This is version 2.3.1 of the core CIF dictionary (coreCIF). A commentary on the use of this dictionary may be found in Chapter 3.2.

The data names defined here are central to the description and reporting of any crystal structure determination, and this dictionary collects the natural set of descriptors for small-unit-cell structures (typically inorganic or small-molecular organic and metal-organic compounds) determined in single-crystal experiments. These data items may be supplemented by additional items designed for use in powder-diffraction experiments (Chapter 3.3), modulated and composite structures (Chapter 3.4), or electron-density studies (Chapter 3.5).

The data items in this dictionary also form a suitable basis for the description of biological macromolecular structures, but the complexity of such structures requires a more extensive dictionary (Chapter 3.5).

Categories are described in alphabetic order; data items are arranged alphabetically within each category.

### 4.1. Core dictionary (coreCIF)

**By S. R. Hall, F. H. Allen and I. D. Brown**

Data items in the ATOM_SITE category record details about the atom sites in a crystal structure, such as the positional coordinates, atomic displacement parameters, and magnetic moments and directions.


```
loop_
  _atom_site_label
  _atom_site_type
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_aniso_B_11
  _atom_site_aniso_B_12
  _atom_site_aniso_B_13
  _atom_site_aniso_B_22
  _atom_site_aniso_B_23
  _atom_site_aniso_B_33
  _atom_site_chemical_conn_number
  _atom_site_label
  _atom_site_disorder_group
  _atom_site_disorder_assembly
  _atom_site_occupancy
  _atom_site_thermal_displace_type
```


```
loop_
  _atom_site_label
  _atom_site_chemical_conn_number
  _atom_site_fract_x
  _atom_site_aniso_B_11
  _atom_site_aniso_B_12
  _atom_site_aniso_B_13
  _atom_site_aniso_B_22
  _atom_site_aniso_B_23
  _atom_site_aniso_B_33
  _atom_site_aniso_label
  _atom_site_disorder_group
  _atom_site_disorder_assembly
  _atom_site_occupancy
  _atom_site_thermal_displace_type
```

**Example 3 – hypothetical example to illustrate the description of a disordered methyl group.**

```
loop_
  _atom_site_label
  _atom_site_type
  _atom_site_label # _assembly M is a disordered methyl
  _atom_site_occupancy # with configurations 'A' and 'B':
  _atom_site_disorder_assembly
  _atom_site_thermal_displace_type
```

**Example 4 – hypothetical code to describe the type of atomic displacement parameters used for the site.**

Appears in list containing _atom_site_label.

Related item: _atom_site_thermal_displace_type(alternate).

The data value must be one of the following:

- **Uani**: anisotropic U
- **Uiso**: isotropic U
- **Uovl**: overall U
- **Bani**: anisotropic B
- **Biso**: isotropic B
- **Bovl**: overall B

Appears in list containing _atom_site_label.
These are the standard anisotropic atomic displacement components in ångströms squared which appear in the structure-factor terms to the atom site to which the ‘geometry-calculated’ atom site is attached.

Appears in list containing _atom_site_label. Where no value is given, the assumed value is ‘.’.

Related item: _atom_site_calc_attached_atom (alternate).

Appears in list containing _atom_site_label. Where no value is given, the assumed value is ‘d’.

The data value must be one of the following:
- d determined from diffraction measurements
- calc calculated from molecular geometry
- c abbreviation for ‘calc’
- dum dummy site with meaningless coordinates

Related items: _atom_site_label where no value is given, the assumed value is ‘c’.

The IUCr Commission on Nomenclature recommends against the use of _atom_site_type_symbol codes in this list.

Appears in list containing _atom_site_aniso_label. Must match parent data name _atom_site_label

The unique elements of the real symmetric matrix are entered by row.

Appears in list containing _atom_site_aniso_label. Must match parent data name _atom_site_label

These are the standard anisotropic atomic displacement components in ångströms squared which appear in the structure-factor term

\[
T = \exp\left\{ -\frac{(1/4)}{2} \sum_i \sum_j (B^{ij}h_i h_j a_i^* a_j^*) \right\},
\]

where \( h = \) the Miller indices and \( a^* = \) the reciprocal-space cell lengths.

The unique elements of the real symmetric matrix are entered by row.

Appears in list containing _atom_site_aniso_label. Related item: _atom_site_aniso_U_ (conversion).

Anisotropic atomic displacement parameters are usually looped in a separate list. If this is the case, this code must match the _atom_site_aniso_label of the associated atom in the atom coordinate list and conform with the same rules described in _atom_site_aniso_label.

Appears in list as an essential element of loop structure. Must match parent data name _atom_site_label

Ratio of the maximum to minimum principal axes of displacement (thermal) ellipsoids.

Appears in list containing _atom_site_aniso_label. The permitted range is 1.0 → ∞.

This _atom_type_symbol code links the anisotropic atom parameters to the atom-type data associated with this site and must match one of the _atom_type_symbol codes in this list.

Appears in list containing _atom_site_aniso_label. Must match parent data name _atom_site_type_symbol

The number of hydrogen atoms attached to the atom at this site excluding any hydrogen atoms for which coordinates (measured or calculated) are given.

Appears in list containing _atom_site_label. The permitted range is 0 → 8. Where no value is given, the assumed value is ‘0’.

Examples: ‘2’ (water oxygen), ‘1’ (hydroxyl oxygen), ‘4’ (ammonium nitrogen).

Equivalent isotropic atomic displacement parameter, \( B_{\text{equiv}} \), in ångströms squared, calculated as the geometric mean of the anisotropic atomic displacement parameters.

\[
B_{\text{equiv}} = \left( \frac{B_{11} + B_{22} + B_{33}}{3} \right)^{1/2},
\]

where \( B_{ij} = \) the principal components of the orthogonalized \( B^{ij} \).

The IUCr Commission on Nomenclature recommends against the use of _atom_site_aniso_label for reporting atomic displacement parameters. \( U \), being directly proportional to \( B \), is preferred.

Appears in list containing _atom_site_label. The permitted range is 0.0 → ∞.

Isotropic atomic displacement parameter, or equivalent isotropic atomic displacement parameter, \( B_{\text{equiv}} \), in ångströms squared, calculated from anisotropic displacement components.

\[
B_{\text{equiv}} = \left( \frac{1}{3} \sum_i \sum_j (B^{ij}A_i A_j a_i^* a_j^*) \right)^{1/2},
\]

where \( A = \) the real-space cell lengths and \( a^* = \) the reciprocal-space cell lengths; \( B^{ij} = 8\pi^2 U^{ij} \).


The IUCr Commission on Nomenclature recommends against the use of _atom_site_aniso_label for reporting atomic displacement parameters. \( U \), being directly proportional to \( B \), is preferred.

Appears in list containing _atom_site_label. The permitted range is 0.0 → ∞.

The IUCr Commission on Nomenclature recommends against the use of _atom_site_aniso_label for reporting atomic displacement parameters. \( U \), being directly proportional to \( B \), is preferred.

Appears in list containing _atom_site_label. Where no value is given, the assumed value is ‘c’.

