from processing along with a justification of why the data points were not used. Example: ‘20 to 21 degrees unreliable due to beam dump.’

**_pd_proc_info_special_details_** (char)
Detailed description of any non-routine processing steps applied due to any irregularities in this particular data set.

**_pd_proc_intensity_net_**

**_pd_proc_intensity_total_**

**_pd_proc_intensity_bkg_calc_**

**_pd_proc_intensity_bkg_fix_**

**_pd_proc_intensity_incident_**

**_pd_proc_intensity_corrected_**

**_pd_proc_intensity_norm_** (numb, su)

_**_pd_proc_intensity_net_** contains intensity values for the processed diffractogram for each data point (see _pd_proc_2theta, _pd_proc_wavelength_ etc.) after correction and normalization factors have been applied (in contrast to _pd_meas_counts_ values, which are uncorrected). _**_pd_proc_intensity_total_** contains intensity values for the processed diffractogram for each data point where background, normalization and other corrections have not been applied. Inclusion of s.u.’s for these values is strongly recommended. _**_pd_proc_intensity_bkg_calc_** is intended to contain the background intensity for every data point where the background function has been fitted or estimated (for example, in all Rietveld and profile fits). If the background is estimated for a limited number of points and the calculated background is then extrapolated from these fixed points, indicate the background values for these points with _pd_proc_intensity_bkg_fix_. Use a value of ‘.’ for data points where a fixed background has not been defined.

The extrapolated background at each point may be specified using _**_pd_proc_intensity_bkg_calc_**. Background values should be on the same scale as the _pd_proc_intensity_net_ values. Thus normalization and correction factors should be applied before background subtraction (or should be applied to the background values equally). If the intensities have been corrected for a variation of the incident intensity as a function of a data-collection variable (examples: source fluctuations in synchrotrons, \(\theta\)-compensated slits in conventional diffractometers, spectral corrections for white-beam experiments), the correction function should be specified as _pd_proc_intensity_incident_. The normalization should be specified in _**_pd_proc_intensity_incident_** as a value to be used to divide the measured intensities to obtain the normalized diffractogram. Thus, the _**_pd_proc_intensity_incident_** values should increase as the incident flux is increased. The other normalization factors applied to the data set (for example, Lp corrections, compensation for variation in counting time) may be specified in _**_pd_proc_intensity_norm_**. The function should be specified as the one used to divide the measured intensities.

Appears in list.
The permitted range is \(0.0 \rightarrow \infty\).

**_pd_proc_2theta_corrected_** (numb)
The 2\(\theta\) diffraction angle in degrees of an intensity measurement where 2\(\theta\) is not constant. Used if corrections such as for nonlinearity, zero offset etc. have been applied to the _pd_meas_2theta_ values or if 2\(\theta\) values are computed. If the 2\(\theta\) values are evenly spaced, _pd_proc_2theta_range_min, _pd_proc_2theta_range_max and _pd_proc_2theta_range_inc may be used to specify the 2\(\theta\) values.

Appears in list.
The permitted range is \(-180.0 \rightarrow 180.0\).

**_pd_proc_2theta_range_min_**

**_pd_proc_2theta_range_max_**

**_pd_proc_2theta_range_inc_** (numb)
The range of 2\(\theta\) diffraction angles in degrees for the measurement of intensities. These may be used in place of the _**_pd_proc_2theta_corrected_** values, or in the case of white-beam experiments it will define the fixed 2\(\theta\) value.

The permitted range is \(-180.0 \rightarrow 180.0\).

**_pd_proc_ls_background_function_** (char)
Description of the background treatment mechanism used to fit the data set. For refinements where the background is computed as a function that is fitted to minimize the difference between the observed and calculated patterns, it is recommended that in addition to a description of the function (e.g. Chebychev polynomial), the actual equation(s) used are included in TeX, or a programming language such as Fortran or C. Include also the values used for the coefficients used in the background function with their s.u.’s. The background values for each data point computed from the function should be specified in _**_pd_proc_intensity_bkg_calc_**. If background correction is performed using extrapolation from a set of points at fixed locations, these points should be defined using _**_pd_proc_intensity_bkg_calc_** and _**_pd_proc_ls_background_function_** should indicate the extrapolation method (linear extrapolation, spline etc.). _**_pd_proc_ls_background_function_** should also indicate how the points were determined (automatically, by visual estimation etc.) and whether the values were refined to improve the agreement. The extrapolated background intensity value for each data point should be specified in _**_pd_proc_intensity_bkg_calc_**.

