diffraction measurements were made, how the refinement was performed *etc.* While reflection tables for each phase can be placed in each phase block, it is better to include a single reflection table in the block that contains the diffraction data. This block will also contain a phase table that uses the block pointer `_pd_block_diffractogram_id` to link to the phase blocks. The phase blocks can also be linked to the data block using the block pointer `_pd_phase_block_id`. For most Rietveld refinements, each phase is allowed to have different profile parameters, so `_pd_proc_ls_profile_function` should also be included in the phase-table loop.

3.3.9.3. One phase, multiple sets of measurements

It is fairly common to use more than one diffraction data set to determine a model for a single phase. Some examples include: combined refinement using both neutron and X-ray powder diffraction; use of multiple X-ray wavelengths to make use of anomalous dispersion; and the use of single-crystal X-ray and powder neutron diffraction data in a single refinement. For these cases, there will be a CIF block for each data set. Each of these blocks will contain a reflection table and a loop with the observed and calculated diffraction intensities, as described in Section 3.3.9.1.

As explained in Section 3.3.7, the resulting structural parameters could be placed in a block with one of the sets of diffraction data. However, it is better practice to create one additional block for these parameters, as it then becomes clear that the result is from a combined refinement. This is indicated by linking the phase block and the data-set blocks using a loop of `_pd_block_diffractogram_id` values in the phase block. The data-set blocks can also have a link to the phase information using the block pointer `_pd_phase_block_id`.

3.3.9.4. Multiple sets of measurements and phases

Multiple data sets may be used for mixtures as well as single phases. This is becoming increasingly common as more complex materials are studied using powder diffraction. The treatment of this case follows logically from that of Sections 3.3.9.2 and 3.3.9.3. If there are M diffraction data sets and P phases, there will be P blocks containing the crystallographic parameters for each phase. There will be M blocks with the observed and calculated diffraction intensities, as well as reflection tables. Depending on the Rietveld software, there may be $M \times P$ sets of some parameters, for example phase fractions and profile descriptions. These parameters may be placed in the phase table loop within the data-set block(s).

Ideally, the same specimen, or at least the same sample, will be used for all measurements. Sometimes, however, different samples are used for combined refinements to extend the number of observations, despite the possibility that the samples might have slightly different structures or compositions. If there are S samples, there will be an additional S blocks that record the sample and specimen preparation and characterization information. Thus, in this case there will be a total of $M + P + S$ blocks.

As before, the phase blocks will use the block pointers `_pd_block_diffractogram_id` to link to the data-set blocks. Likewise, the data-set blocks will have phase tables with `_pd_phase_block_id` values that link to the phase blocks. The sample blocks can use both `_pd_block_diffractogram_id` values and `_pd_phase_block_id` values to link to the the diffraction data and the analysis results. This is shown in the CIF in Example 3.3.7.1. The program *GSAS2CIF* (Toby *et al.*, 2003) can create CIFs for multiple sets of measurements and phases.

Example 3.3.10.1. *Phase identification using a reflection table and a phase table.*

```
loop_
  _pd_peak_2theta_centroid
  _pd_peak_id
     3 A1
     4 B1
     6 A2
     8 B2
     9 A3
    12 A4
    15 A5
    16 B3

loop_
  _refln_index_h
  _refln_index_k
  _refln_index_l
  _pd_refln_peak_id
  _pd_refln_phase_id
  ? ? ? A1 Phase1
  ? ? ? A2 Phase1
  ? ? ? A3 Phase1
  ? ? ? A4 Phase1
  ? ? ? A5 Phase1

loop_
  _pd_phase_id
  _pd_phase_name
  Phase1  'component 1'
```

3.3.10. Other pdCIF applications

As mentioned above, there are other applications for pdCIF than the storage of unprocessed measurements and the reporting of the results of a Rietveld refinement. This section describes the use of data items in other common pdCIF applications.

3.3.10.1. Simulated intensities

It is common to simulate a diffraction pattern from a known or hypothetical structural model. The structural model is recorded in CIF using core data items, such as `_atom_site_label`, `_atom_site_fract_x`, `_atom_site_fract_y`, `_atom_site_fract_z`, `_atom_site_U_iso_or_equiv` and `_atom_site_occupancy`, as well as the unit cell in `_cell_length_*` and `_cell_angle_*`. Calculated reflection intensities can be recorded using `_refln_index_*` and `_refln_F_squared_calc`, as described in Section 3.3.5.4. The simulated pattern can be recorded using `_pd_calc_*` data items, as described in Section 3.3.5.2.

The simulated diffraction pattern will be determined not only by the structural parameters, but also by the type of experiment that is being simulated. For example, it is good practice to define data items to specify the type of radiation in `_diffrn_radiation_probe`, the wavelength in `_diffrn_radiation_wavelength` and the profile in `_pd_proc_ls_profile_function`.

3.3.10.2. Phase identification and indexing

For phase identification, a CIF will include unprocessed measurements, as described in Section 3.3.8. Sample characterization information, for example chemical analysis information, can often aid phase determination. Characterization information is described in Section 3.3.4.1. Similarly, sample preparation information can also be quite valuable (see Section 3.3.4.1). Since preferred orientation or other artifacts of the measurement can make phase