A standard code to signal whether the site coordinates have been determined from the intensities or calculated from the geometry of surrounding sites, or have been assigned dummy coordinates. The abbreviation ‘c’ may be used in place of ‘calc’.

Appears in list containing _atom_site_label. Where no value is given, the assumed value is ‘d’.

The data value must be one of the following:
- d determined from diffraction measurements
- calc calculated from molecular geometry
- c abbreviation for ‘calc’
- dum dummy site with meaningless coordinates

Where no value is given, the assumed value is ‘d’.
**ATOM_SITE**

`atom_site_label` *(char)*

The `atom_site_label` is a unique identifier for a particular site in the crystal. This code is made up of a sequence of up to seven components, `atom_site_label_component_0` to `atom_site_label_component_6`, which may be specified as separate data items. Component 0 usually matches one of the specified `atom_type_symbol` codes. This is not mandatory if an `atom_site_type_symbol` item is included in the atom-site list. The `atom_site_type_symbol` always takes precedence over an `atom_site_label` in the identification of the atom type. The label components 1 to 6 are optional, and normally only components 0 and 1 are used. Note that components 0 and 1 are concatenated, while all other components, if specified, are separated by an underscore. Underscore separators are only used if higher-order components exist. If an intermediate component is not used, it may be omitted provided the underscore separators are inserted. For example, the label 'C233_ggg' is acceptable and represents the components C, 233, 'g' and ggg. Different labels may have a different number of components.

Appears in list as essential element of loop structure. May match child data name(s): _atom_site_aniso_label, _geom_angle_atom_site_label_1, _geom_angle_atom_site_label_2, _geom_angle_atom_site_label_3, _geom_bond_atom_site_label_1, _geom_bond_atom_site_label_2, _geom_contact_atom_site_label_1, _geom_contact_atom_site_label_2, _geom_bond_atom_site_label_D, _geom_bond_atom_site_label_R, _geom_bond_atom_site_label_A, _geom_contact_atom_site_label_1, _geom_contact_atom_site_label_2, _geom_contact_atom_site_label_3, _geom_contact_atom_site_label_4, _geom_torsion_atom_site_label_1, _geom_torsion_atom_site_label_2, _geom_torsion_atom_site_label_3, _geom_torsion_atom_site_label_4, _atom_site_disorder_assembly, _atom_site_disorder_group, _atom_site_disorder_atom_number, _atom_site_chemical_conn_number, _atom_site_label_component_0, _atom_site_label_component_1, _atom_site_label_component_2, _atom_site_label_component_3, _atom_site_label_component_4, _atom_site_label_component_5, _atom_site_label_component_6.

Examples: 'C12', 'Ca3g28', 'Fe3+17', 'H*251', 'boron2a', 'C_3pGe_33_A', 'Zn,En,101_A,0'.

**4. DATA DICTIONARIES**

**cif.core.dic**

`atom_site_chemical_conn_number` *(numb, su)*

This field is used to identify the component 0 number specified by _chemical_conn_atom_number_.

Appears in list containing _atom_site_label. Must match parent data name _chemical_conn_atom_number_.

The permitted range is $1 \rightarrow \infty$.

**atom_site_constraints** *(char)*

A description of the constraints applied to parameters at this site during refinement. See also _atom_site_refinement_flags_ and _refine_SET_number constraints_.

Appears in list containing _atom_site_label. Where no value is given, the assumed value is ' '.

Example: 'pop=1.0-pop(Zn3)'.

**atom_site_description** *(char)*

A description of special aspects of this site. See also _atom_site_refinement_flags_.

Appears in list containing _atom_site_label.

Example: 'Ag/Si disordered'.

**atom_site_disorder_assembly** *(char)*

A code which identifies a cluster of atoms that show long-range positional disorder but are locally ordered. Within each such cluster of atoms, _atom_site_disorder_group_ is used to identify the sites that are simultaneously occupied. This field is only needed if there is more than one cluster of disordered atoms showing independent local order.

Appears in list containing _atom_site_label.

Examples: 'X' (disordered methyl assembly with groups 1 and 2), 'Y' (disordered sites related by a mirror), 'Z' (disordered sites independent of symmetry).

**atom_site_disorder_group** *(char)*

A code which identifies a group of positionally disordered atom sites that are locally simultaneously occupied. Atoms that are positionally disordered over two or more sites (e.g. the hydrogen atoms of a methyl group that exists in two orientations) can be assigned to two or more groups. Sites belonging to the same group are simultaneously occupied, but those belonging to different groups are not. A minus prefix (e.g. '-1') is used to indicate sites disordered about a special position.

Appears in list containing _atom_site_label.

Examples: '1' (unique disordered site in group 1), '2' (unique disordered site in group 2), '-1' (symmetry-independent disordered site).

**atom_site_frac_x**

**atom_site_frac_y**

**atom_site_frac_z** *(numb, su)*

Atom-site coordinates as fractions of the _cell_length_ values.

Appears in list containing _atom_site_label.

Related item _atom_site_Cartn_ (alternate).
4.1. CORE DICTIONARY (coreCIF)  

**ATOM SITE**

- **atom_site_symmetry_multiplicity** (numb)
  - The multiplicity of a site due to the space-group symmetry as given in International Tables for Crystallography Vol. A (2002).
  - Appears in list containing _atom_site_label.
  - The permitted range is $1 \rightarrow 192$.

- **atom_site_thermal_displace_type** (char)
  - A code used to describe the type of atomic displacement parameters used for the site.
  - Appears in list containing _atom_site_label.
  - The data value must be one of the following:
    - Uani: anisotropic $U_{ij}$
    - Uiso: isotropic $U$
    - Uovl: overall $U$
    - Umpe: multipole expansion $U$
    - Baniso: anisotropic $B$
    - Biso: isotropic $B$
    - Bovl: overall $B$

- **atom_site_label** (char)
  - A code which identifies the atom species (singular or plural) occupying this site. This code must match a corresponding **atom_type_symbol**. The specification of this code is optional if component 0 of the **atom_site_label** is used for this purpose.
  - See **atom_type_symbol**.
  - Appears in list containing _atom_site_label.
  - Must match parent data name _atom_type_symbol.

- **atom_site_U_equiv_geom_mean** (numb, su)
  - Equivalent isotropic atomic displacement parameter, $U_{eq}$, in ångströms squared, calculated as the geometric mean of the anisotropic atomic displacement parameters.
  - Appears in list containing _atom_site_label.
  - The permitted range is $0 \rightarrow \infty$.
  - The data value must be one of the following:
    - $U_{eq} = (U_{11}U_{22}U_{33})^{1/3}$,
    - where $U_{ij}$ = the principal components of the orthogonalized $U_{ij}$.

- **atom_site_U_iso_or_equiv** (numb, su)
  - Isotropic atomic displacement parameter, or equivalent isotropic atomic displacement parameter, $U_{eq}$, in ångströms squared, calculated from anisotropic atomic displacement parameters.
  - Appears in list containing _atom_site_label.
  - The permitted range is $0 \rightarrow \infty$.
  - The data value must be one of the following:
    - $U_{eq} = (1/3) \sum_i \left[ \sum_j \left( U_{ij}a_i^*a_j^* \right) \right]$, 
    - where $a_i^*$ = the reciprocal-space cell lengths and $a_i^* = a_i^*$ = the reciprocal-space cell lengths.


