

Dictionary name: **cif\_pd.dic**

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**\_pd\_block\_[pd]**  
**\_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\_diffraction\_id**, **\_pd\_calib\_std\_external\_block\_id** and **\_pd\_phase\_block\_id**).

Note that a data block may contain only a single diffraction dataset or information about a single crystalline phase. Yet a single diffraction measurement may yield structural information on more than one phase, or a single structural determination may use more than one dataset. Alternatively, results from a single dataset, 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 datasets may be preserved when the file is exported from the laboratory where 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 id's, if that site wishes to resolve these references.

**\_pd\_block\_diffraction\_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 most frequently occur when more than one set of diffraction data is used for a structural determination. The data block containing the diffraction data will contain a **\_pd\_block\_id** code matching the code in **\_pd\_block\_diffraction\_id**.

Appears in list. [pd\_proc]

**\_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 dataset 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 later made to the block, a new id may be assigned, but the original name should be retained.

The format for the id code is:

`<date-time>|<block-name>|<creator-name>|<instr-name>`

`<date-time>` is the date and time the CIF was created or modified. `<block-name>` is an arbitrary name assigned by the originator of the dataset. It will usually match the name of the phase and possibly the name of the current CIF data block (*i.e.* the string `xxx` in a `data_xxx` identifier). It may be a sample name. `<creator-name>` is the name of the person who measured the diffraction, prepared or modified the CIF. `<instr-name>` is a unique name (so 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.* `<block-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-Z a-z 0-9 # & \* . : , - \_ + / ( ) \ [ ]

The sections are separated with vertical bars '|' which are not allowed within the sections. Blank spaces may also not be used. Capitalisation may be used within the id code but should not be considered significant – searches for dataset id names should be case insensitive.

Date-time entries are in the standard CIF format 'yyyy-mm-ddThh: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 ensure that the id code is unique.

An archive site that wishes to make CIF files available via WWW 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 on-line indefinitely.

May appear in list.

Example(s):

```
'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\_meas\_[pd]**

This section contains the measured diffraction and information about conditions used for measurement of the diffraction dataset, 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 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 (normalisations, corrections, smoothing, zero-offset corrections, *etc.*). Such corrected measurements should be recorded in the `_pd_proc_` section.

Datasets 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_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_2theta_fixed` (numb)  
 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_meas_2theta_range_min`  
`_pd_meas_2theta_range_max`  
`_pd_meas_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_meas_2theta_scan` values for datasets measured with a constant step size.  
 The permitted range is  $-180.0 \rightarrow 360.0$ . [pd\_meas\_method]

`_pd_meas_2theta_scan` (numb)  
 $2\theta$  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 item `_pd_meas_scan_method`. For fixed  $2\theta$  (white-beam) experiments, use `_pd_meas_2theta_fixed`. In the case of continuous scan datasets, the  $2\theta$  value should be the value at the mid-point of the counting period. Associated with each `_pd_meas_2theta_scan` value will be `_pd_meas_counts_` items. The  $2\theta$  values should not be corrected for non-linearity, zero offset, *etc.* Corrected values may be specified using `_pd_proc_2theta_corrected`.  
 Note that for datasets taken 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_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*, Vol. IV (1974), 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_...`). 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 dataset measurement. Entries follow the standard CIF format 'yyyy-mm-ddThh: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 completed.

Example(s): '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, 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 id's should be the number to be used in the equation.

Appears in list. **Must** match data name `_pd_calib_detector_id`. [pd\_data]

`_pd_meas_info_author_address` (char)  
 The address of the person who measured the dataset. 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 email address of the person who measured the dataset. 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 dataset. If there is more than one person this will be looped with `_pd_meas_info_author_name`. The recommended style includes the international dialing prefix, 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 dataset. 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) May appear in list. The permitted range is 0→360.0. [pd\_data]  
 The telephone number of the person who measured the dataset. If there is more than one person this will be looped with `_pd_meas_info_author_name`. The recommended style includes the international dialing prefix, 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)  
 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→∞. [pd\_meas\_method]
- `_pd_meas_position` (numb)  
 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 non-linear, 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` (numb)  
 The angular range in degrees a sample is rotated or oscillated during a measurement step (see `_pd_meas_rocking_axis`).
- `_pd_meas_rocking_axis` (char)  
 Description of the axis (or axes) used to rotate or rock the specimen for better randomisation of crystallites (see `_pd_meas_rocking_angle`).  
 chi  
 omega  
 phi  
 May appear in list. [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.  
 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)  
 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→∞. [pd\_data]
- `_pd_meas_time_of_flight` (numb)  
 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→∞. [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 to be strongly discouraged – convert the intensity measurements to counts and use `_pd_meas_counts_` and `_pd_meas_step_count_time` instead of `_pd_meas_intensity_`.  
 Example(s): ‘estimated from strip chart’,  
 ‘arbitrary, from film density’,  
 ‘counts, with automatic deadtime correction applied’  
 [pd\_meas\_method]

`_pd_calib_[pd]`

This section defines parameters used for calibration of the instrument used directly or indirectly in the interpretation of this dataset. 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 -  $2\theta_{actual} = 2\theta_{setting} + \arctan(\cos(P_1)/(1/(P_0(CC - CH_0 - P_2CC^2)) - \sin(P_1)))$*

*This allows for the calibration of  $2\theta$  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 non-linearities 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_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  $2\theta$  (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  $2\theta$ , 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  $-180.0 \rightarrow 180.0$ . [pd\_calib]

`_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 subsidiary 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  $0.0 \rightarrow \infty$ . [pd\_calib]

`_pd_calib_std_external_block_id`  
`_pd_calib_std_external_name` (char)

Identifies the dataset 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 dataset 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)

Percent 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  $0.0 \rightarrow 100.0$ . [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`.

Example(s): 'NIST 640a Silicon standard', 'A1203' [pd\_calib]

`_pd_calibration_conversion_eqn` (char)

The calibration function to convert 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... Use `_pd_calib_std_external_` to define a pointer to the file or data block containing the information used to define this function.

Example(s):

