4.2. Powder dictionary (pdCIF)

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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.

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 designed to ensure uniqueness. It is the responsibility of a data archive site or local laboratory to create a catalogue of block IDs if that site wishes to resolve these references.

_pd_block_diffractogram_id *(char)*

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**.

Appears in list. **[pd_proc]**

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_pd_block_id *(char)*

Used to assign a unique character string to a block. Note that this code is not intended to be parsed; the concatenation of several strings is used in order to generate a string that can reasonably be expected to be unique.

This code is assigned by the originator of the data set and is used for references between different CIF blocks. The ID will normally be created when the block is first created. It is possible to loop more than one ID for a block: if changes or additions are made to the block later, a new ID may be assigned, but the original name should be retained.

The format for the ID code is

$$\langle\textit{date-time}\rangle | \langle\textit{block\_name}\rangle | \langle\textit{creator\_name}\rangle | \langle\textit{instr\_name}\rangle.$$

$\langle\textit{date-time}\rangle$ is the date and time the CIF was created or modified. $\langle\textit{block\_name}\rangle$ is an arbitrary name assigned by the originator of the data set. It will usually match the name of the phase and possibly the name of the current CIF data block (*i.e.* the string *xxxx* in a **data_xxxx** identifier). It may be a sample name. $\langle\textit{creator\_name}\rangle$ is the name of the person who measured the diffractogram, or prepared or modified the CIF. $\langle\textit{instr\_name}\rangle$ is a unique name (as far 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.* $\langle\textit{block\_name}\rangle$) should be retained, but the $\langle\textit{creator\_name}\rangle$ may be changed and the $\langle\textit{date-time}\rangle$ will always change. The $\langle\textit{date-time}\rangle$ 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-Z a-z 0-9 # & * . : , - _ + / ( ) \ [ ]
```

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 '*yyyy-mm-dd*T*hh*:*mm*:*ss*+*zz*'. 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 ID 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 ($\langle\textit{creator\_name}\rangle$ and $\langle\textit{instr\_name}\rangle$). Note that this should not be done unless the archive site is prepared to keep the file available online indefinitely.

May appear in list.

Examples: '`1991-15-09T16:54|Si-std|B.Toby|D500#1234-987`', '`1991-15-09T16:54|SEPD7234|B.Toby|SEPD.IPNS.ANL.GOV`'. **[pd_block]**

PD_CALC

This section is used for storing a computed diffractogram trace. This may be a simulated powder pattern for a material from a program such as *LAZY/PULVERIX* or the computed intensities from a Rietveld refinement.

_pd_calc_intensity_net
_pd_calc_intensity_total   (*numb*)

Intensity values for a computed diffractogram at each angle setting. Values should be computed at the same locations as the processed diffractogram, and thus the numbers of points will be defined by **_pd_proc_number_of_points** and point positions may be defined using **_pd_proc_2theta_range_** or **_pd_proc_2theta_corrected**. Use **_pd_calc_intensity_net** if the computed diffractogram does not contain background or normalization corrections and thus is specified on the same scale as the **_pd_proc_intensity_net** values. Use **_pd_calc_intensity_total** if the computed diffraction pattern includes background or normalization corrections (or both) and thus is specified on the same scale as the observed intensities (**_pd_meas_counts_** or **_pd_meas_intensity_**). If an observed pattern is included, **_pd_calc_intensity_** should be looped with either **_pd_proc_intensity_net**, **_pd_meas_counts_** or **_pd_meas_intensity_**.

Appears in list.

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

_pd_calc_method   (*char*)

A description of the method used for the calculation of the intensities in **_pd_calc_intensity_**. If the pattern was calculated from crystal structure data, the atom coordinates and other crystallographic information should be included using the core CIF **_atom_site_** and **_cell_** data items.

     [pd_calc]

_pd_calc_point_id   (*char*)

Arbitrary label identifying a calculated data point. Used to identify a specific entry in a list of values forming the calculated diffractogram. 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_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.