**_pd_proc_ls_peak_cutoff_** (numb)
Describes where peak-intensity computation is discontinued as a fraction of the intensity of the peak at maximum. Thus for a value of 0.005, the tails of a diffraction peak are neglected after the intensity has dropped below 0.5% of the diffraction intensity at the maximum.

**_pd_proc_ls_pref_orient_corr_** (char)
Description of the preferred-orientation correction if such a correction is used. Omitting this entry implies that no preferred-orientation correction has been used. If a function form is used, it is recommended that the actual equation in TeX, or a programming language, is used to specify the function as well as a giving a description. Include the value(s) used for the correction with s.u.’s.
Rietveld/profile fit R factors. Note that the R factor computed for Rietveld refinements using the extracted reflection intensity values (often called the Rietveld or Bragg R factor, $R_p$) is not properly a profile R factor. This R factor may be specified using \_refine\_ls\_R\_I\_factor. (Some authors report \_refine\_ls\_Fsqd\_factor or \_refine\_ls\_R\_I\_factor all as the Rietveld or Bragg R factor. While it is appropriate to compute and report any or all of these R factors, the names ‘Rietveld or Bragg R factor’ refer strictly to \_refine\_ls\_R\_I\_factor.)

\_pd\_proc\_ls\_prof\_R\_factor, often called $R_p$, is an unweighted fitness metric for the agreement between the observed and computed diffraction patterns.

$$R_p = \sum_i |I_{\text{obs}}(i) - I_{\text{calc}}(i)| / \sum_i |I_{\text{obs}}(i)|.$$

\_pd\_proc\_ls\_prof\_wr\_factor, often called $R_{wp}$, is a weighted fitness metric for the agreement between the observed and computed diffraction patterns.

$$R_{wp} = \left( \frac{\sum_i (w(i)|I_{\text{obs}}(i) - I_{\text{calc}}(i)|^2)}{\sum_i (w(i)|I_{\text{obs}}(i)|^2) \right)^{1/2}.$$

\_pd\_proc\_ls\_prof\_wr\_expected, sometimes called the theoretical $R_{wp}$ or $R_{wp}$, is a weighted fitness metric for the statistical precision of the data set. For an idealized fit, where all deviations between the observed intensities and those computed from the model are due to statistical fluctuations, the observed $R_{wp}$ should match the expected $R$ factor. In reality, $R_{wp}$ will always be higher than $R_{exp}$.

$$R_{exp} = \left( \frac{n - p}{\sum_i (w(i)|I_{\text{obs}}(i)|^2) \right)^{1/2}.$$

Note that in the above equations, $w(i)$ is the weight for the $i$th data point (see \_pd\_proc\_ls\_weight). $I_{\text{obs}}(i)$ is the observed intensity for the $i$th data point, sometimes referred to as $y_i(\text{obs})$ or $y_{xi}$. (See \_pd\_meas\_count\_total, \_pd\_meas\_intensity\_total or \_pd\_proc\_intensity\_total) $I_{\text{calc}}(i)$ is the computed intensity for the $i$th data point with background and other corrections applied to match the scale of the observed data set, sometimes referred to as $y_i(\text{calc})$ or $y_x$. (See \_pd\_calc\_intensity\_total.) $n$ is the total number of data points (see \_pd\_proc\_number\_of\_points) less the number of data points excluded from the refinement. $p$ is the total number of refined parameters.

The permitted range is 0.0 → ∞.

\_pd\_proc\_ls\_weight (numb)

Weight applied to each profile point. These values may be omitted if the weights are 1/u^2, where u is the s.u. for the \_pd\_proc\_intensity\_net values. A weight value of zero is used to indicate a data point not used for refinement (see \_pd\_proc\_info\_excluded\_regions).

Appears in list. The permitted range is 0 → ∞.

\_pd\_proc\_number\_of\_points (numb)

The total number of data points in the processed diffractogram.

The permitted range is 1 → ∞.

\_pd\_proc\_point\_id (char)

Arbitrary label identifying a processed data point. Used to identify a specific entry in a list of processed intensities. The role of this identifier may be adopted by \_pd\_data\_point\_id if measured, processed and calculated intensity values are combined in a single list, or by \_pd\_meas\_point\_id if measured and processed lists are combined.

Related items:
\_pd\_data\_point\_id(alternate), \_pd\_meas\_point\_id(alternate).

\_pd\_proc\_recip\_len\_Q (numb)

Length in reciprocal space ($|Q| = 2\pi/d$) corresponding to an intensity point. Units are inverse angstroms.