```
; 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)

Descriptive information about 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_spec_[pd]	
This section contains information about the specimen used for measurement of the diffraction dataset. Note that information about the sample (the batch of material where the specimen was obtained), is specified in <code>_pd_prep_</code> .	
<i>Example 1</i>	
<code>_pd_spec_mounting</code>	?
<code>_pd_spec_mount_mode</code>	transmission
<code>_pd_spec_orientation</code>	horizontal
<code>_pd_spec_preparation</code>	?

`_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.

reflection  
transmission [pd\_spec]

`_pd_spec_mounting` (char)

A description of how the specimen is mounted.

Example(s): '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  $\omega$  ( $\theta$ ) 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 (the  $2\theta$  axis is perpendicular to the ground). 'Both' is appropriate for experiments where measurements are made in both planes, for example using 2-D detectors.

horizontal  
vertical  
both [pd\_spec]

`_pd_spec_preparation` (char)

A description of 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 synthesised, use the `_pd_prep_` entries.

Example(s): 'wet grinding in acetone',  
'sieved through a 44 micron (325mesh/inch) sieve',  
'spray dried in water with 1% clay' [pd\_spec]

`_pd_spec_shape` (char)

A code describing the specimen shape.

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]

_pd_instr_[pd]	
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 dataset.	
Note that several definitions in the core CIF dictionary are relevant here. For example, use: <code>_diffrn_radiation_wavelength</code> for the source wavelength, <code>_diffrn_radiation_type</code> for the X-ray wavelength type, <code>_diffrn_radiation_source</code> for the radiation source, <code>_diffrn_radiation_polarisn_ratio</code> for the source polarisation, <code>_diffrn_radiation_probe</code> for the radiation type. For datasets measured with partially monochromatised radiation, for example, where both $K\alpha_1$ and $K\alpha_2$ are present, it is important that all wavelengths present be included using a loop_ for <code>_diffrn_radiation_wavelength</code> , possibly with <code>_diffrn_radiation_wavelength_id</code> and <code>_diffrn_radiation_wavelength_wt</code> . It may also be useful to create a "dummy" id to use for labeling peaks/reflections where the $K\alpha_1$ and $K\alpha_2$ wavelengths are not resolved. Set <code>_diffrn_radiation_wavelength_wt</code> to be 0 for such a dummy id.	
In the <code>_pd_instr_</code> 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 specific wavelength or may be capable of being scanned.	
For multiple-detector instruments it may be necessary to loop the <code>*_anal/detc</code> or <code>*_spec/detc</code> values (for <code>_pd_instr_dist_</code> , <code>_pd_instr_divg_</code> , <code>_pd_instr_slit_</code> and <code>_pd_instr_soller_</code> ) with the detector id's ( <code>_pd_calib_detector_id</code> ).	
It is strongly recommended that the core dictionary term <code>_diffrn_radiation_probe</code> (specifying the nature of the radiation used) be employed for all datasets.	
<i>Example 1</i>	
<code>_pd_instr_slit_eq_src/spec</code>	1.
<code>_pd_instr_slit_eq_anal/detc</code>	0.2
<code>_pd_instr_geometry</code>	Bragg-Brentano
<code>_pd_instr_monochr_post_spec</code>	'graphite (0001)'
<code>_pd_instr_cons_illum_flag</code>	no

`_pd_instr_2theta_monochr_pre`  
`_pd_instr_2theta_monochr_post` (numb)

The  $2\theta$  angle for 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_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  $\theta$ -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  $2\theta$ , specify 'no'. Note that if the length is known, it may be specified using '`_pd_instr_var_illum_len`'.