**atom_site_restraints** (char)
- A description of restraints applied to specific parameters at this site during refinement. See also _atom_site_refinement_flags and _refine_ls_number_restraints.
  - Appears in list containing _atom_site_label.
  - Example: ‘restrained to planar ring’. (alternate).
**ATOM_SITES**

Data items in the ATOM_SITES category record details about the crystallographic cell and cell transformations, which are common to all atom sites.

Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.

<table>
<thead>
<tr>
<th>ATOM_SITES Cartn transform axes</th>
<th>'c along z, astar along x, b along y'</th>
</tr>
</thead>
<tbody>
<tr>
<td>atom_sites_Cartn_tran_matrix_11</td>
<td>58.39</td>
</tr>
<tr>
<td>atom_sites_Cartn_tran_matrix_12</td>
<td>0.00</td>
</tr>
<tr>
<td>atom_sites_Cartn_tran_matrix_13</td>
<td>0.00</td>
</tr>
<tr>
<td>atom_sites_Cartn_tran_matrix_21</td>
<td>86.70</td>
</tr>
<tr>
<td>atom_sites_Cartn_tran_matrix_22</td>
<td>86.70</td>
</tr>
<tr>
<td>atom_sites_Cartn_tran_matrix_31</td>
<td>0.00</td>
</tr>
<tr>
<td>atom_sites_Cartn_tran_matrix_32</td>
<td>0.00</td>
</tr>
<tr>
<td>atom_sites_Cartn_tran_matrix_33</td>
<td>46.27</td>
</tr>
</tbody>
</table>

Matrix elements used to transform fractional coordinates in the ATOM_SITE category to Cartesian coordinates. The axial alignments of this transformation are described in `atom_sites_Cartn_transform_axes`. The $3 \times 1$ translation is defined in `atom_sites_Cartn_tran_vector_1`.

\[
\begin{pmatrix}
  x' \\
  y' \\
  z'
\end{pmatrix}
\_{\text{Cartesian}} =
\begin{pmatrix}
  11 & 12 & 13 \\
  21 & 22 & 23 \\
  31 & 32 & 33
\end{pmatrix}
\begin{pmatrix}
  x \\
  y \\
  z
\end{pmatrix}
\_{\text{fractional}} +
\begin{pmatrix}
  1 \\
  2 \\
  3
\end{pmatrix}.
\]

**atom_sites_Cartn_tran_matrix_1**

**atom_sites_Cartn_tran_matrix_2**

**atom_sites_Cartn_tran_matrix_3**

**atom_sites_Cartn_tran_matrix_11**

**atom_sites_Cartn_tran_matrix_12**

**atom_sites_Cartn_tran_matrix_13**

Elements of a $3 \times 1$ translation vector used in the transformation of Cartesian coordinates in the ATOM_SITE category to fractional coordinates. The axial alignments of this transformation are described in `atom_sites_Cartn_transform_axes`. The $3 \times 1$ translation is defined in `atom_sites_Cartn_tran_vector_2`.

\[
\begin{pmatrix}
  x' \\
  y' \\
  z'
\end{pmatrix}
\_{\text{Cartesian}} =
\begin{pmatrix}
  11 & 12 & 13 \\
  21 & 22 & 23 \\
  31 & 32 & 33
\end{pmatrix}
\begin{pmatrix}
  x \\
  y \\
  z
\end{pmatrix}
\_{\text{fractional}} +
\begin{pmatrix}
  1 \\
  2 \\
  3
\end{pmatrix}.
\]

**atom_sites_Cartn_tran_vector_1**

**atom_sites_Cartn_tran_vector_2**

**atom_sites_Cartn_tran_vector_3**

**atom_sites_Cartn_tran_vector_1**

**atom_sites_Cartn_tran_vector_2**

**atom_sites_Cartn_tran_vector_3**

**atom_sites_solution_primary**

**atom_sites_solution_secondary**

**atom_sites_solution_hydrogens**

Covers which identify the methods used to locate the initial atom sites. The *primary* code identifies how the first atom sites were determined; the *secondary* code identifies how the remaining non-hydrogen sites were located; and the *hydrogens* code identifies how the hydrogen sites were located.

The data value must be one of the following:

- difmap: difference Fourier map
- vecmap: real-space vector search
- heavy: heavy-atom method
- direct: structure-invariant direct methods
- geom: inferred from neighbouring sites
- disper: anomalous-dispersion techniques
- isomor: isomorphous structure methods

**atom_sites_special_details**

Additional information about the atomic coordinates not coded elsewhere in the CIF.

**ATOM_TYPE**

Data items in the ATOM_TYPE category record details about properties of the atoms that occupy the atom sites, such as the atomic scattering factors.


<table>
<thead>
<tr>
<th>atom_type_symbol</th>
<th>atom_type_oxidation_number</th>
<th>atom_type_number_in_cell</th>
<th>atom_type_scat Dispersion Real</th>
<th>atom_type_scat Dispersion Imag</th>
<th>atom_type_scat Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>C 0 72 0.357 0.009 International Tables Vol IV Table 2.2B</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H 0 100 0 0 International Tables Vol IV Table 2.2B</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>O 0 12 0.047 0.032 International Tables Vol IV Table 2.2B</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>N 0 0.029 0.018 International Tables Vol IV Table 2.2B</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Example: 'International Tables Vol. IV Table 2.4.6B'.
Example: 'International Tables Vol. IV, Table 2.2B; 1991-04-18 adjustments based on second referee report.'
Example: 'International Tables Vol. IV Table 2.3.1'.

Highlights:
- The Cromer–Mann scattering-factor coefficients used to calculate the scattering factors for this atom type.
- The imaginary and real components of the anomalous-dispersion coefficients.
- The bound coherent scattering length in femtometres for the atom type at the isotopic composition used for the diffraction experiment.

References:

Data items in the AUDIT category record details about the creation and subsequent updating of the data block.


| AUDIT | 
|---|---|
| _audit_block_code | TOZ_1991-03-20 |
| _audit_creation_date | 1991-03-20 |
| _audit_creation_method | from_xtal_archive_file_using_CIFIO |

| AUDIT | 
|---|---|
| _audit_block_code | (char) |
| _audit_creation_date | (char) |
| _audit_creation_method | (char) |
| _audit_update_record | (char) |

A code intended to identify uniquely the current data block.
The date that the data block was created. The date format is yyyy-mm-dd.
A description of how data were entered into the data block.
A record of any changes to the data block. The update format is a date (yyyy-mm-dd) followed by a description of the changes. The latest update entry is added to the bottom of this record.
4. DATA DICTIONARIES

AUDIT_AUTHOR

Data items in the AUDIT_AUTHOR category record details about the author(s) of the data block.

Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.