Appears in list. The permitted range is 0.0 → ∞.

\_pd\_proc\_wavelength (numb)

Wavelength in angstroms for the incident radiation as computed from secondary calibration information. This will be most appropriate for time-of-flight and synchrotron measurements. This will be a single value for continuous-wavelength methods or may vary for each data point and be looped with the intensity values for energy-dispersive measurements.

May appear in list. The permitted range is 0.0 → ∞.

PD_REFLN

This section provides a mechanism to identify each peak in the peak-table section (\_pd\_peak\_) with the phase(s) (\_pd\_phase\_id) and the reflection indices (\_refln\_index\_) associated with the peak. There are no restrictions on the number of phases or reflections associated with an observed peak. Reflections may also be included that are not observed; use ‘.’ for the \_pd\_refln\_peak\_id.

\_pd\_refln\_peak\_id (char)

Code which identifies the powder diffraction peak that contains the current reflection. This code must match a \_pd\_peak\_id code.

Appears in list containing \_refln\_index\_h \_refln\_index\_k \_refln\_index\_l. Must match parent data name \_pd\_peak\_id.

\_pd\_refln\_phase\_id (char)

Code which identifies the crystal phase associated with this reflection. This code must match a \_pd\_phase\_id code.

Appears in list containing \_refln\_index\_h \_refln\_index\_k \_refln\_index\_l. Must match parent data name \_pd\_phase\_id.

\_pd\_refln\_wavelength\_id (char)

Code which identifies the wavelength associated with the reflection and the peak pointed to by \_pd\_refln\_peak\_id. This code must match a \_diffrn\_radiation\_wavelength\_id code.

Appears in list containing \_refln\_index\_h \_refln\_index\_k \_refln\_index\_l. Must match parent data name \_diffrn\_radiation\_wavelength\_id.
This section contains information about the specimen used for measurement of the diffraction data set. Note that information about the sample (the batch of material from which the specimen was obtained) is specified in \_pd_prep\_.

**Example 1.**

<table>
<thead>
<tr>
<th>pd_spec_montaging</th>
<th>?</th>
</tr>
</thead>
<tbody>
<tr>
<td>pd_spec_mount_mode</td>
<td>transmission</td>
</tr>
<tr>
<td>pd_spec_orientation</td>
<td>horizontal</td>
</tr>
<tr>
<td>pd_spec_preparation</td>
<td>?</td>
</tr>
</tbody>
</table>

**pd_spec_description**  
A description of the specimen, such as the source of the specimen, identification of standards, mixtures etc.

**pd_spec_mont_mode**  
A code describing the beam path through the specimen.
The data value must be one of the following:
- reflection
- transmission

**pd_spec_montaging**  
A description of how the specimen is mounted.
Examples: 'vanadium can with He exchange gas', 'quartz capillary', 'packed powder pellet', 'drifted powder on off-cut Si', 'drifted powder on Kapton film'.

**pd_spec_orientation**  
The orientation of the $\omega$ ($\theta$) and $2\theta$ axis. Note that this axis is parallel to the specimen axial axis and perpendicular to the plane containing the incident and scattered beams. Thus for a horizontal orientation, scattering measurements are made in a plane perpendicular to the ground (the $2\theta$ axis is parallel to the ground); for vertical orientation, scattering measurements are made in a plane parallel with the ground. 'Both' is appropriate for experiments where measurements are made in both planes, for example using two-dimensional detectors.
The data value must be one of the following:
- horizontal
- vertical
- both

**pd_spec_preparation**  
A description of the preparation steps for producing the diffraction specimen from the sample. Include any procedures related to grinding, sieving, spray drying etc. For information relevant to how the sample is synthesized, use the \_pd_prep\_ entries.
Examples: 'wet grinding in acetone', 'sieved through a 44 micron (325 mesh/inch) sieve', 'spray dried in water with 1% clay'.

**pd_spec_shape**  
A code describing the specimen shape.
The data value must be one of the following:
- cylinder
- flat_sheet
- irregular

**pd_spec_size_axial**  
**pd_spec_size_equat**  
**pd_spec_size_thick**  
The size of the specimen in three mutually perpendicular directions in millimetres. The perpendicular to the plane containing the incident and scattered beam is the *axial direction. In transmission geometry, the scattering vector is parallel to *equat and in reflection geometry the scattering vector is parallel to *thick. The permitted range is 0.0 → ∞.

**pd_spec_special_details**  
Descriptive information about the specimen that cannot be included in other data items.