Example 3.2.3.2. *Structure-factor listing.*

```
loop_
     _refln_index_h
     _refln_index_k
     _refln_index_l
     _refln_F_squared_calc
     _refln_F_squared_meas
     _refln_F_squared_sigma
     _refln_include_status
    2   0   0       85.57       58.90      1.45 o
    3   0   0    15718.18    15631.06     30.40 o
    4   0   0    55613.11    49840.09     61.86 o
    5   0   0      246.85      241.86     10.02 o
    6   0   0       82.16       69.97      1.93 o
    7   0   0     1133.62      947.79     11.78 o
    8   0   0     2558.04     2453.33     20.44 o
    9   0   0      283.88      393.66      7.79 o
    10  0   0      283.70      171.98      4.26 o
```

the exception of $R(I)$ in Rietveld refinements against powder data, where it is generally called the Bragg R factor, $R_{\rm Bragg}$ or R_B.

The data items in the REFINE_LS_CLASS category are similar to several in the general REFINE category, but correspond to values for separate reflection classes as described in the REFLNS_CLASS category. The data name **_refine_ls_class_code** identifies the individual classes through a direct match with a corresponding value of **_reflns_class_code**.

3.2.3.2. Reflection measurements

The categories describing the reflections used in the refinement are as follows:

REFLN group

Individual reflections (§3.2.3.2.1)

REFLN

Groups of reflections (§3.2.3.2.2)

REFLNS

REFLNS_CLASS

REFLNS_SCALE

REFLNS_SHELL

The main category in this group is REFLN, which stores the list of reflections used in the structure refinement process, their associated structure factors and information about how each reflection was handled. The distinction between the REFLN (singular) category and the REFLNS (plural) category parallels the distinction between the categories DIFFRN_REFLN and DIFFRN_REFLNS: data items in the REFLN category store information about individual reflections, while data items in the REFLNS category store information about the complete set of reflections, or about subsets of reflections selected by shells of resolution, scaling factors or other criteria.

3.2.3.2.1. *Individual reflections*

The data items in this category are as follows:

REFLN

```
• _refln_index_h
• _refln_index_k
• _refln_index_l
  _refln_A_calc
  _refln_A_meas
  _refln_B_calc
  _refln_B_meas
  _refln_class_code
        → _reflns_class_code
  _refln_crystal_id
        → _exptl_crystal_id
  _refln_d_spacing
  _refln_F_calc
  _refln_F_meas
  _refln_F_sigma
  _refln_F_squared_calc
  _refln_F_squared_meas
  _refln_F_squared_sigma
  _refln_include_status
  _refln_intensity_calc
  _refln_intensity_meas
  _refln_intensity_sigma
  _refln_mean_path_length_tbar
† _refln_observed_status
  _refln_phase_calc
  _refln_phase_meas
  _refln_refinement_status
  _refln_scale_group_code
        → _reflns_scale_group_code
  _refln_sint/lambda
  _refln_symmetry_epsilon
  _refln_symmetry_multiplicity
  _refln_wavelength
  _refln_wavelength_id
        → _diffrn_radiation_wavelength_id
```

The bullet (•) indicates a category key. Where multiple items within a category are marked with a bullet, they must be taken together to form a compound key. 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.

Example 3.2.3.2 shows a typical structure-factor listing produced by a refinement program. This kind of structure-factor listing is suitable for deposition with a journal or a database. The Miller indices for each reflection are accompanied by the calculated and measured values of the quantity used in the refinement, and the standard uncertainty derived from the measurement. There is also an indication of whether each reflection was included in the refinement and in the calculation of R factors.

In this example, the squared structure factors $|F|^2$ are listed. When refinement is performed against the structure factors F or the intensities I, the data items **_refln_F_calc** or **_refln_intensity_calc** and the corresponding data names for the measured values and uncertainties should be used.

Individual calculated structure-factor components $A = |F|\cos\varphi$ and $B = |F|\sin\varphi$ may also be listed, along with the phase φ, using the data names **_refln_A_calc**, **_refln_B_calc** and **_refln_phase_calc**. Corresponding measured values have equivalent ***_meas** names.

The **_refln_include_status** flag is used to indicate whether reflections were used in the refinement and in the calculation of R factors, and if they were not used, to give the reason for exclusion of the reflection from the refinement. The flag o, which indicates that a reflection was used in the refinement, was originally chosen to indicate that the value of the reflection was higher than the limit specified by **_reflns_observed_criterion** and that the reflection was thus 'observed'. The data item **_reflns_observed_criterion** is now deprecated in favour of **_reflns_threshold_status**, and the value o is now taken to indicate not only that the reflection has an intensity suitable for inclusion in the refinement, but also that the reflection satisfies all other criteria used to select reflections for inclusion in the refinement.

Various other flags indicate reflections that were not included in the refinement. Reflections outside the range of d spacings bounded by the values **_refine_ls_d_res_high** and **_refine_ls_d_res_low** are flagged with h or l, respectively. Reflections within the resolution limits but below the intensity threshold are flagged with <. Systematically absent reflections are flagged with -. Sometimes a value can be identified as having a systematic error; these reflections can be flagged with x. However, great care must be taken in excluding reflections with apparently 'anomalous' structure factors (*i.e.* where the measured values are substantially different from the calculated ones), so as not to introduce bias into the refinement.

The flag **_refln_refinement_status** is used specifically to indicate whether a reflection was included in or excluded from

the refinement. Use of **_refln_include_status** to provide more information about each reflection is greatly preferred.