<table>
<thead>
<tr>
<th>_audit_author_name</th>
<th>_audit_author_address</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fitzgerald, Paula M. D.</td>
<td>Merck Research Laboratories</td>
</tr>
<tr>
<td>2000, Sy80203</td>
<td>Rahway</td>
</tr>
<tr>
<td>New Jersey 07065</td>
<td>USA</td>
</tr>
</tbody>
</table>

_Audit_author_address_ (char)
The address of an author of this data block. If there are multiple authors, _audit_author_address_ is looped with _audit_author_name_.

Appears in list containing _audit_author_name_.

Example:

; Department
Institute
City and postcode
COUNTRY ;

_Audit_author_name_ (char)
The name of an author of this data block. If there are multiple authors, _audit_author_name_ is looped with _audit_author_address_. The family name(s), followed by a comma and including any dynastic components, precedes the first name(s) or initial(s).

Appears in list as essential element of loop structure.


AUDIT_CONFORM

Data items in the AUDIT_CONFORM category describe the dictionary versions against which the data names appearing in the current data block are conformant.

Example 1 – any file conforming to the current CIF core dictionary.

<table>
<thead>
<tr>
<th>_audit_conform_dict_name</th>
<th>_audit_conform_dict_location</th>
</tr>
</thead>
<tbody>
<tr>
<td>cif_core.dic</td>
<td>ftp://ftp.iucr.org/pub/cif_core.2.3.1.dic</td>
</tr>
</tbody>
</table>

_Audit_conform_dict_location_ (char)
A file name or uniform resource locator (URL) for the dictionary to which the current data block conforms.

May appear in list containing _audit_conform_dict_name_. [audit_conform]

_Audit_conform_dict_name_ (char)
The string identifying the highest-level dictionary defining data names used in this file.

May appear in list as essential element of loop structure. [audit_conform]
4.1. CORE DICTIONARY (coreCIF)

**CELL**

- cell_formula_units_Z (numb)
  - The number of the formula units in the unit cell as specified by _chemical_formula_structural_ or _chemical_formula_moiety_.
  - The permitted range is $0 \rightarrow \infty$.

- cell_length_a (numb, su)
  - Unit-cell lengths in ångströms corresponding to the structure reported.
  - The values of _diffrn_refln_index_h_ *k* _l* must correspond to the cell defined by these values and _cell_angle_ values.
  - The values of _diffrn_refln_index_h_ *k* _l* may not correspond to these values if a cell transformation took place following the measurement of the diffraction intensities. See also _diffrn_reflns_transf_matrix_.

- cell_measurement_theta_max (numb)
  - The maximum and minimum $\theta$ angles of reflections used to measure the unit cell in degrees.
  - The permitted range is $0 \rightarrow 180.0$.

- cell_measurement_theta_min (numb)
  - Where no value is given, the assumed value is '90.0'.

- cell_measurement_temperature (numb, su)
  - The temperature in kelvins at which the unit-cell parameters were measured (not the temperature at which the sample was synthesized).
  - The permitted range is $0 \rightarrow \infty$.

- cell_measurement_wavelength (char)
  - The wavelength in ångströms of the radiation used to measure the unit-cell parameters.
  - The permitted range is $0 \rightarrow \infty$.

- _diffrn_reflns_transf_matrix_ (char)
  - The wavelength in ångströms of the radiation used to measure the unit-cell parameters.
  - The permitted range is $0 \rightarrow \infty$.

**DATA ITEMS**

- audit_contact_author_phone (char)
  - The telephone number of the author of the data block to whom correspondence should be addressed.
  - The recommended style starts with the international dialing prefix, followed by the area code in parentheses, followed by the local number and any extension number prefixed by ‘x’, with no spaces.

Examples: '12(34)9477330', '12(3)49477330','12(34)9477330x5543'.

- audit_link (link)
  - A textual description of the relationship of the referenced data to the current file related to the current data block. See also _audit_link_block_code_, _audit_link_block_description_, _audit_link_block_code_, _audit_link_block_description_, _audit_link_block_code_, _audit_link_block_description_.


Example 2 – example file for the one-dimensional incommensurately modulated structure of K$_2$SeO$_4$.

- audit_link_block_code (char)
  - The value of _audit_block_code_ associated with a data block in the current file related to the current data block. The special value '*' may be used to refer to the current data block for completeness.

  Appears in list as essential element of loop structure.

- audit_link_block_description (char)
  - A textual description of the relationship of the referenced data block to the current one.

  Appears in list containing _audit_link_block_code_.

- audit_block_code (char)
  - The telephone number of the author of the data block to whom correspondence should be addressed. The recommended style starts with the international dialing prefix, followed by the area code in parentheses, followed by the local number and any extension number prefixed by ‘x’, with no spaces.

Examples: '12(34)9477330', '12(3)49477330','12(34)9477330x5543'. [audit_contact_author]
4. DATA DICTIONARIES

CHEMICAL

Data items in the CHEMICAL category record details about the composition and chemical properties of the compound. The formula data items must agree with those that specify the density, unit-cell and Z values.


 absolute_configuration (char)

Necessary conditions for the assignment of absolute_configuration are given by H. D. Flack and G. Bernardinelli (1999, 2000).


The data value must be one of the following:

rm Absolute configuration established by the structure determination of a compound containing a chiral reference molecule of known absolute configuration.
ad Absolute configuration established by anomalous-dispersion effects in diffraction measurements on the crystal. 
rmad Absolute configuration established by the structure determination of a compound containing a chiral reference molecule of known absolute configuration and confirmed by anomalous-dispersion effects in diffraction measurements on the crystal.

syn Absolute configuration has not been established by anomalous-dispersion effects in diffraction measurements on the crystal. The enantiomer has been assigned by reference to an unchanging chiral centre in the synthetic procedure.

unk Absolute configuration is unknown, there being no firm chemical evidence for its assignment to hand and it having not been established by anomalous-dispersion effects in diffraction measurements on the crystal. An arbitrary choice of enantiomer has been made.

Inapplicable.

CHEMICAL

Data items in the CHEMICAL category record details about the composition and chemical properties of the compound. The formula data items must agree with those that specify the density, unit-cell and Z values.


 absolute_configuration (char)

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unk Absolute configuration is unknown, there being no firm chemical evidence for its assignment to hand and it having not been established by anomalous-dispersion effects in diffraction measurements on the crystal. An arbitrary choice of enantiomer has been made.

Inapplicable.

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Inapplicable.

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unk Absolute configuration is unknown, there being no firm chemical evidence for its assignment to hand and it having not been established by anomalous-dispersion effects in diffraction measurements on the crystal. An arbitrary choice of enantiomer has been made.

Inapplicable.
4.1. CORE DICTIONARY (coreCIF)

**CHEMICAL.MELTING POINT**

- **_chemical_melting_point_gt** (num)
  - A temperature in kelvins below which (*_lt*) or above which (*_gt*) the melting point (the temperature at which the crystalline solid changes to a liquid) lies. These items allow a range of temperatures to be given. _chemical_melting_point should always be used in preference to these items whenever possible.
  - The permitted range is 0 → ∞.
  - Related item: _chemical_melting_point (alternate).

