Table A3.3.1.1. *Categories in the powder CIF dictionary*
Numbers in parentheses refer to the section of this chapter where each category is described in detail.

PD_BLOCK group (§3.3.7)	PD_MEAS group (§3.3.4.4)
PD_BLOCK (§3.3.7)	PD_DATA (*part of category*) (§3.3.4.4(*a*))
PD_CALC group (§3.3.5.2)	PD_MEAS_INFO (§3.3.4.4(*b*))
PD_CALC (§3.3.5.2(*b*))	PD_MEAS_METHOD (§3.3.4.4(*c*))
PD_DATA (*part of category*) (§3.3.5.2(*a*))	PD_PEAK group (§3.3.5.3)
PD_CALIB group (§3.3.4.3)	PD_PEAK (§3.3.5.3(*a*))
PD_CALIB (§3.3.4.3(*a*))	PD_PEAK_METHOD (§3.3.5.3(*b*))
PD_CALIBRATION (§3.3.4.3(*b*))	PD_PHASE group (§3.3.6.1)
PD_CHAR group (§3.3.4.1)	PD_PHASE (§3.3.6.1)
PD_CHAR (§3.3.4.1(*a*))	PD_PREP group (§3.3.4.1)
PD_DATA group	PD_PREP (§3.3.4.1(*b*))
_pd_calc_* items (§3.3.5.2(*a*))	PD_PROC group (§3.3.5.1)
_pd_instr_var_illum_len (§3.3.4.3(*d*))	PD_DATA (*part of category*) (§3.3.5.1(*a*))
_pd_meas_* items (§3.3.4.4(*a*))	PD_PROC_INFO (§3.3.5.1(*b*))
_pd_proc_* items (§3.3.5.1(*a*))	PD_PROC_LS (§3.3.5.1(*c*))
PD_INSTR group (§3.3.4.3)	PD_SPEC group (§3.3.4.2)
PD_DATA (*part of category*) (§3.3.4.3(*d*))	PD_SPEC (§3.3.4.2)
PD_INSTR (§3.3.4.3(*c*))	REFLN group (§3.3.5.4)
	REFLN (§3.3.5.4)

identification more difficult, it is a good idea to include specimen preparation and mounting information, as described in Section 3.3.4.2.

Peaks will be located and documented in the peak table, as discussed in Section 3.3.5.3. In this case, it can be very helpful to specify **_pd_peak_wavelength_id** for peaks that are clearly a $K\alpha_2$ component. Similarly, recording a peak width can also be helpful for some autoindexing programs.

To identify peaks by phase in the case where at least one phase in a material is known but other peaks remain unidentified requires the use of a reflection table and a phase table, as shown in Example 3.3.10.1. This example shows a diffraction pattern with eight peaks, of which five have been identified as arising from a phase where the unit cell has not yet been determined. The peaks labelled B1, B2 and B3 are referenced in the peak table, but are not defined in the reflection loop. This implies that they arise from an unknown phase or phases. The remaining peaks A1 to A5 are referenced in the peak table. Note that the reflection table must include the **_refln_index_*** data items, even though no reflection indices are assigned. This is because CIF rules require that the **_refln_index_*** data items be present in this loop, as noted in the pdCIF dictionary definitions for **_pd_refln_peak_id** and **_pd_refln_phase_id**. The place holder **?** is used to indicate that the reflection indices are not yet known.

Appendix 3.3.1
Category structure of the powder CIF dictionary

Table A3.3.1.1 provides an overview of the structure of the powder CIF dictionary by informal category group.

Many people contributed to the creation of this dictionary, most notably Syd Hall, I. David Brown and Brian McMahon. Ian Langford helped considerably with the evolution of the dictionary. This project also benefited from the efforts of many members of the PDF-3 Database Format Subcommittee of the International Centre for Diffraction Data; I am particularly indebted to Walter Schriener for useful concepts and discussions. My initial involvement with powder diffraction file formats was prompted by the encouragement of Richard Harlow; I may someday forgive him.

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