† **_pd_refln_wavelength_id** (***_refln_wavelength_id***)
→ ***_diffrn_radiation_wavelength_id***

The arrow (→) *is a reference to a parent data item. The dagger* (†) *indicates a deprecated item, which should not be used in the creation of new CIFs. Items in italics are defined in the core CIF dictionary.*

In a single-crystal experiment, a reflection table contains the initial experimental observations for structural analysis. In contrast, the reflection table for a powder-diffraction experiment is a derived result that depends on the model used to apportion intensity between overlapping reflections. Another difference is that in a single-crystal experiment, the reflection list will refer to only one phase (one hopes), while it is common to have reflections from more than one phase in a powder-diffraction reflection list.

A list of reflections in a powder-diffraction pattern is commonly generated by Rietveld analysis, where Hugo Rietveld's algorithm (Rietveld, 1967, 1969) is used to estimate the intensity of each reflection. Alternatively, when the structure of one or more phases is not known, it is possible to use full-pattern intensity-extraction methods such as the algorithms developed by Pawley (1981) or Le Bail *et al.* (1988). In fact, intensity information obtained by full-pattern intensity extraction is often used for *ab initio* structure determination.

Most of the information in the reflection table will be defined using data items from the core CIF dictionary (see Section 3.2.2.2 and Chapter 4.1). For example, **_refln_index_h**, **_refln_index_k** and **_refln_index_l** will be used for the indices. The structure factors and reflection intensities are specified using **_refln_intensity_calc**, **_refln_intensity_meas**, **_refln_F_squared_calc** and **_refln_F_squared_meas**; reflection positions are defined using **_refln_d_spacing**. To link a reflection with a powder-diffraction peak, the pdCIF data item **_pd_refln_peak_id** is used. The value for **_pd_refln_peak_id** serves as a pointer to an entry in the peak table which has been labelled, using the data name **_pd_peak_id**, with the same symbol. Likewise, to link a reflection to a phase, the pdCIF data item **_pd_refln_phase_id** points to a phase defined using **_pd_phase_id** in the phase table. Since a single reflection may be observed with more than one wavelength, for example, with $\lambda/2$ or $K\alpha_2$ wavelengths, the pdCIF dictionary defines a wavelength link, **_pd_refln_wavelength_id**, that defines a wavelength label. However, since version 2.1, the core CIF dictionary defines **_refln_wavelength_id** and this should be used in preference to **_pd_refln_wavelength_id**. The data items **_refln_wavelength_id** and **_pd_refln_wavelength_id** both point to a wavelength label defined using **_diffrn_radiation_wavelength_id**.

The International Centre for Diffraction Data abstracts peak positions and heights for inclusion in the Powder Diffraction File. This information would be found in the **_pd_peak** section of a pdCIF. However, in many studies, particularly in Rietveld refinements, peak tables are never generated. In principle, it should be possible to calculate peak positions and peak heights (or better still, peak areas) from the information in a reflection table. An algorithm for this would be very useful.

3.3.6. Atomicity, chemistry and structure

The structural model of a compound determined by powder-diffraction methods can be described by the data items in the core CIF dictionary. However, for a powder-diffraction study of a mixture of phases, the PD_PHASE category is used to list the phases present. This is the only category in the pdCIF dictionary that extends the description of the structural model beyond that covered by items in the core CIF dictionary.

3.3.6.1. Table of phases

The data items in this category are as follows:

PD_PHASE
- **_pd_phase_id**

_pd_phase_block_id
_pd_phase_mass_%
_pd_phase_name

The bullet (•) *indicates a category key.*

When a sample contains more than one phase, the PD_PHASE data items are used to create a table describing the phases present. For example, the name and abundance of each phase can be specified using **_pd_phase_name** and **_pd_phase_mass_%**, respectively.

Two types of pointers can also be defined:

(i) Since the crystallographic description of each phase must be incorporated in a separate data block, **_pd_phase_block_id** contains the unique block ID (see Section 3.3.7) pointing to the block containing the data for the phase.

(ii) An arbitrary label is assigned to every phase using **_pd_phase_id** so that reflections can be assigned to a phase using **_pd_refln_phase_id**. This is discussed further in Section 3.3.5.4.

3.3.7. File metadata

The many data items in the core dictionary that decribe file auditing and history cover most of the metadata requirements of a pdCIF, but two new data items in the pdCIF category PD_BLOCK are introduced to provide a specific mechanism for identifying and relating individual data blocks.

Data items in this category are as follows:

PD_BLOCK
_pd_block_diffractogram_id
_pd_block_id

The data item **_pd_block_id** is used to define a unique name for each data block. This name is used so that one data block may reference another data block. Since CIF blocks may be separated into different files, or many CIFs from different sources may be grouped into a single file, the block ID provides a robust mechanism for maintaining references between blocks, independent of how CIF blocks have been arranged between files. The intent is that a site that archives pdCIFs will construct an index to **_pd_block_id** names that can be used to resolve block ID references.

The definition for **_pd_block_id** gives a procedure for creating a **_pd_block_id** name that is extremely unlikely to be duplicated. Other mechanisms for creating unique names can also be used: for example, using a web page name (URL) could be appropriate if care is taken never to reuse the URL.

The need for the block ID/block pointer mechanism is demonstrated by the following example. Consider a case where a neutron powder diffraction data set and an X-ray powder diffraction data set have been used together to determine a single structural model for a single crystalline phase. CIF does not allow the two data sets to be placed in a single block, since this would require two independent loops of observations where each loop uses some of the same data names. One can create a CIF with two blocks and include the structural model in the block that contains either of the two data sets. However, if this is done, a logical link is needed between the two blocks to make it clear that the structural model was derived from both data sets. It is better practice to place the