- **_chemical_melting_point_lt** (num)
  - The temperature in kelvins at which the solid decomposes.
  - The permitted range is 0 → ∞.
  - Example: '350'.

**CHEMICAL.PROPERTY**

- **_chemical_temperature_decomposition** (num, su)
  - The temperature in kelvins at which the solid decomposes.
  - The permitted range is 0 → ∞.
  - Example: '350'.

**CHEMICAL.MELTING POINT**

- **_chemical_temperature_decomposition_gt** (num)
  - A temperature in kelvins below which (*_lt*) or above which (*_gt*) the solid is known to decompose. These items allow a range of temperatures to be given. _chemical_temperature_decomposition should always be used in preference to these items whenever possible.
  - The permitted range is 0 → ∞.
  - Related item: _chemical_temperature_decomposition (alternate).

- **_chemical_temperature_decomposition_lt** (num)
  - A temperature in kelvins below which (*_lt*) or above which (*_gt*) the solid is known to decompose. These items allow a range of temperatures to be given. _chemical_temperature_decomposition should always be used in preference to these items whenever possible.
  - The permitted range is 0 → ∞.

**CHEMICAL.CONNECTED ATOM**

- **_chemical_conn_atom_**
  - Related item: _chemical_conn_bond (alternate).

**CHEMICAL.THERMAL**

- **_chemical_temperature_sublimation** (num, su)
  - The temperature in kelvins at which the solid sublime.
  - The permitted range is 0 → ∞.
  - Example: '350'.

**CHEMICAL.THERMAL**

- **_chemical_temperature_sublimation_gt** (num)
  - A temperature in kelvins below which (*_lt*) or above which (*_gt*) the solid is known to sublimate. These items allow a range of temperatures to be given. _chemical_temperature_sublimation should always be used in preference to these items whenever possible.
  - The permitted range is 0 → ∞.
  - Related item: _chemical_temperature_sublimation (alternate).

**CHEMICAL.THERMAL**

- **_chemical_temperature_sublimation_lt** (num)
  - A temperature in kelvins below which (*_lt*) or above which (*_gt*) the solid is known to sublimate. These items allow a range of temperatures to be given. _chemical_temperature_sublimation should always be used in preference to these items whenever possible.
  - The permitted range is 0 → ∞.

**CHEMICAL.THERMAL**

- **_chemical_temperature_decomposition** (num, su)
  - The temperature in kelvins at which the solid decomposes.
  - The permitted range is 0 → ∞.
  - Example: '350'.

**CHEMICAL.THERMAL**

- **_chemical_temperature_decomposition_gt** (num)
  - A temperature in kelvins below which (*_lt*) or above which (*_gt*) the solid is known to decompose. These items allow a range of temperatures to be given. _chemical_temperature_decomposition should always be used in preference to these items whenever possible.
  - The permitted range is 0 → ∞.
  - Related item: _chemical_temperature_decomposition (alternate).

**CHEMICAL.THERMAL**

- **_chemical_temperature_decomposition_lt** (num)
  - A temperature in kelvins below which (*_lt*) or above which (*_gt*) the solid is known to decompose. These items allow a range of temperatures to be given. _chemical_temperature_decomposition should always be used in preference to these items whenever possible.
  - The permitted range is 0 → ∞.
  - Related item: _chemical_temperature_decomposition (alternate).
CHEMICAL_CONN_ATOM

The net integer charge assigned to this atom. This is the formal charge assignment normally found in chemical diagrams. Appears in list containing _chemical_conn_atom_type_symbol.
The permitted range is $-\infty \rightarrow 0$. Where no value is given, the assumed value is ‘0’.
Examples: ‘1’ (for an ammonium nitrogen), ‘-1’ (for a chloride ion).

CHEMICAL_CONN_BOND

Data items in the _chemical_conn_atom and _chemical_conn_bond categories record details about the two-dimensional (2D) chemical structure of the molecular species. They allow a 2D chemical diagram to be reconstructed for use in a publication or in a database search for structural and substructural relationships. The _chemical_conn_bond data items specify the connections between the atoms in the _chemical_conn_atom list and the nature of the chemical bond between these atoms.


\[
\]

\[
\]

\[
\]
CHEMICAL FORMULA

_formula_element_ items specify the composition and chemical properties of the formula. The formula data items must agree with those that specify the density, unit-cell and Z values. The following rules apply to the construction of the data items _analytical, *_structural and *_sum. For the data item *_moiety*, the formula construction is broken up into residues or moieties, i.e., groups of atoms that form a molecular unit or molecular ion. The rules given below apply within each moiety but different requirements apply to the way that moieties are connected (see _formula moiety_). (1) Only recognized element symbols may be used. (2) Each element symbol is followed by a 'count' number. A count of '1' may be omitted. (3) A space or parenthesis must separate each cluster of (element symbol + count). (4) Where a group of elements is enclosed in parentheses, the multiplier for the group must follow the closing parenthesis. That is, all element and group multipliers are assumed to be printed as subscripted numbers. (An exception to this rule exists for *moiety* formulae where pre- and post-multipliers are permitted for molecular units.) (5) Unless the elements are ordered in a manner that corresponds to their chemical structure, as in _formula structural_, the order of the elements within any group or moiety depends on whether carbon is present or not. If carbon is present, the order should be: C, then H, then the other elements in alphabetical order of their symbol. If carbon is not present, the elements are listed purely in alphabetical order of their symbol. This is the 'Hill' system used by _Chemical Abstracts_. This ordering is used in _formula and _sum_.


_formula_moiety_ 'C18 H25 N O3'
_formula_sum_ 'C18 H25 N O3'
_formula_weight_ 303.40


_formula_iupac_ 'Mo, 4 (C O) 4 (C18 H33 P) 2'
_formula_moiety_ 'Mo, 4 (C O) 4 (C18 H33 P) 2'
_formula_structural_ (C O) 4 (F, (C5 H11) 3) 2 Mo'
_formula_sum_ 'C40 H66 Mo O4 P2'
_formula_weight_ 768.81

FORMULA category description for the rules for writing chemical formulae. Parentheses are assumed to be printed as subscripted numbers. (An exception to this rule exists for _moiety_ formulae where pre- and post-multipliers are permitted for molecular units.) (5) Unless the elements are ordered in a manner that corresponds to their chemical structure, as in _formula structural_, the order of the elements within any group or moiety depends on whether carbon is present or not. If carbon is present, the order should be: C, then H, then the other elements in alphabetical order of their symbol. If carbon is not present, the elements are listed purely in alphabetical order of their symbol. This is the ‘Hill’ system used by _Chemical Abstracts_. This ordering is used in _formula and _sum_.

See the _CHEMICAL FORMULA category description for the rules for writing chemical formulae in which all discrete bonded residues and ions are summed over the constituent elements, following the ordering given in general rule (5) in the _CHEMICAL FORMULA category description. Parentheses are not normally used._

Example: 'Co Re (C12 H22 P) 2 (C O) 6, 0.5C H3 O H'.

