4.2. Powder dictionary (pdCIF)

BY B. H. TOBY

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_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

\[
\langle\text{date-time}\rangle|\langle\text{block_name}\rangle|\langle\text{creator_name}\rangle|\langle\text{instr_name}\rangle.
\]

(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 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. (creator_name) is the name of the person who measured the diffractogram, or prepared or modified the CIF. (instr_name) 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. (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 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 ‘yyyyMMdd-mm-ddThh:mm:ss+zzz’. 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 ((creator_name) and (instr_name)). Note that this should not be done unless the archive site is prepared to keep the file available online indefinitely. May appear in list.


**PD_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 _LAZYPULVERIX_ or the computed intensities from a Rietveld refinement.
4.2. POWDER DICTIONARY (pdCIF)

**_pd_calc_intensity_net_**

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_ or _pd_meas_counts_ or _pd_meas_intensity_.

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

**_pd_meas_counts_**

Same scale as the _pd_meas_intensity_. If the computed diffractogram does not contain 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_), an observed pattern is included, _pd_calc_intensity_ should be looped with either _pd_proc_counts_ or _pd(Meas_counts)_.

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

**_pd_meas_position_**

Position of the measured intensity.

**_pd_meas_detector_id_**

Position of the measured intensity, if measured, processed and calculated intensity identifies in _pd_calc_intensity_. If an observed pattern is included, _pd_calc_intensity_ should be looped with either _pd_proc_counts_ or _pd_meas_counts_.

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

**_pd_calc_method_**

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_calib_detector_id_**

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_.

The permitted range is 0 → ∞.

**_pd_calib_detector_response_**

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 → ∞.

**_pd_calib_std_external_block_id_**

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_.

The permitted range is 0 → 100.

**_pd_calib_std_external_name_**

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

May appear in list containing _pd_calib_detector_id_.

Examples: ‘HIST 640a Silicon standard’, ‘Al2O3’. For cases where the _pd_calib_2theta_offset value is not a constant, but rather varies with _2theta_, 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 → 180.0.

**_pd_calib_2theta_offset_**

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_.

The permitted range is 0 → ∞.

**_pd_calib_2theta_off_point_**

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_.

The permitted range is 0 → ∞.

**_pd_calib_2theta_off_min_**

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 → ∞.

**_pd_calib_2theta_off_max_**

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 → ∞.

**_pd_calib_std_internal_mass_%_**

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 → 100.

**_pd_calib_std_internal_name_**

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

May appear in list containing _pd_calib_detector_id_.
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 not in one-to-one correspondence.

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

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.).

Additional characterization information relevant to the sample or documentation of non-routine processing steps used for characterization.
**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: _diffn_radiation_wavelength_ for the source wavelength, _diffn_radiation_type_ for the X-ray wavelength type, _diffn_source_ for the radiation source, _diffn_radiation_polarisation_ratio_ for the source polarization, _diffn_radiation_probe_ for the radiation type.

For data sets measured with partially monochromated radiation, for example, where both Kα1 and Kα2 are present, it is important that all wavelengths present are included in a loop using _diffn_radiation_wavelength_ to define the wavelength and _diffn_radiation_wavelength wt_ to define the relative intensity of that wavelength. It is required that _diffn_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/reflectons where the Kα1 and Kα2 wavelengths are not resolved. Set _diffn_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_divg_ _pd_instr_soller_ _pd_instr_monochr_post_spec_ and _pd_instr_soller_ with the detector IDs (_pd_instr detector_id_). It is strongly recommended that the core dictionary term _diffn_radiation_probe_ (specifying the nature of the radiation used) is employed for all data sets.

Example 1.

<table>
<thead>
<tr>
<th>_pd_instr_divg_eq</th>
<th>src/mono</th>
<th>_pd_instr_divg_eq</th>
<th>src/mono</th>
</tr>
</thead>
<tbody>
<tr>
<td>_pd_instr_divg_eq</td>
<td>spec</td>
<td>_pd_instr_divg_eq</td>
<td>spec</td>
</tr>
<tr>
<td>_pd_instr_divg_eq</td>
<td>anal</td>
<td>_pd_instr_divg_eq</td>
<td>anal</td>
</tr>
<tr>
<td>_pd_instr_divg_eq</td>
<td>detc</td>
<td>_pd_instr_divg_eq</td>
<td>detc</td>
</tr>
<tr>
<td>_pd_instr_divg_eq</td>
<td>_spec/anal</td>
<td>_pd_instr_divg_eq</td>
<td>_spec/anal</td>
</tr>
<tr>
<td>_pd_instr_divg_eq</td>
<td>_spec/detc</td>
<td>_pd_instr_divg_eq</td>
<td>_spec/detc</td>
</tr>
</tbody>
</table>

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 → ∞.