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  $2\theta$ , by adjustment of the divergence slits (sometimes known as  $\theta$ -compensated slits). Use `_pd_instr_var_illum_len` for instruments where the divergence slit is fixed so that the illumination length varies with  $2\theta$  when the length is known.

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, `*_src/spec` is used in place of `*_src/mono` and `*_mono/spec`, if there is no monochromator in use. Also, `*_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 other beam-line 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, `*_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 other beam-line 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, `*_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.

Example(s): 'Bragg-Brentano', 'Guinier',  
; Parallel beam non-focussing 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 datasets measured away from the author's home facility, at shared resources such as a reactor or spallation source.

Example(s):

'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 and R. Snyder, *Introduction to X-ray Powder Diffraction*, Wiley (1996), pp. 164–5.

May appear in list.

Example(s): '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, `*_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→∞. [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, `*_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→∞. [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, `*_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→∞. [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, \*\_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→∞. [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→∞. [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\_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  $2\theta$  (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  $\theta$ -compensated to yield a constant illumination length.

Appears in list. The permitted range is 0.0→∞. [pd\_data]

#### \_pd\_proc\_[pd]

This section contains the diffraction dataset after processing and application of correction terms. If the dataset is reprocessed, this section may be replaced (with addition of a new \_pd\_block\_id entry).

\_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 non-linearity, 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→180.0. [pd\_data]

\_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→180.0. [pd\_proc\_info]

\_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→∞. [pd\_data]

\_pd\_proc\_energy\_incident  
\_pd\_proc\_energy\_detection (numb)

Incident energy in electron-volts of the source computed from secondary calibration information (time-of-flight and synchrotron). Detection energy in electron-volts 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→∞. [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 email 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 includes the international dialing prefix, 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 dataset. 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 includes the international dialing prefix, 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 processing steps applied in the data reduction process (background subtraction,  $\alpha$ -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 dataset 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+zz'. Use of seconds and a time zone is optional, but use of hours and minutes is strongly encouraged.

May appear in list.

Example(s): '1990-07-13T14:40' [pd\_proc\_info]

`_pd_proc_info_excluded_regions` (char)  
Description of regions in the diffractogram excluded from processing along with a justification of why the datapoints were not used.

Example(s):

'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 dataset.

[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)

`_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 normalisation 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, normalisation 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 fit 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 normalisation 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 normalisation should be specified in `_pd_proc_intensity_incident` as a value to be used to divide the measured intensities to obtain the normalised diffractogram. Thus, the `_pd_proc_intensity_incident` values should increase as the incident flux is increased.

The other normalisation factors applied to the dataset (for example,  $L_p$  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_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_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_proc_ls_[pd]`

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 dictionary for structural 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/esd_`).

`_pd_proc_ls_background_function` (char)  
Description of the background treatment mechanism used to fit the dataset.

For refinements where background is computed from a function fit to the difference between *obs* and *calc*, it is recommended that in addition to a description of the function (e.g. Chebyshev polynomial), the actual equation(s) used be included in  $\text{\TeX}$ , 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 no preferred orientation correction has been used. If a function form is used, it is recommended that the actual equation in  $\text{\TeX}$ , or a programming language, be used to specify the function as well as 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

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

`_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

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

`_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 dataset. For an idealised 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  $R_{exp}$ .

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

Note that in the above equations,  $w(i)$  is the weight for the *i*th data point (see `_pd_proc_ls_weight`).  $I_{obs}(i)$  is the observed intensity for the *i*th data point, sometimes referred to as  $y_i(obs)$  or  $y_{oi}$ . (See `_pd_meas_count_total`, `_pd_meas_intensity_total` or `_pd_proc_intensity_total`.)  $I_{calc}(i)$  is the computed intensity for the *i*th data point with background and other corrections applied to match the scale of the observed dataset, sometimes referred to as  $y_i(calc)$  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 dataset. If a function form is used, it is recommended that the actual equation in  $\text{\TeX}$ , or a programming language, be used to specify the function as well as 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 characterisation 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_calc_[pd]`

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 normalisation corrections and thus is specified on the same scale as the `_pd_proc_intensity_net`.