```
_pd_calib_std_external_block_id
      QuartzPlate|D500#1234-987|B.Toby|91-15-09|14:02
_pd_calib_std_external_name
      'Arkansas Stone quartz plate'
```

Example 2.

$2\theta_{actual} = 2\theta_{setting} + arctan(cos(P_1) / \{1/[P_0 (CC - CH_0 - P_2 CC^2)] - sin(P_1)\})$.
This allows for the calibration of 2θ for a linear position-sensitive detector (PSD) where the PSD has been set so 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 nonlinearities in the detector.*

```
_pd_calibration_conversion_eqn
; 2\q~actual~ = 2\q~setting~ + arctan(
cos(P~1~)/{1/[P~0~ (CC - CH~0~ - P~2~ CC^2^)] - sin(P~1~)})
;
```

_pd_calib_detector_id   (*char*)

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):
_pd_meas_detector_id.   **[pd_calib]**

_pd_calib_detector_response   (*numb*)

A value that indicates the relative sensitivity of each detector. This can compensate for differences in electronics, size and collimation. Usually, one detector or the mean for all detectors will be assigned the value of 1.

Appears in list containing **_pd_calib_detector_id**.

The permitted range is $0.0 \to \infty$.   **[pd_calib]**

_pd_calib_std_external_block_id
_pd_calib_std_external_name   (*char*)

Identifies the data set used as an external standard for the diffraction angle or the intensity calibrations. *_name specifies the name of the material and *_id the **_pd_block_id** for the CIF containing calibration measurements. If more than one data set is used for calibration, these fields may be looped.

May appear in list containing **_pd_calib_detector_id**.   **[pd_calib]**

_pd_calib_std_internal_mass_%   (*numb, su*)

Per cent presence of the internal standard specified by the data item **_pd_calib_std_internal_name** expressed as 100 times the ratio of the amount of standard added to the original sample mass.

May appear in list containing **_pd_calib_detector_id**.

The permitted range is $0.0 \to 100.0$.   **[pd_calib]**

_pd_calib_std_internal_name   (*char*)

Identity of material(s) used as an internal intensity standard.

May appear in list containing **_pd_calib_detector_id**.

Examples: 'NIST 640a Silicon standard', 'Al2O3'.   **[pd_calib]**

_pd_calib_2theta_offset
_pd_calib_2theta_off_point
_pd_calib_2theta_off_min
_pd_calib_2theta_off_max   (*numb*)

_pd_calib_2theta_offset defines an offset angle (in degrees) used to calibrate 2θ (as defined in **_pd_meas_2theta_**). Calibration is done by adding the offset:

$$2\theta_{calibrated} = 2\theta_{measured} + 2\theta_{offset}.$$

For cases where the **_pd_calib_2theta_offset** value is not a constant, but rather varies with 2θ, a set of offset values can be supplied in a loop. In this case, the value where the offset has been determined can be specified as **_pd_calib_2theta_off_point**. Alternatively, a range where the offset is applicable can be specified using **_pd_calib_2theta_off_min** and **_pd_calib_2theta_off_max**.

May appear in list containing **_pd_calib_detector_id**.

The permitted range is $-180.0 \to 180.0$.   **[pd_calib]**

_pd_calibration_conversion_eqn   (*char*)

The calibration function for converting a channel number supplied in **_pd_meas_detector_id** for a position-sensitive or energy-dispersive detector or the distance supplied in **_pd_meas_position** to Q, energy, angle *etc*. Use **_pd_calib_std_external_** to define a pointer to the file or data block containing the information used to define this function.

Example:
```
; 2\q~actual~ = 2\q~setting~ + arctan(
cos(P~1~) / {1/[P~0~ (CC - CH~0~ - P~2~ CC^2^)] - sin(P~1~)})
;
```
     [pd_calibration]

_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

This section contains experimental (non-diffraction) information relevant to the chemical and physical nature of the material.

_pd_char_atten_coef_mu_obs
_pd_char_atten_coef_mu_calc   (*numb*)

The observed and calculated linear attenuation coefficient, μ, 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 μ will be obtained from the atomic content of the cell, the average density (allowing for specimen packing) and the radiation wavelength. The observed μ will be determined by a transmission measurement. Note that **_pd_char_atten_coef_mu_calc** will differ from **_exptl_absorpt_coefficient_mu** if the packing density is not unity.

The permitted range is $0.0 \rightarrow \infty$.   **[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.

Examples: 'dark_green', 'orange_red', 'brownish_red', 'yellow_metallic'.   **[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

The PD_DATA category contains raw, processed and calculated data points in a diffraction data set. In many cases, it is convenient to tabulate calculated values against the raw and processed measurements, and so the various **_pd_meas_**, **_pd_proc_** and **_pd_calc_** data items belonging to this category may be looped together. In some instances, however, it makes more sense to maintain separate tables of the data contributing to the measured and processed diffractograms (for example, a profile may be calculated at 2θ values different from those of the measured data points). To facilitate the identification of equivalent points in these separate tables, separate identifiers are defined.

Example 1 – data set collected for a two-phase sample (Al_2O_3/Si) by B. H. Toby, '1997-01-29T16:37|POWSET_01|B.Toby|..NIST-D5000'.