Other data names in this category allow the recording of specific information about each reflection, such as the symmetry reinforcement factor ε, the number of reflections symmetry-equivalent under the Laue symmetry, the d spacing, the mean path length through the crystal $\bar{t}$, the $(\sin\theta)/\lambda$ value and, in the case of Laue experiments, the mean wavelength of the radiation. (For polychromatic radiation, the wavelength information might instead be given by **_refln_wavelength_id**, which is a code identifying a matching entry in the DIFFRN_RADIATION category.)

Other codes provide links to identifiers in other categories. The **_refln_class_code** identifies a set of reflections binned as described by entries in the REFLNS_CLASS category. **_refln_scale_group_code** identifies groups of reflections to which the same structure-factor scaling has been applied.

Note that the values of the Miller indices in this list must correspond to the cell defined by the lengths and angles recorded in the CELL category; they may, however, be different from the Miller indices in the DIFFRN_REFLN list if a transformation of the original cell has taken place. In this case, the transformation matrix is given using the **_diffrn_reflns_transf_matrix_*** items.

The usual use of a CIF as an archive of a completed structure determination implies that the values given in the REFLN list are derived from the final cycle of refinement, but this is not a formal requirement. Care should be taken when preparing a CIF for archiving that the structural model corresponds to the refinement cycle summarized in the accompanying REFLN table, especially if the file is constructed from fragments output from different programs.

3.2.3.2.2. *Groups of reflections*

The data items in these categories are as follows:

(*a*) REFLNS

```
  _reflns_d_resolution_high
  _reflns_d_resolution_low
  _reflns_Friedel_coverage
  _reflns_limit_h_max
  _reflns_limit_h_min
  _reflns_limit_k_max
  _reflns_limit_k_min
  _reflns_limit_l_max
  _reflns_limit_l_min
  _reflns_number_gt
† _reflns_number_observed
  _reflns_number_total
† _reflns_observed_criterion
  _reflns_special_details
  _reflns_threshold_expression
```

(*b*) REFLNS_CLASS

```
• _reflns_class_code
  _reflns_class_d_res_high
  _reflns_class_d_res_low
  _reflns_class_description
  _reflns_class_number_gt
  _reflns_class_number_total
  _reflns_class_R_factor_all
  _reflns_class_R_factor_gt
  _reflns_class_R_Fsqd_factor
  _reflns_class_R_I_factor
  _reflns_class_wR_factor_all
```

(*c*) REFLNS_SCALE

```
• _reflns_scale_group_code
  _reflns_scale_meas_F
  _reflns_scale_meas_F_squared
  _reflns_scale_meas_intensity
```

(*d*) REFLNS_SHELL

```
• _reflns_shell_d_res_high
• _reflns_shell_d_res_low
† _reflns_shell_meanI_over_sigI_all
† _reflns_shell_meanI_over_sigI_gt
† _reflns_shell_meanI_over_sigI_obs
  _reflns_shell_meanI_over_uI_all
  _reflns_shell_meanI_over_uI_gt
  _reflns_shell_number_measured_all
  _reflns_shell_number_measured_gt
† _reflns_shell_number_measured_obs
  _reflns_shell_number_possible
  _reflns_shell_number_unique_all
  _reflns_shell_number_unique_gt
† _reflns_shell_number_unique_obs
  _reflns_shell_percent_possible_all
  _reflns_shell_percent_possible_gt
† _reflns_shell_percent_possible_obs
  _reflns_shell_Rmerge_F_all
  _reflns_shell_Rmerge_F_gt
† _reflns_shell_Rmerge_F_obs
  _reflns_shell_Rmerge_I_all
  _reflns_shell_Rmerge_I_gt
† _reflns_shell_Rmerge_I_obs
```

The bullet (•) indicates a category key. Where multiple items within a category are marked with a bullet, they must be taken together to form a compound key. The dagger (†) indicates a deprecated item, which should not be used in the creation of new CIFs.

The data items in the REFLNS category describe properties or attributes of the complete set of reflections used in the structure refinement. Several are derivative and may be obtained from the information in the reflections list, but it is convenient to present them separately so that they do not need to be calculated again. They can also be used to check the consistency of the reflections list.

The **_reflns_limit_*** data items define the upper and lower bounds on the Miller indices and on the interplanar d spacings.

The **_reflns_threshold_expression** is a text field describing the criterion applied to mark individual reflections as 'significantly intense' (*i.e.* distinct from the background level). This is typically expressed as a multiple of the standard uncertainty on the quantity used in refinement, *e.g.* `I>2u(I)`.

The number of reflections with values higher than the threshold is reported in **_reflns_number_gt**. The total number of reflections measured is given by **_reflns_number_total**. Although the use of these data names appears to be obvious, different practices have been used in the past to report total numbers (*e.g.* by neglecting symmetry-equivalent reflections) and the definitions in the dictionary should be consulted. Both numbers may contain Friedel-equivalent reflections (those which are symmetry-equivalent under the Laue symmetry but inequivalent under the crystal class).

The proportion of Friedel-related reflections present is reported separately by **_reflns_Friedel_coverage**, defined as $(N_C - N_L)/N_L$, where N_C is the number of reflections obtained on averaging under the symmetry of the crystal class and N_L is the number obtained on averaging under the Laue class. The definition in the dictionary provides examples of how the value of this data name may be used as an indicator of the fraction of the available reciprocal space sampled in the diffraction experiment.

The deprecated data names **_reflns_observed_criterion** and **_reflns_number_observed** reflect the old use of 'observed' as a term describing significantly intense reflections. They should not be used in the creation of new CIFs, but are retained to ensure that the information can be extracted from old CIFs.

The free-text field **_reflns_special_details** can be used to discuss any aspects of the reflections list not covered by other data names. It is recommended that information about the averaging of symmetry-equivalent reflections (including Friedel pairs) should be given here.