Example 3.3.8.3. *Identifying intensities from multiple detectors.*

```
loop_
  _pd_meas_2theta_scan
  _pd_meas_intensity_total
  _pd_meas_detector_id
  5.0   10 A    25.0   16 B   45.0 23 C   65.0 18 D
  5.02 16 A    25.02 30 B   ...   ... ...
```

Example 3.3.8.4. *Measurements from an energy-dispersive X-ray diffraction experiment.*

```
_pd_meas_scan_method       disp
_pd_meas_2theta_fixed      6.5
_pd_calib_2theta_offset    0.1071
loop_
  _pd_meas_detector_id
  _pd_meas_counts_total
  _pd_proc_energy_detection
  _pd_proc_recip_len_Q
      0  180   6114.0 .714
      1  166   6141.2 .717
      2   11   6168.4 .721
      3   11   6195.5 .724
```

In Example 3.3.8.3, four detectors placed 20° apart are referenced with arbitrarily chosen labels A, B, C and D. Note that the detector characteristics will typically be specified in a separate calibration loop containing terms such as `_pd_calib_detector_id`, `_pd_calib_detector_response` and `_pd_calib_2theta_offset`. The labels given for `_pd_calib_detector_id` should match those in `_pd_meas_detector_id`.

3.3.8.4. Energy-dispersive X-ray detection

For energy-dispersive X-ray diffraction, an X-ray detector is placed at a fixed value of 2θ and a diffractogram is measured on a multichannel analyser. The channel number is then calibrated to yield photon energies. From the energy and 2θ angle, a d-spacing or Q value ($Q = 4\pi \sin\theta/\lambda$) is calculated for each diffraction point. Note that energy, d spacing or Q are not the experimental independent variable. Rather, they result from processing, since calibration information is required. The calibration equation should be described in `_pd_calibration_conversion_eqn`.

In Example 3.3.8.4, the nominal 2θ setting is 6.5°, but the actual position (determined by prior calibration) is 6.6071°, so the difference is indicated using a `_pd_calib_2theta_offset` value (see Section 3.3.4.3).

3.3.8.5. Neutron time-of-flight detection

Neutron time-of-flight (TOF) detection in theory should be no different from energy-dispersive X-ray detection, but TOF instruments record complex three-dimensional data structures, where diffraction intensities are recorded as a function of time for as many as several hundred detectors. For some instruments, both the position along the detector and the time of flight are recorded, so there may be effectively thousands of detectors. To add even further complexity, the data may be binned in different time steps for detectors at different 2θ values. CIF is likely to be cumbersome for the storage of unprocessed measurements from TOF instruments, owing to the one-dimensional nature of CIF, but it could be useful to translate files from one binary format to another using CIF as a common intermediate. To do this, a single loop is used for all data points, where each detector (or detector section, in the case of a position-sensitive detector) is assigned a detector ID. In a second loop, the detector ID values are defined. In addition to 2θ, `_pd_meas_angle_omega` and `_pd_meas_angle_chi` are defined where needed (Example 3.3.8.5).

Example 3.3.8.5. *Measurements from a neutron time-of-flight diffraction experiment.*

```
_pd_meas_scan_method       tof
loop_
  _pd_meas_detector_id
  _pd_meas_time_of_flight
  _pd_proc_d_spacing
  _pd_meas_counts_total
  _pd_proc_intensity_incident
    88  1101.6  0.251658559  11843  4003
    88  1103.2  0.25202477   11934  4001
    88  1104.8  0.252391011  11906  3999
    88  1106.4  0.252757192  11773  3997
    88  1108.0  0.253123432  11707  3995
    ...
    150 1500.0  0.257258087   6559  3185
    ...

loop_
  _pd_calib_detector_id
  _pd_meas_2theta_fixed
     88  88.05
     150 148.29
```

TOF data are usually reduced to a small number of 'banks' consisting of intensity as a function of d space or Q, where multiple detectors are summed. Data in this form can be recorded using a loop containing `_pd_proc_d_spacing` and `_pd_proc_intensity_net`. A data block is needed for each bank.

3.3.8.6. Digitized film and image plates

To record intensities from digitized X-ray film or from image plates properly requires the storing of two-dimensional data structures, which in some cases can be accommodated through imgCIF (see Chapters 2.3 and 3.7). However, it is possible to record a one-dimensional scan using `_pd_meas_position` and `_pd_meas_intensity_total` (not `_pd_meas_counts_total`!). `_pd_proc_2theta_corrected` values can then be assigned using calibration information, and they can then be included in the same loop, as in Section 3.3.8.4.

3.3.8.7. Direct background measurements

For some diffraction experiments, particularly for the determination of radial distribution functions, measurements are made for background scattering from the diffraction instrument and from the sample container. When this is done, the values can be included in a single loop using `_pd_meas_counts_background`, `_pd_meas_counts_container` and `_pd_meas_counts_total`.

3.3.8.8. Noting sample orientation

For texture measurements, intensity measurements can be made as a function of different sample setting angles. These setting angles can be specified using `_pd_meas_angle_chi`, `_pd_meas_angle_omega` and `_pd_meas_angle_phi`. The change in these values may be specified by including these data items in the loop with the diffraction intensities. In some cases, it may be more convenient to separate measurements with different setting angles into different blocks. In this case, the values for the setting angle(s) that are invariant will be set outside of a loop.

It is common in powder diffraction to reduce preferred orientation and improve crystallite averaging by rocking or rotating the sample. This is indicated by specifying the axis used for rocking, usually φ for capillary specimens or χ for flat-plate specimens, as `_pd_meas_rocking_axis`. The data item