```
loop_
  _pd_data_point_id
  _pd_meas_intensity_total
  _pd_proc_ls_weight
  _pd_proc_intensity_bkg_calc
  _pd_calc_intensity_total
    1     240(15)      0.00417      214.5    214.5
    2     219(15)      0.00457      214.3    214.2
    3     206(14)      0.00485      214.0    214.0
    4     212(15)      0.00472      213.8    213.7
    5     190(14)      0.00526      213.5    213.5
    6     203(14)      0.00493      213.2    213.2
# - - - - data truncated for brevity - - - -
```

Example 2 – the data of Example 1 split into three separate tables.

```
loop_
  _pd_meas_point_id
  _pd_meas_intensity_total
    1  240(15) 2  219(15) 3  206(14) 4  212(15) 5  190(14)
    6  203(14)

loop_
  _pd_proc_point_id
  _pd_proc_ls_weight
  _pd_proc_intensity_bkg_calc
    1  0.00417  214.5      2  0.00457  214.3
    3  0.00485  214.0      4  0.00472  213.8
    5  0.00526  213.5      6  0.00493  213.2
loop_
  _pd_calc_point_id
  _pd_calc_intensity_total
    1    214.5 2    214.2 3    214.0 4    213.7 5    213.5
    6    213.2
```

Example 3 – hypothetical example where the measured and calculated points are not in one-to-one correspondence.

```
  loop_
_pd_meas_point_id
_pd_meas_2theta_scan
_pd_meas_intensity_total
     1   21.0    24
     2   21.2    32
     3   21.4    67
     4   21.6    98