_formula_analytical_ (char)

Formula determined by standard chemical analysis including trace elements. See the _CHEMICAL FORMULA category description for rules for writing chemical formulae. Parentheses are used only for standard uncertainties (e.s.d.’s).

Example: 'Fe 2.45(2) Ni 1.60(3) S 47'.

_formula_iupac_ (char)

Formula expressed in conformance with IUPAC rules for inorganic and metal-organic compounds where these conflict with the rules for any other _formula_ entries. Typically used for formatting a formula in accordance with journal rules. This should appear in the data block in addition to the most appropriate of the other _formula_ data names.


Example: 'Ca ((Cl O3)2 O)2 (H2 O)6'.

_formula_weight_ (numb)

Formula mass in daltons. This mass should correspond to the formula given under _formula structural_. *moiety or *sum and, together with the Z value and cell parameters, should yield the density given as _exp1_crystal_density_diffrn_.

The permitted range is 1.0 → ∞.

_formula_weight_meas_ (numb)

Formula mass in daltons measured by a non-diffraction experiment.

The permitted range is 1.0 → ∞.
Data items in the CITATION category record details about the literature cited as being relevant to the contents of the data block.

Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP:

<table>
<thead>
<tr>
<th>loop_</th>
</tr>
</thead>
<tbody>
<tr>
<td>_citation_id</td>
</tr>
<tr>
<td>_citation_coordinate_linkage</td>
</tr>
<tr>
<td>_citation_title</td>
</tr>
<tr>
<td>_citation_country</td>
</tr>
<tr>
<td>_citation_page_first</td>
</tr>
<tr>
<td>_citation_page_last</td>
</tr>
<tr>
<td>_citation_year</td>
</tr>
<tr>
<td>_citation_journal_abbr</td>
</tr>
<tr>
<td>_citation_journal_volume</td>
</tr>
<tr>
<td>_citation_journal_issue</td>
</tr>
<tr>
<td>_citation_journal_id_ASTM</td>
</tr>
<tr>
<td>_citation_journal_id_ISSN</td>
</tr>
<tr>
<td>_citation_book_title</td>
</tr>
<tr>
<td>_citation_book_publisher</td>
</tr>
<tr>
<td>_citation_book_id_ISBN</td>
</tr>
</tbody>
</table>

Citation for example:

- Title: "Crystallographic analysis of a complex between human immunodeficiency virus type I protease and acetyl-pepstatin at 2.0-Angstroms resolution.
- Year: 1990
- Location: New York

Example 2:

- Title: "Three-dimensional structure of aspartyl-protease from human immunodeficiency virus HIV-1.
- Year: 1990
- Location: UK

Example 3:

- Title: "Determination of the structure of the unliganded enzyme.
- Year: 1990
- Location: UK

Abstract for the citation. This is used most when the citation is extracted from a bibliographic database that contains full text or abstract information.

Example from PubMed:

- Title: "Crystallographic analysis of a complex between human immunodeficiency virus type I protease and acetyl-pepstatin at 2.0-Angstroms resolution.
- Year: 1990
- Location: New York

Example from Medline:

- Title: "Three-dimensional structure of aspartyl-protease from human immunodeficiency virus HIV-1.
- Year: 1990
- Location: UK

Example from CSD:

- Title: "Determination of the structure of the unliganded enzyme.
- Year: 1990
- Location: UK


Example:

- ISBN: "0221-9258"
CITATION_EDITOR

Data items in the CITATION_EDITOR category record details about the editor associated with the book or book chapter citations in the _citation_list.

Example 1 – hypothetical example.

loop
_citation_editor_citation_id _citation_editor_name
5 'McKeever, B.M.'
5 'Navia, M.A.'
5 'Fitzgerald, P.M.D.'
5 'Springer, J.P.'

_citation_editor_citation_id (char)
The value of _citation_editor_citation_id must match an identifier specified by _citation_id in the _citation_list.
Appears in list as essential element of loop structure. Must match parent data name _citation_id.

_citation_editor_name (char)
Name of an editor of the citation; relevant for books and book chapters. The family name(s), followed by a comma and including any dynastic components, precedes the first name(s) or initial(s).
Appears in list as essential element of loop structure.

DATABASE

Data items in the DATABASE category record details about the database identifiers of the data block. These data items are assigned by database managers and should only appear in a CIF if they originate from that source.


_database_code_CSD 'VOBYDD'
_database_code_CAS
_database_code_ICSD
_database_code_MDF
_database_code_PB
_database_code_PDB
_database_code_PDF (char)
The codes are assigned by databases: Chemical Abstracts; Cambridge Structural Database (organic and metal-organic compounds); Inorganic Crystal Structure Database; Metals Data File (metal structures); NBS (NIST) Crystal Data Database (lattice parameters); Protein Data Bank; and the Powder Diffraction File (JCPDS/ICDD).

_database_code_depnum_ccdc_archive (char)
Deposition numbers assigned by the Cambridge Crystallographic Data Centre (CCDC) to files containing structural information archived by the CCDC.

_database_code_depnum_ccdc_fiz (char)
Deposition numbers assigned by the Fachinformationszentrum Karlsruhe (FIZ) to files containing structural information archived by the Cambridge Crystallographic Data Centre (CCDC).

_database_code_depnum_ccdc_journal (char)
Deposition numbers assigned by various journals to files containing structural information archived by the Cambridge Crystallographic Data Centre (CCDC).

_computing_cell_refinement
_computing_cell_refinement (char)
Software used in the processing of the data. Give the program or package name and a brief reference.
The permitted range is 0 out to 1.

_diffrn_reflns_theta_max
q scan width (1.0 + 0.14tan(q)/2), q scan rate 1.2%/min"-1". Background counts for 5 s on each side every scan.

_diffrn_ambient_temperature 293

_diffrn_ambient_environment (char)
The gas or liquid surrounding the sample, if not air.

Examples: 'He', 'vacuum', 'mother liquor'.

_diffrn_ambient_pressure (numb, su)
The mean hydrostatic pressure in kilopascals at which the intensities were measured.

The permitted range is 0 → ∞.

_diffrn_ambient_pressure_gt _diffrn_ambient_pressure_lt
The mean hydrostatic pressure in kilopascals above which (*_gt) or below which (*_lt) the intensities were measured. These items allow for a pressure range to be given. _diffrn_ambient_pressure should always be used in preference to these items whenever possible.

The permitted range is 0 → ∞.

_diffrn_ambient_temperature (numb, su)
The mean temperature in kelvins at which the intensities were measured.

The permitted range is 0 → ∞.

_diffrn_ambient_temperature_gt _diffrn_ambient_temperature_lt
The mean temperature in kelvins above which (*_gt) or below which (*_lt) the intensities were measured. These items allow a range of temperatures to be given. _diffrn_ambient_temperature should always be used in preference to these items whenever possible.

The permitted range is 0 → ∞.

_diffrn_crystal_treatment (char)
Remarks about how the crystal was treated prior to the intensity measurements. Particularly relevant when intensities were measured at low temperature.