<table>
<thead>
<tr>
<th>_pd_instr_dist_src/mono</th>
<th>_pd_instr_dist_monospec/mono</th>
<th>_pd_instr_dist_src/spec</th>
<th>_pd_instr_divg_eq/src/mono</th>
</tr>
</thead>
<tbody>
<tr>
<td>_pd_instr_divg_ax_eq</td>
<td>src/mono</td>
<td>_pd_instr_divg_ax_eq</td>
<td>spec</td>
</tr>
<tr>
<td>_pd_instr_divg_ax_eq</td>
<td>spec</td>
<td>_pd_instr_divg_ax_eq</td>
<td>anal</td>
</tr>
<tr>
<td>_pd_instr_divg_ax_eq</td>
<td>detc</td>
<td>_pd_instr_divg_ax_eq</td>
<td>detc</td>
</tr>
<tr>
<td>_pd_instr_divg_ax_eq</td>
<td>_spec/anal</td>
<td>_pd_instr_divg_ax_eq</td>
<td>_spec/anal</td>
</tr>
<tr>
<td>_pd_instr_divg_ax_eq</td>
<td>_spec/detc</td>
<td>_pd_instr_divg_ax_eq</td>
<td>_spec/detc</td>
</tr>
</tbody>
</table>

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_). _*_src/mono_, collimation between the radiation source and the monochromator; _*_mono/spec, collimation between the monochromator and the specimen; _*_spec/anal, collimation between the radiation source and the specimen; _*_spec/anal, collimation between the specimen and the analyser; _*_anal/detc, collimation between the analyser and the detector; _*_spec/detc, collimation between the specimen and the detector. Note that _*_src/mono and _*_mono/spec if there is no monochromator in use, and _*_spec/detc or _*_spec/anal if there is no analyser in use.

May appear in list.

The permitted range is 0.0 → ∞.

<table>
<thead>
<tr>
<th>_pd_instr_divg_eq</th>
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<td>anal</td>
</tr>
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<td>_pd_instr_divg_eq</td>
<td>detc</td>
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<td>_spec/anal</td>
<td>_pd_instr_divg_eq</td>
<td>_spec/anal</td>
</tr>
<tr>
<td>_pd_instr_divg_eq</td>
<td>_spec/detc</td>
<td>_pd_instr_divg_eq</td>
<td>_spec/detc</td>
</tr>
</tbody>
</table>

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_). _*_src/mono_ and _*_mono/spec if there is no monochromator in use, and _*_spec/detc or _*_spec/anal if there is no analyser in use.

May appear in list.

The permitted range is 0.0 → ∞.

<table>
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<tr>
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<td>_spec/anal</td>
<td>_pd_instr_divg_eq</td>
<td>_spec/anal</td>
</tr>
<tr>
<td>_pd_instr_divg_eq</td>
<td>_spec/detc</td>
<td>_pd_instr_divg_eq</td>
<td>_spec/detc</td>
</tr>
</tbody>
</table>

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_). _*_src/mono_ and _*_mono/spec if there is no monochromator in use, and _*_spec/detc or _*_spec/anal if there is no analyser in use.

May appear in list.

The permitted range is 0.0 → ∞.

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<td>_pd_instr_divg_eq</td>
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</tr>
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<td>_pd_instr_divg_eq</td>
<td>_spec/anal</td>
</tr>
<tr>
<td>_pd_instr_divg_eq</td>
<td>_spec/detc</td>
<td>_pd_instr_divg_eq</td>
<td>_spec/detc</td>
</tr>
</tbody>
</table>

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_). _*_src/mono_ and _*_mono/spec if there is no monochromator in use, and _*_spec/detc or _*_spec/anal if there is no analyser in use.

May appear in list.

The permitted range is 0.0 → ∞.