  loop_
_pd_calc_point_id
_pd_proc_2theta_corrected
_pd_calc_intensity_total
     1    21.0   26
     1a   21.3   56
     4    21.6   76
     4a   21.9   90
```

_pd_data_point_id   (*char*)

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

[pd_data]

PD_INSTR

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_polarisn_ratio` for the source polarization, `_diffrn_radiation_probe` for the radiation type. For data sets measured with partially monochromatized radiation, for example, where both $K\alpha_1$ and $K\alpha_2$ 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 $K\alpha_1$ and $K\alpha_2$ 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 $0.0 \rightarrow \infty$.   **[pd_data]**

_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]**

_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 $0.0 \rightarrow \infty$.   **[pd_instr]**

_pd_instr_dist_src/mono
_pd_instr_dist_mono/spec
_pd_instr_dist_src/spec
_pd_instr_dist_spec/anal
_pd_instr_dist_anal/detc
_pd_instr_dist_spec/detc   (*numb*)
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 $0.0 \rightarrow \infty$.   **[pd_instr]**

_pd_instr_divg_ax_src/mono
_pd_instr_divg_ax_mono/spec
_pd_instr_divg_ax_src/spec
_pd_instr_divg_ax_spec/anal
_pd_instr_divg_ax_anal/detc
_pd_instr_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 $0.0 \rightarrow \infty$.   **[pd_instr]**

_pd_instr_divg_eq_src/mono
_pd_instr_divg_eq_mono/spec
_pd_instr_divg_eq_src/spec
_pd_instr_divg_eq_spec/anal
_pd_instr_divg_eq_anal/detc
_pd_instr_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 `_pd_instr_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, 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 $0.0 \rightarrow \infty$. **[pd_instr]**

_pd_instr_geometry (*char*)

A description of the diffractometer type or geometry.

Examples: 'Bragg-Brentano', 'Guinier',
; Parallel-beam non-focusing optics with
  channel-cut monochromator and linear
  position-sensitive detector
; **[pd_instr]**

_pd_instr_location (*char*)

The name and location of the instrument where measurements were made. This is used primarily to identify data sets measured away from the author's home facility, at shared resources such as a reactor or spallation source.

Example: 'SEPD diffractometer, IPNS, Argonne National Lab (USA)'.
[pd_instr]

_pd_instr_monochr_pre_spec
_pd_instr_monochr_post_spec (*char*)

Indicates the method used to obtain monochromatic radiation. Use **_pd_instr_monochr_pre_spec** to describe the primary beam monochromator (pre-specimen monochromation). Use **_pd_instr_monochr_post_spec** to specify the post-diffraction analyser (post-specimen monochromation). When a monochromator crystal is used, the material and the indices of the Bragg reflection are specified. Note that monochromators may have either 'parallel' or 'antiparallel' orientation. It is assumed that the geometry is parallel unless specified otherwise. In a parallel geometry, the position of the monochromator allows the incident beam and the final post-specimen and post-monochromator beam to be as close to parallel as possible. In a parallel geometry, the diffracting planes in the specimen and monochromator will be parallel when $2\theta_{\text{monochromator}}$ is equal to $2\theta_{\text{specimen}}$. For further discussion see R. Jenkins & R. Snyder (1996). *Introduction to X-ray Powder Diffraction*, pp. 164–165. New York: Wiley.

May appear in list.

Examples: 'Zr filter', 'Ge 220', 'none',
'equatorial mounted graphite (0001)', 'Si (111), antiparallel'.
[pd_instr]

_pd_instr_slit_ax_src/mono
_pd_instr_slit_ax_mono/spec
_pd_instr_slit_ax_src/spec
_pd_instr_slit_ax_spec/anal
_pd_instr_slit_ax_anal/detc
_pd_instr_slit_ax_spec/detc (*numb*)

Describes collimation in the axial direction (perpendicular to 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/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 $0.0 \rightarrow \infty$. **[pd_instr]**

_pd_instr_slit_eq_src/mono
_pd_instr_slit_eq_mono/spec
_pd_instr_slit_eq_src/spec
_pd_instr_slit_eq_spec/anal
_pd_instr_slit_eq_anal/detc
_pd_instr_slit_eq_spec/detc (*numb*)

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/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 $0.0 \rightarrow \infty$. **[pd_instr]**

_pd_instr_soller_ax_src/mono
_pd_instr_soller_ax_mono/spec
_pd_instr_soller_ax_src/spec
_pd_instr_soller_ax_spec/anal
_pd_instr_soller_ax_anal/detc
_pd_instr_soller_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 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/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 $0.0 \rightarrow \infty$. **[pd_instr]**

_pd_instr_soller_eq_src/mono
_pd_instr_soller_eq_mono/spec
_pd_instr_soller_eq_src/spec
_pd_instr_soller_eq_spec/anal
_pd_instr_soller_eq_anal/detc
_pd_instr_soller_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 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/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 $0.0 \rightarrow \infty$. **[pd_instr]**

_pd_instr_source_size_ax
_pd_instr_source_size_eq (*numb*)
Axial 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 $0.0 \rightarrow \infty$. **[pd_instr]**

_pd_instr_special_details (*char*)
A brief description of the instrument giving details that cannot be given in other _pd_instr_ entries.
[pd_instr]

_pd_instr_2theta_monochr_pre
_pd_instr_2theta_monochr_post (*numb*)
The 2θ angle for a pre-specimen or post-specimen monochromator (see _pd_instr_monochr_pre_spec and _pd_instr_monochr_post_spec).
May appear in list.
The permitted range is $-180.0 \rightarrow 180.0$. **[pd_instr]**

_pd_instr_var_illum_len (*numb*)
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 $0.0 \rightarrow \infty$. **[pd_data]**

PD_MEAS

This section contains the measured diffractogram and information about the conditions used for the measurement of the diffraction data set, prior to processing and application of correction terms. While additional information may be added to the CIF as data are processed and transported between laboratories (possibly with the addition of a new _pd_block_id entry), the information in this section of the CIF will rarely be changed once data collection is complete. Where possible, measurements in this section should have no post-collection processing applied (normalizations, corrections, smoothing, zero-offset corrections *etc.*). Such corrected measurements should be recorded in the _pd_proc_ section. Data sets that are measured as counts, where a standard uncertainty can be considered equivalent to the standard deviation and where the standard deviation can be estimated as the square root of the number of counts recorded, should use the _pd_meas_counts_ fields. All other intensity values should be recorded using _pd_meas_intensity_.

Example 1.