Examples: 'equilibrated in batch for 24 hours', 'flash frozen in liquid nitrogen', 'slow cooled with direct air stream'.

_diffrn_measured_fraction_theta_full (numb)
Fraction of unique (symmetry-independent) reflections measured out to _diffrn_reflns_theta_full.

The permitted range is 0 → 1.0.

_diffrn_measured_fraction_theta_max (numb)
Fraction of unique (symmetry-independent) reflections measured out to _diffrn_reflns_theta_max.

The permitted range is 0 → 1.0.

_diffrn_special_details (char)
Special details of the intensity-measurement process. Should include information about source instability, crystal motion, degradation and so on.

Example: "The results may not be entirely reliable as the measurement was made during a heat wave when the air-conditioning had failed."

_diffrn_symmetry_description (char)
Observed diffraction point symmetry, systematic absences and possible space group(s) or superspace group(s) compatible with these.

_diffrn_detector_type 'Siemens'
detector used to measure the scattered radiation, including any analyser and post-sample collimation.

_example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.

_diffrn_detector 'multiwire'
_data items in the DIFFRN category record details about the intensity measurements.

_data items in the DIFFRN_ATTENUATOR category record details about the diffraction attenuator scales employed.

_data items in the DIFFRN_DETECTOR category describe the detector used to measure the scattered radiation, including any analyser and post-sample collimation.
4. DATA DICTIONARIES

<table>
<thead>
<tr>
<th>DIFFRN.DETECTOR</th>
<th></th>
<th>DIFFRN.ORIENT_MATRIX</th>
</tr>
</thead>
<tbody>
<tr>
<td><em>diffrn_detector_area_resol_mean</em></td>
<td>(numb)</td>
<td>The resolution of an area detector, in pixels mm⁻¹. The permitted range is 0 → ∞.</td>
</tr>
<tr>
<td><em>diffrn_detector_details</em></td>
<td>(char)</td>
<td>A description of special aspects of the radiation detector.</td>
</tr>
<tr>
<td><em>diffrn_detector_dtime</em></td>
<td>(numb)</td>
<td>The deadtime in microseconds of the detector used to measure the diffraction intensities. The permitted range is 0 → ∞. Related item: <em>diffrn_radiation_detector_dtime</em>(alternate).</td>
</tr>
<tr>
<td><em>diffrn_detector_type</em></td>
<td>(char)</td>
<td>The make, model or name of the detector device used.</td>
</tr>
<tr>
<td><em>diffrn_radiation_detector</em></td>
<td>(char)</td>
<td>This definition has been superseded and is retained here only for archival purposes. Use instead <em>diffrn_detector</em>. The detector used to measure the diffraction intensities.</td>
</tr>
<tr>
<td><em>diffrn_radiation_detector_dtime</em></td>
<td>(numb)</td>
<td>This definition has been superseded and is retained here only for archival purposes. Use instead <em>diffrn_detector_dtime</em>. The deadtime in microseconds of the detector used to measure the diffraction intensities. The permitted range is 0 → ∞.</td>
</tr>
</tbody>
</table>

**DIFFRN.MEASUREMENT**

Data items in the DIFFRN.MEASUREMENT category refer to the mounting of the sample and to the goniometer on which it is mounted.


<table>
<thead>
<tr>
<th><em>diffrn_measurement_device_type</em></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>'Philips PW1100/20 diffractometer'</td>
<td></td>
<td></td>
</tr>
<tr>
<td><em>diffrn_measurement_method</em></td>
<td>(char)</td>
<td>Method used to measure the intensities. Example: 'profile data from $</td>
</tr>
<tr>
<td><em>diffrn_measurement_specimen_support</em></td>
<td>(char)</td>
<td>The physical device used to support the crystal during data collection. Examples: 'glass capillary', 'quartz capillary', 'fiber', 'metal loop'.</td>
</tr>
</tbody>
</table>

| _diffrn_measurement_details_ | (char) | A description of special aspects of the intensity measurement. Example: '440 frames of 0.25°'. |
| _diffrn_measurement_device_ | (char) | The general class of goniometer or device used to support and orient the specimen. Examples: 'three-circle diffractometer', 'four-circle diffractometer', '$\kappa$-geometry diffractometer', 'oscillation camera', 'precession camera'. |
| _diffrn_measurement_device_details_ | (char) | A description of special aspects of the device used to measure the diffraction intensities. Example: ', commercial goniometer modified locally to allow for 90° $\kappa \pm$ arc'. |

**DIFFRN.ORIENT_MATRIX**

Data items in the DIFFRN.ORIENT_MATRIX category record details about the orientation matrix used in the measurement of the diffraction intensities.


| _diffrn_orient_matrix_UB_11_ |  |  |
|_diffrn_orient_matrix_UB_12_ |  |  |
|_diffrn_orient_matrix_UB_13_ |  |  |
|_diffrn_orient_matrix_UB_21_ |  |  |
|_diffrn_orient_matrix_UB_22_ |  |  |
|_diffrn_orient_matrix_UB_23_ |  |  |
|_diffrn_orient_matrix_UB_31_ |  |  |
|_diffrn_orient_matrix_UB_32_ |  |  |
|_diffrn_orient_matrix_UB_33_ |  |  |

| _diffrn_orient_matrix_type_ | (char) | A description of the orientation matrix type and how it should be applied to define the orientation of the crystal precisely with respect to the diffractometer axes. |

| _diffrn_orient_matrix_type_ |  |  |
|_TEKSAN convention (MSC, 1989)_ |  |  |
**DIFFRN.ORIENT.REFLN**

Data items in the DIFFRN. ORIENT. REFLN category record details about the reflections that define the orientation matrix used in the measurement of the diffraction intensities.

Example 1 – typical output listing from an Enraf-Nonius CAD-4 diffractometer.

<table>
<thead>
<tr>
<th>loop</th>
</tr>
</thead>
<tbody>
<tr>
<td>_diffrn_orient_refln_index_h</td>
</tr>
<tr>
<td>_diffrn_orient_refln_angle_theta</td>
</tr>
<tr>
<td>_diffrn_orient_refln_angle_chi</td>
</tr>
<tr>
<td>_diffrn_orient_refln_angle_kappa</td>
</tr>
<tr>
<td>_diffrn_orient_refln_angle_omega</td>
</tr>
</tbody>
</table>

Appears in list containing _diffrn_orient_refln_index_.

**DIFFRN.RADIATION**

Data items in the DIFFRN. RADIATION category describe the radiation used in measuring the diffraction intensities, its collimation and monochromatization before the sample. Post-sample treatment of the beam is described by data items in the DIFFRN. DETECTOR category.


<table>
<thead>
<tr>
<th>_diffrn_radiation_type</th>
<th>_diffrn_radiation_monochromator</th>
</tr>
</thead>
</table>

**DIFFRN.RADIATION.WAVELENGTH**

Half-width in millimetres of the incident beam in the direction perpendicular to the diffraction plane.

The permitted range is $0 \rightarrow \infty$.