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<td>anal</td>
</tr>
<tr>
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<td>detc</td>
<td>_pd_instr_divg_eq</td>
<td>detc</td>
</tr>
<tr>
<td>_pd_instr_divg_eq</td>
<td>_spec/anal</td>
<td>_pd_instr_divg_eq</td>
<td>_spec/anal</td>
</tr>
<tr>
<td>_pd_instr_divg_eq</td>
<td>_spec/detc</td>
<td>_pd_instr_divg_eq</td>
<td>_spec/detc</td>
</tr>
</tbody>
</table>

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_). _*_src/mono_ and _*_mono/spec if there is no monochromator in use, and _*_spec/detc or _*_spec/anal if there is no analyser in use.

May appear in list.

The permitted range is 0.0 → ∞.
4. DATA DICTIONARIES

**_pd_instr_divg_eq_src/mono_**

* _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 $0 \rightarrow \infty$.

**_pd_instr_geometry_**

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_location_**

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_monochr_pre_spec_**

**_pd_instr_monochr_post_spec_**

Indicates the method used to obtain monochromatic radi-
tion. 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
analyzer (post-specimen monochromation). When a monochro-
mator 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 geo-
metry 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

May appear in list.

‘equatorial mounted graphite (0001)’, ‘Si (111), antiparallel’;

**_pd_instr_soller_ax_src/mono_**

**_pd_instr_soller_ax_mono/spec_**

**_pd_instr_soller_ax_src/spec_**

**_pd_instr_soller_ax_anal/detc_*
in use, and *

May appear in list.

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

**_pd_instr_slit_eq_spec/anal_**

**_pd_instr_slit_eq_src/mono_**

**_pd_instr_slit_eq_src/spec_**

**_pd_instr_slit_eq spec/anal_**

**_pd_instr_slit_eq anal/detc_*
Describes collimation in the equatorial plane (the plane contain-
ing 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: *

May appear in list.

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

**_pd_instr_soller_ax/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_*
Describes collimation in the equatorial plane (the plane contain-
ing 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: *

May appear in list.

The permitted range is $0 \rightarrow \infty$.
4.2. POWDER DICTIONARY (pdCIF)

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 measurement was started rather than when it was completed. Example: '1990-07-13T14:40'. The date and time of the data-set measurement. Entries follow the standard CIF format 'yyyy-mm-ddTThh: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 1.

<table>
<thead>
<tr>
<th>Field</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>_pd_meas_info_author_name</td>
<td>'Cranswick, Lachlan'</td>
</tr>
<tr>
<td>_pd_meas_info_author_email</td>
<td><a href="mailto:lachlan@mp.dmp.csiro.au">lachlan@mp.dmp.csiro.au</a></td>
</tr>
<tr>
<td>_pd_meas_info_author_address</td>
<td>?</td>
</tr>
<tr>
<td>_pd_meas_datetime_initiated</td>
<td>1992-01-23T17:20</td>
</tr>
<tr>
<td>_pd_meas_scan_method</td>
<td>step</td>
</tr>
<tr>
<td>_pd_meas_2theta_range_min</td>
<td>6.0</td>
</tr>
<tr>
<td>_pd_meas_2theta_range_max</td>
<td>164.0</td>
</tr>
<tr>
<td>_pd_meas_2theta_range_inc</td>
<td>0.025</td>
</tr>
<tr>
<td>_pd_meas_step_count_time</td>
<td>2.0</td>
</tr>
</tbody>
</table>

The permitted range is −180.0 → 360.0.

The date and time of the data-set measurement. Entries follow the standard CIF format 'yyyy-mm-ddTThh: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'.

The date and time of the data-set measurement. Entries follow the standard CIF format 'yyyy-mm-ddTThh: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'.

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_calibration_conversion_eqn 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]

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_calibration_conversion_eqn values. If _pd_calibration_conversion_eqn is used, the detector IDs should be the number to be used in the equation.

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

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

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_email [pd_meas_info]

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

_cif_pd_dic_

_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._

Applies in list containing _pd_meas_info_author_name_. [pd_meas_info]

_pd_meas_position_

_A linear distance in millimetres corresponding to the location where an intensity measurement is made. Used for detectors where a distance measurement is made as a direct observable, such as from a microdensitometer trace from film or a strip chart recorder._

May appear in list containing _pd_meas_info_author_name_. [pd_meas_info]

_pd_meas_focal_distance_

_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._

Appears in list containing _pd_meas_info_author_name_. [pd_meas_info]

_theta_range_theta_ (numb, su)

_The angular range in degrees through which a sample is rotated or oscillated during a measurement step (see _pd_meas_rocking_axis)._

The permitted range is 0 → 360.0. May appear in list. [pd_data]

_theta_omega_ (char)

_Description of the axis (or axes) used to rotate or rock the specimen for better randomization of crystallites (see _pd_meas_rocking_axis)._

The data value must be one of the following:

- chi
- omega
- phi

Appears in list. [pd_meas_method]

_theta_tof_ (numb, char)

_Description of the distance measurement.