```
_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_scan_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
```

_pd_meas_angle_chi
_pd_meas_angle_omega
_pd_meas_angle_phi
_pd_meas_angle_2theta (*numb*)
The diffractometer angles in degrees for an instrument with an Euler circle. The definitions for these angles follow the convention of *International Tables for X-ray Crystallography* (1974), Vol. IV, p. 276.
May appear in list.
The permitted range is $-180.0 \rightarrow 360.0$. **[pd_data]**

_pd_meas_counts_total
_pd_meas_counts_background
_pd_meas_counts_container
_pd_meas_counts_monitor (*numb*)
Counts measured at the measurement point as a function of angle, time, channel or some other variable (see _pd_meas_2theta_ *etc.*). The defined fields are: _pd_meas_counts_total, scattering from the specimen (with background, specimen mounting or container scattering included); _pd_meas_counts_background, scattering measured without a specimen, specimen mounting *etc.*, often referred to as the instrument background; _pd_meas_counts_container, the specimen container or mounting without a specimen, includes background; _pd_meas_counts_monitor, counts measured by an incident-beam monitor to calibrate the flux on the specimen. Corrections for background, detector deadtime *etc.* should not have been made to these values. Instead use _pd_proc_intensity_ for corrected diffractograms. Note that counts-per-second values should be converted to total counts. If the counting time varies for different points, it may be included in the loop using _pd_meas_step_count_time. Standard uncertainties should not be quoted for these values. If the standard uncertainties differ from the square root of the number of counts, _pd_meas_intensity_ should be used.
Appears in list.
The permitted range is $0 \rightarrow \infty$. **[pd_data]**

_pd_meas_datetime_initiated (*char*)
The date and time of the data-set measurement. Entries follow the standard CIF format '*yyyy-mm-dd*T*hh*:*mm*:*ss*+*zz*'. 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.
Example: '1990-07-13T14:40'. **[pd_meas_method]**

_pd_meas_detector_id (*char*)
A code or number which identifies the measuring detector or channel number in a position-sensitive, energy-dispersive or other 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]**

_pd_meas_info_author_address (*char*)
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_name.
May appear in list containing _pd_meas_info_author_name. **[pd_meas_info]**

_pd_meas_info_author_email (*char*)
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_name.
May appear in list containing _pd_meas_info_author_name. **[pd_meas_info]**

_pd_meas_info_author_fax   (*char*)

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   (*char*)

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   (*char*)

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   (*numb, su*)

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   (*numb*)

The total number of points in the measured diffractogram.

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

_pd_meas_point_id   (*char*)

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   (*numb, su*)

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 2θ. 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 2θ 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   (*numb*)

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   (*char*)

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   (*char*)

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   (*char*)

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   (*numb, su*)

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   (*numb, su*)

The 2θ diffraction angle in degrees for measurements in a white-beam fixed-angle experiment. For measurements where 2θ 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_meas_2theta_range_min
_pd_meas_2theta_range_max
_pd_meas_2theta_range_inc   (*numb*)

The range of 2θ diffraction angles in degrees for the measurement of intensities. These may be used in place of the **_pd_meas_2theta_scan** values for data sets measured with a constant step size.

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

_pd_meas_2theta_scan   (*numb, su*)

2θ diffraction angle (in degrees) for intensity points measured in a scanning method. The scan method used (*e.g.* continuous or step scan) should be specified in the item **_pd_meas_scan_method**. For fixed 2θ (white-beam) experiments, use **_pd_meas_2theta_fixed**. In the case of continuous-scan data sets, the 2θ value should be the value at the midpoint of the counting period. Associated with each **_pd_meas_2theta_scan** value will be **_pd_meas_counts_** items. The 2θ values should not be corrected for nonlinearity, zero offset *etc*. Corrected values may be specified using **_pd_proc_2theta_corrected**. Note that for data sets collected with constant step size, **_pd_meas_2theta_range_** (*_min, *_max and *_inc) may be used instead of **_pd_meas_2theta_scan**.

Appears in list.

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

_pd_meas_time_of_flight   (*numb, su*)

Measured time in microseconds for time-of-flight neutron measurements. Note that the flight distance may be specified using **_pd_instr_dist_** values.

Appears in list.

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

_pd_meas_units_of_intensity   (*char*)

Units for intensity measurements when **_pd_meas_intensity_** is used. Note that use of 'counts' or 'counts per second' here is strongly discouraged: convert the intensity measurements to counts and use **_pd_meas_counts_** and **_pd_meas_step_count_time** instead of **_pd_meas_intensity_**.

Examples: 'estimated from strip chart',
'arbitrary, from film density',
'counts, with automatic deadtime correction applied'.

     [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.

Appears in list containing **_pd_peak_id**.

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

_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]**

_pd_peak_intensity   (*numb, su*)

Integrated area for the peak, with the same scaling as the **_pd_proc_intensity_** values. It is good practice to include s.u.'s for these values.

Appears in list containing **_pd_peak_id**.

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

_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**.

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

_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.

     [pd_peak_method]

_pd_peak_2theta_centroid
_pd_peak_2theta_maximum   (*numb, su*)

Position of the centroid and maximum of a peak as a 2θ angle in degrees.

Appears in list containing **_pd_peak_id**.

The permitted range is $0.0 \rightarrow 180.0$.   **[pd_peak]**

_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**.) Most commonly used to distinguish $K\alpha_1$ peaks from $K\alpha_2$ or to designate where $K\alpha_1$ and $K\alpha_2$ peaks cannot be resolved. 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]**

_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**.

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

_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**.

The permitted range is $0.0 \rightarrow 180.0$.   **[pd_peak]**

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.

_pd_phase_block_id   (*char*)

A block ID code identifying the phase contributing to the diffraction peak. The data block containing the crystallographic information for this phase will be identified with a **_pd_block_id** code matching the code in **_pd_phase_block_id**.

