describe how the measurements were processed using **_pd_proc_info_data_reduction**.

The **_pd_proc_*** data items in this list may be used to calibrate the 2θ or energy values of the data. These are defined in the items **_pd_proc_2theta_corrected**, **_pd_proc_2theta_range_***, **_pd_proc_d_spacing**, **_pd_proc_energy_***, **_pd_proc_recip_len_Q** and **_pd_proc_wavelength**.

When corrections, scaling or other processing, such as averaging or smoothing, are applied to the intensities, the results are stored using the **_pd_proc_intensity_*** data items. Note that if the number of data points does not change, it might be most convenient to include the processed intensities in the same loop as the observed values. This is not always possible, so these items can be placed in a separate loop if there is no longer a one-to-one correspondence between the 2θ or energy positions for the **_pd_proc_intensity_*** values and the **_pd_meas_counts_*** or **_pd_meas_intensity_*** values.

For energy-dispersive measurements, the incident spectrum must be determined for normalization. This can be recorded using **_pd_proc_intensity_incident**. For other types of normalization, **_pd_proc_intensity_norm** should be used.

For full-pattern fitting, there is a series of **_pd_proc_ls_*** data items for recording settings and results. For example, agreement factors can be recorded using the **_pd_proc_ls_prof_*_factor** data items. Some data items may be included in the loop(s) containing the measured or the processed data: **_pd_proc_ls_weight** specifies the weight assigned to each point and **_pd_proc_intensity_bkg_calc** specifies the fitted background. Note that background values are usually generated by extrapolation from fixed values set during the refinement or are determined from a function that is fitted to the observations, and occasionally both are used together. The function that has been fitted can be described using **_pd_proc_ls_background_function**, while fixed points are listed using **_pd_proc_intensity_bkg_fix**. If sections of the pattern are not fitted, this is indicated using **_pd_proc_info_excluded_regions**.

3.3.5.2. Simulated data

The data items in these categories are as follows:

(*a*) Part of PD_DATA

_pd_calc_intensity_net
_pd_calc_intensity_total
_pd_calc_point_id

(*b*) PD_CALC

_pd_calc_method

It is common to calculate powder-diffraction intensities from a crystallographic model. This is necessary for Rietveld refinements, where the model is fitted to the experimentally observed intensities. It is also used to simulate the diffraction pattern of a material for which the structure is known, perhaps for comparison with a measured diffraction pattern.

A crystallographic model can be described in CIF using data items from the core CIF dictionary, as described in Chapter 3.2. To record the results of the simulation, the data items **_pd_calc_intensity_net** or **_pd_calc_intensity_total** are used. The difference between these two data items depends on the treatment of background. If the pattern is simulated with a fitted background added to it, **_pd_calc_intensity_total** is used; otherwise **_pd_calc_intensity_net** is used. The values will typically be placed in a loop with the processed (**_pd_proc_***) data items or the observed (**_pd_meas_***) data items. If neither observed nor processed data are present (*e.g.* for a simulation), or if, for some reason, the simulation has been performed with a different 2θ range or step size, the appropriate **_pd_proc_*** data items are used to define the 2θ values *etc.* used for the simulation.

3.3.5.3. Diffraction peak table

The data items in these categories are as follows:

(*a*) PD_PEAK

- **_pd_peak_id**
  _pd_peak_2theta_centroid
  _pd_peak_2theta_maximum
  _pd_peak_d_spacing
  _pd_peak_intensity
  _pd_peak_pk_height
  _pd_peak_wavelength_id
  → ***_diffrn_radiation_wavelength_id***
  _pd_peak_width_2theta
  _pd_peak_width_d_spacing

(*b*) PD_PEAK_METHOD

_pd_peak_special_details

The bullet (•) indicates a category key. The arrow (→) is a reference to a parent data item. Items in italics are defined in the core CIF dictionary.

When diffraction intensities are first measured, particularly when attempting to identify unknown phases in a material, the first step in the analysis is often to compile a list of peak positions. These peak positions are commonly used to search the Powder Diffraction File, which contains lists of peak heights and positions for approximately 100 000 materials (International Centre for Diffraction Data, 2004).

Information on diffraction peaks is recorded in the PD_PEAK section of the pdCIF. Peak positions are recorded using **_pd_peak_2theta_maximum** or **_pd_peak_2theta_centroid**, for positions determined from the intensity maxima or from the peak centroids, respectively. It is also possible to record peak positions using **_pd_peak_d_spacing**. Peak intensities are recorded using **_pd_peak_intensity** and **_pd_peak_pk_height**, for the integrated peak area or the intensity value at the peak maximum, respectively. Peak widths are recorded using **_pd_peak_width_2theta** and **_pd_peak_width_d_spacing**.

A separate loop is used to list reflections, as will be discussed in Section 3.3.5.4. To link reflections to peaks (one peak may consist of many reflections), each peak is assigned a unique code using **_pd_peak_id**, which is then referenced in the reflection table using **_pd_refln_peak_id**.

When intensities are measured using radiation with more than one wavelength, for example when both Cu $K\alpha_1$ and $K\alpha_2$ radiation are used or when a monochromator passes both λ and $\lambda/2$ radiation, peaks may be assigned a wavelength symbol using **_pd_peak_wavelength_id**, where the wavelength symbol is defined in a separate **_diffrn_radiation_wavelength_id** loop. However, for many experiments, the assignment of wavelengths to peaks will be impractical owing to reflection overlap. It is usually better practice to specify wavelength labels in the reflection table using **_pd_refln_wavelength_id**.

3.3.5.4. Reflection assignments and intensities

In addition to the REFLN data items defined in the core CIF dictionary, the following items are defined:

REFLN

_pd_refln_peak_id
→ **_pd_peak_id**
_pd_refln_phase_id
→ **_pd_phase_id**