Use `_pd_calc_intensity_total` if the computed diffraction pattern includes background or normalisation 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  $0.0 \rightarrow \infty$ . [pd\_data]

`_pd_calc_method` (char)

A description of the method used for 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_peak_[pd]`

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 a later section (see the `_pd_refl_n_` 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_2theta_centroid`  
`_pd_peak_2theta_maximum` (numb)

Position of the centroid and maximum of a peak as a  $2\theta$  angle in degrees.

Appears in list containing `_pd_peak_id`. The permitted range is  $0.0 \rightarrow 180.0$ . [pd\_peak]

`_pd_peak_d_spacing` (numb)

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_refl_n_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. Uniqueness of loop packet tested on `_pd_peak_id`. May match subsidiary data name(s): `_pd_refl_n_peak_id`. [pd\_peak]

`_pd_peak_intensity` (numb)

Integrated area for the peak, with the same scaling as the `_pd_proc_intensity_` values. Good practice is 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)

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. Good practice is 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 described elsewhere.

[pd\_peak\_method]

`_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 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_refl_n_wavelength_id` rather than identifying peaks by wavelength.

Appears in list containing `_pd_peak_id`. **Must** match data name `_diffrn_radiation_wavelength_id`. [pd\_peak]

`_pd_peak_width_2theta` (numb)

Peak width as full-width at half-maximum expressed as  $2\theta$  value in degrees.

Appears in list containing `_pd_peak_id`. The permitted range is  $0.0 \rightarrow 180.0$ . [pd\_peak]

`_pd_peak_width_d_spacing` (numb)

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\_phase\_[pd]**

This section contains a description of the crystalline phases present in the powder diffraction dataset. 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_refl_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_refl_phase_id`.

Appears in list as essential element of loop structure. Uniqueness of loop packet tested on `_pd_phase_id`. May match subsidiary data name(s): `_pd_refl_phase_id`. [pd\_phase]

**\_pd\_phase\_mass\_%** (numb)

Percent 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→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\_refl\_[pd]**

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_refl_peak_id`.

**\_pd\_refl\_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 data name `_pd_peak_id`. [refln]

**\_pd\_refl\_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 data name `_pd_phase_id`. [refln]

**\_pd\_refl\_wavelength\_id** (char)

Code which identifies the wavelength associated with the reflection and the peak pointed to by `_pd_refl_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 data name `_diffrn_radiation_wavelength_id`. [refln]

**\_pd\_prep\_[pd]**

This section contains descriptive information on how the sample is prepared.

**\_pd\_prep\_conditions** (char)

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

[pd\_prep]

**\_pd\_prep\_cool\_rate** (numb)

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 instead in `_pd_prep_conditions`.

The permitted range is 0.0→∞. [pd\_prep]

**\_pd\_prep\_pressure** (numb)

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→∞. [pd\_prep]

**\_pd\_prep\_temperature** (numb)

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

The permitted range is 0.0→∞. [pd\_prep]

**\_pd\_char\_[pd]**

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,  $\mu$  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 `_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 standardised use of names, the following guidelines for colour naming developed by Peter Bayliss for the ICDD should be used. 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 description of a single sample.

Example(s): '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. . .).

[pd\_char]

`_pd_char_special_details` (char)

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

[pd\_char]

`_pd_char_special_details` (char)

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

[pd\_char]

`_pd_data_[pd]`

The PD\_DATA category contains raw, processed and calculated data points in a diffraction dataset. 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 two-theta 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_meas_intensity_total
  _pd_proc_ls_weight
  _pd_proc_intensity_bkg_calc
  _pd_calc_intensity_total
240(15)      0.00417      214.5      214.5
219(15)      0.00457      214.3      214.2
206(14)      0.00485      214.0      214.0
212(15)      0.00472      213.8      213.7
190(14)      0.00526      213.5      213.5
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_calc_2theta_scan
  _pd_calc_intensity_total
1 21.0 26
1a 21.3 56
4 21.6 76
4a 21.9 90
```

`_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

diffraction. 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(s): `_pd_data_point_id` (alternate). [pd\_data]

`_pd_data_point_id` (char)

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

[pd\_data]

`_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(s): `_pd_data_point_id` (alternate). [pd\_data]

`_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 item(s): `_pd_data_point_id` (alternate), `_pd_meas_point_id` (alternate). [pd\_data]