Appears in list containing **_pd_phase_id**.   **[pd_phase]**

_pd_phase_id   (*char*)

A code for each crystal phase used to link with **_pd_refln_phase_id**.

Appears in list as essential element of loop structure. May match child data name(s):
_pd_refln_phase_id.   **[pd_phase]**

_pd_phase_mass_%   (*numb, su*)

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 permitted range is $0.0 \rightarrow 100.0$.   **[pd_phase]**

_pd_phase_name   (*char*)

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**.   **[pd_phase]**

PD_PREP

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

_pd_prep_conditions   (*char*)

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

                                                                        [pd_prep]

_pd_prep_cool_rate   (*numb, su*)

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 $0.0 \rightarrow \infty$.   **[pd_prep]**

_pd_prep_pressure   (*numb, su*)

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 $0.0 \rightarrow \infty$.   **[pd_prep]**

_pd_prep_temperature   (*numb, su*)

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 $0.0 \rightarrow \infty$.   **[pd_prep]**

PD_PROC

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).

_pd_proc_d_spacing   (*numb*)

d-spacing corresponding to an intensity point from Bragg's law, $d = \lambda/(2 \sin \theta)$, in units of ångströms.

Appears in list.
The permitted range is $0.0 \rightarrow \infty$.   **[pd_data]**

_pd_proc_energy_incident
_pd_proc_energy_detection   (*numb*)

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).

May appear in list.
The permitted range is $0.0 \rightarrow \infty$.   **[pd_data]**

_pd_proc_info_author_address   (*char*)

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**.

May appear in list containing **_pd_proc_info_author_name**.   **[pd_proc_info]**

_pd_proc_info_author_email   (*char*)

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_name**.

May appear in list containing **_pd_proc_info_author_name**.   **[pd_proc_info]**

_pd_proc_info_author_fax   (*char*)

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_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_proc_info_author_name**.   **[pd_proc_info]**

_pd_proc_info_author_name   (*char*)

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.

May appear in list.   **[pd_proc_info]**

_pd_proc_info_author_phone   (*char*)

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_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_proc_info_author_name**.   **[pd_proc_info]**

_pd_proc_info_data_reduction   (*char*)

Description of the processing steps applied in the data-reduction process (background subtraction, α_2 stripping, smoothing *etc.*). Include details of the program(s) used *etc.*

                                                                   [pd_proc_info]

_pd_proc_info_datetime   (*char*)

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-dd*T*hh*:*mm*:*ss*+*zz*'. Use of seconds and a time zone is optional, but use of hours and minutes is strongly encouraged.

May appear in list.
Example: '1990-07-13T14:40'.   **[pd_proc_info]**

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_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]

_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_info]

_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_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 every 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, θ-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 obtained 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_data]**

_pd_proc_2theta_corrected   (*numb*)

The 2θ diffraction angle in degrees of an intensity measurement where 2θ is not constant. Used if corrections such as for nonlinearity, zero offset *etc.* have been applied to the **_pd_meas_2theta_** values or if 2θ values are computed. If the 2θ 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 2θ values.

Appears in list.

The permitted range is $-180.0 \rightarrow 180.0$.   **[pd_data]**

_pd_proc_2theta_range_min
_pd_proc_2theta_range_max
_pd_proc_2theta_range_inc   (*numb*)

The range of 2θ 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 2θ value.

The permitted range is $-180.0 \rightarrow 180.0$.   **[pd_proc_info]**

PD_PROC_LS

This section is used to define parameters relevant to a least-squares fit to a powder diffractogram, using a Rietveld or other full-profile (*e.g.* Pawley or Le Bail methods) fit. Note that values in this section refer to full-pattern fitting. Use the appropriate items for single-crystal analyses from the core CIF dictionary for structure refinements using diffraction intensities estimated from a powder diffractogram by pattern-decomposition methods. Also note that many entries in the core **_refine_ls_** entries may also be useful (for example **_refine_ls_shift/su_***).

_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_fix**, 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]

_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]

_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.

                                       [pd_proc_ls]

_pd_proc_ls_prof_R_factor
_pd_proc_ls_prof_wR_factor
_pd_proc_ls_prof_wR_expected   (*numb*)

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_B) is not properly a profile *R* factor. This *R* factor may be specified using **_refine_ls_R_I_factor**. (Some authors report **_refine_ls_R_Fsqd_factor** or **_refine_ls_R_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.

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

_pd_proc_ls_prof_wR_expected, sometimes called the theoretical R_{wp} or R_{exp}, 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}.

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

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_{oi}. (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_{ci}. (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 $0.0 \rightarrow \infty$.   **[pd_proc_ls]**

_pd_proc_ls_profile_function   (*char*)
Description of the profile function used to fit the data set. 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 giving a description. Include the values used for the profile-function coefficients and their s.u.'s.

     [pd_proc_ls]

_pd_proc_ls_special_details   (*char*)
Additional characterization information relevant to non-routine steps used for refinement of a structural model that cannot be specified elsewhere.

     [pd_proc_ls]

_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 $0 \rightarrow \infty$.   **[pd_data]**

_pd_proc_number_of_points   (*numb*)
The total number of data points in the processed diffractogram.
The permitted range is $1 \rightarrow \infty$.   **[pd_proc_info]**

_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_data]**

_pd_proc_recip_len_Q   (*numb*)
Length in reciprocal space ($|Q| = 2\pi/d$) corresponding to an intensity point. Units are inverse ångströms.
Appears in list.
The permitted range is $0.0 \rightarrow \infty$.   **[pd_data]**

_pd_proc_wavelength   (*numb*)
Wavelength in ångströms 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 $0.0 \rightarrow \infty$.   **[pd_data]**

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**.   **[refln]**

_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**.   **[refln]**

_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**.   **[refln]**

PD_SPEC

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.