The data value must be one of the following:

- step
- tof
- fixed
- disp
- cont
- scan

Appears in list. [pd_meas_method]

_theta_position_ (numb)

_Description of the position on a scale that has a fixed point.

May appear in list. [pd_meas_method]

_theta_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. [pd_data]

_theta_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 → 360.0. [pd_meas_method]
**PD_PEAK**

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

- **pd_peak_d_spacing**
  - (numb, su)
  - Peak position as a d-spacing in ångströms.
  - Appears in list containing _pd_peak_id_.
  - The permitted range is 0.0 → ∞.

- **pd_peak_id**
  - (char)
  - An arbitrary code is assigned to each peak. Used to link with _pd_refln_peak_id_ so that multiple _pd_peak_ 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_PHASE**

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

**pd_prep_pressure**

Preparation pressure of the sample in kilopascals. This is particularly important for materials which are metastable at the measurement temperature, _diffrn_ambient_pressure. The permitted range is 0 → ∞.

**pd_prep_temperature**

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 → ∞.

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**4. DATA DICTIONARIES**

**cif_pd_dic**

_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**

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.

**pd_proc_info_author_address**

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.

**pd_proc_info_author_email**

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.

**pd_proc_info_author_phone**

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.

---

**PD_PREP**

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

**pd_prep_conditions**

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

**pd_prep_cool_rate**

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 → ∞.

**pd_prep_pressure**

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_temperature**

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 → ∞.

---

**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**

_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 → ∞.

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4.2. POWDER DICTIONARY (pdCIF)

`pd_proc_info_excluded_regions`
Description of regions in the diffractogram excluded from processing along with a justification of why the data points were not used. Example: '20 to 21 degrees unreliable due to beam dump'.

`pd_proc_info_special_details`
Detailed description of any non-routine processing steps applied due to any irregularities in this particular data set.

`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, Lp-compensated slits in conventional diffractometers, spectral corrections for white-beam experiments), the correction function should be specified as _pd_proc_intensity_incident_. The normalization should be specified in _pd_proc_intensity_incident_ as a value to be used to divide the measured intensities to obtain the normalized diffractogram. Thus, _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 → ∞.

`pd_proc_2theta_corrected`
The 2θ diffraction angle in degrees for 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_ and _pd_proc_2theta_range_max_ may be used to specify the 2θ values.

Appears in list.
The permitted range is −180.0 → 180.0.

`pd_proc_ls_background_function`
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 the program 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_. _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_.

Appears in list.

`pd_proc_ls_peak_cutoff`
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.

Appears in list.

`pd_proc_ls_pref_orient_corr`
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.

Appears in list.
4. DATA DICTIONARIES

**pd_proc_ls_weight**

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.

**pd_proc_number_of_points**

The total number of data points in the processed diffractogram.

**pd_proc_point_id**

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.

**pd_proc_recip_len_Q**

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

**pd_proc_wavelength**

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.

**pd_refln_peak_id**

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**

Code which identifies the powder diffraction peak that contains the current reflection. This code must match a _pd_peak_id code.

**pd_refln_phase_id**

Code which identifies the crystal phase associated with this reflection. This code must match a _pd_phase_id code.

**pd_refln_wavelength_id**

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.
### 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**

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

**_pd_spec_mount_mode**

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

**_pd_spec_orientation**

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_preparation**

A description of the preparation steps for producing the diffraction specimen from the sample. Include any procedures related to grinding, sieving, spray drying *etc.*. For information relevant to how the sample is synthesized, use the `_pd_prep_` entries.

Examples: 'wet grinding in acetone', 'sieved through a 44 micron (325 mesh/inch) sieve', 'spray dried in water with 1% clay'.

**_pd_spec_shape**

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

**_pd_spec_size_axial**

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 $0 \rightarrow \infty$.

**_pd_spec_special_details**

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