```
_pd_spec_mounting              ?
_pd_spec_mount_mode            transmission
_pd_spec_orientation           horizontal
_pd_spec_preparation           ?
```

_pd_spec_description   (*char*)
A description of the specimen, such as the source of the specimen, identification of standards, mixtures *etc.*

[pd_spec]

_pd_spec_mount_mode   (*char*)
A code describing the beam path through the specimen.
The data value must be one of the following:
  reflection
  transmission   **[pd_spec]**

_pd_spec_mounting   (*char*)
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]**

_pd_spec_orientation   (*char*)
The orientation of the ω (θ) and 2θ 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 2θ axis is parallel to the ground); for vertical orientation, scattering measurements are made in a plane parallel with the ground (the 2θ axis is perpendicular to

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]**

_pd_spec_preparation   (*char*)
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]**

_pd_spec_shape   (*char*)
A code describing the specimen shape.
The data value must be one of the following:
  cylinder
  flat_sheet
  irregular   **[pd_spec]**

_pd_spec_size_axial
_pd_spec_size_equat
_pd_spec_size_thick   (*numb*)
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 $0.0 \rightarrow \infty$.   **[pd_spec]**

_pd_spec_special_details   (*char*)
Descriptive information about the specimen that cannot be included in other data items.

[pd_spec]

references