**diffrn_radiation_inhomogeneity** (numb)

**diffrn_radiation_monochromator** (char)

The method used to obtain monochromatic radiation. If a monochromator crystal is used, the material and the indices of the Bragg reflection are specified.

Examples: 'Zr filter', 'Ge 220', 'none', 'equatorial mounted graphite'.

**diffrn_radiation_polarisn_ratio** (numb)

The angle in degrees, as viewed from the specimen, between the perpendicular component of the polarization and the diffraction plane. See _diffrn_radiation_polarisn_norm_.

The permitted range is $-180.0 \rightarrow 180.0$.

**diffrn_radiation_polarisn_norm** (numb)

Polarization ratio of the diffraction beam incident on the crystal. It is the ratio of the perpendicularly polarized to the parallel polarized components of the radiation. The perpendicular component forms an angle of _diffrn_radiation_polarisn_ratio_ to the normal to the diffraction plane of the sample (i.e. the plane containing the incident and reflected beams).

The permitted range is $0.0 \rightarrow \infty$.

**diffrn_radiation_type** (char)

The type of the radiation. This is used to give a more detailed description than _diffrn_radiation_.


<table>
<thead>
<tr>
<th>_diffrn_radiation_xray_symbol</th>
<th>_diffrn_radiation_wavelength</th>
</tr>
</thead>
</table>

The IUPAC symbol for the X-ray wavelength for the probe radiation.

The data value must be one of the following:

- x-ray
- neutron
- electron
- gamma
- white-beam

**diffrn_radiation_collimation** (char)

The collimation or focusing applied to the radiation.

Examples: '0.3 mm double-pinhole', '0.5 mm', 'focusing mirrors'.

**diffrn_radiation_filter_edge** (numb)

Absorption edge in ångströms of the radiation filter used.

The permitted range is $0.0 \rightarrow \infty$.
DIFFRN.RADIATION.WAVELENGTH

The radiation wavelength in Ångströms.

**_diffrn_radiation_wavelength_**

The permitted range is 0 → ∞.

**_diffrn_radiation_wavelength_id_**

An arbitrary code identifying each value of *_diffrn_radiation_wavelength_.* Items in the **DIFFRN.RADIATION** category are looped when multiple wavelengths are used. This code is used to link with the **_diffrn_refln_** list. It must match with one of the **_diffrn_refln_wavelength_id_** codes.

The relative weight of a wavelength identified by the code

**_diffrn_radiation_wavelength_id_**

The permitted range is 0 → 1.0. Where no value is given, the assumed value is '1.0'.

**DIFFRN.REFLN**

Data items in the **DIFFRN.REFLN** category record details about the intensities measured in the diffraction experiment. The **DIFFRN.REFLN** data items refer to individual intensity measurements and must be included in looped lists.

(The **DIFFRN.REFLNS** data items specify the parameters that apply to all intensity measurements. The **DIFFRN.REFLNS** data items are not looped.)

**Example 1** – extracted from the CAD-4 listing for Tl₂Cd₂(SO₄)₄ at 85 K (unpublished).

```
loop_
  _diffrn_refln_index_h
  _diffrn_refln_index_k
  _diffrn_refln_index_l
  _diffrn_refln_angle_omega
  _diffrn_refln_angle_psi
  _diffrn_refln_angle_theta
  _diffrn_refln_angle_phi
  _diffrn_refln_counts_total
  _diffrn_refln_counts_peak
  _diffrn_refln_counts_net
  _diffrn_refln_counts_bg_1
  _diffrn_refln_counts_bg_2
  _diffrn_refln_scan_width
  _diffrn_refln_elapsed_time
```

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# - - - - data truncated for brevity - - - -
3 4 -4 0.1.03 69 459 73 30.726 -53.744 46.543 -47.552 1.516 2082.58
3 4 -5 0.1.03 91 465 75 31.407 -54.811 48.519 -42.705 1.516 2084.07
3 14 -6 0.1.03 84 560 79 32.228 -55.841 44.745 -38.092 1.516 2085.57
# - - - - data truncated for brevity - - - -
228
4.1. CORE DICTIONARY (coreCIF)

DIFFRN.REFLNS

_data items in the DIFFRN.REFLNS category record details about the set of intensities measured in the diffraction experiment.

The DIFFRN.REFLNS data items specify the parameters that apply to all intensity measurements. The DIFFRN.REFLNS data items are not looped. (The DIFFRN.REFLNS data items refer to individual intensity measurements and must be included in looped lists.)


<table>
<thead>
<tr>
<th>DIFFRN.REFLNS</th>
<th>Value</th>
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</thead>
<tbody>
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<td>.diffrn_refln_number</td>
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<tr>
<td>.diffrn_reflns_av_R_equivalents</td>
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<tr>
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</table>

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</tr>
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</tr>
</tbody>
</table>
DIFFRN_REFLNS

_\text{diff} \text{frn}\_\text{reflns} \_\text{av} \_\text{R} \_\text{equivalents} \quad \text{(numb)}

The residual \(\frac{\sum |\text{av}(I)|}{\sum |\text{av}(I)|}\) for symmetry-equivalent reflections used to calculate the average intensity \(\text{av}(I)\). The \(|\text{av}(I)|\) term is the average absolute difference between \(\text{av}(I)\) and the individual symmetry-equivalent intensities.

The permitted range is \(0 \rightarrow \infty\).

_\text{diff} \text{frn}\_\text{reflns} \_\text{av} \_\text{sigma}/\text{netI} \quad \text{(numb)}

This definition has been superseded and is retained here only for archival purposes. Use instead _\text{diff} \text{frn}\_\text{reflns} \_\text{av} \_\text{unetI}/\text{netI}.

Measure \(\frac{\sum |\text{std}(I)|}{\sum |\text{netI}|}\) for all measured reflections.

The permitted range is \(0 \rightarrow \infty\).

_\text{diff} \text{frn}\_\text{reflns} \_\text{av} \_\text{unetI}/\text{netI} \quad \text{(numb)}

Measure \(\frac{\sum |\text{unet}(I)|}{\sum |\text{netI}|}\) for all measured reflections.

The permitted range is \(0 \rightarrow \infty\).

Related item _\text{diff} \text{frn}\_\text{reflns} \_\text{av} \_\text{sigma}/\text{netI} (alternate).

_\text{diff} \text{frn}\_\text{reflns} \_\text{limit} \_\text{h} \_\text{max} \quad \text{(numb)}

_\text{diff} \text{frn}\_\text{reflns} \_\text{limit} \_\text{h} \_\text{min}

_\text{diff} \text{frn}\_\text{reflns} \_\text{limit} \_\text{k} \_\text{max}

_\text{diff} \text{frn}\_\text{reflns} \_\text{limit} \_\text{k} \_\text{min}

_\text{diff} \text{frn}\_\text{reflns} \_\text{limit} \_\text{l} \_\text{max}

_\text{diff} \text{frn}\_\text{reflns} \_\text{limit} \_\text{l} \_\text{min}

The limits on the Miller indices of the intensities specified by _\text{diff} \text{frn}\_\text{index} _\text{h}, _\text{k}, _\text{l}.

_\text{diff} \text{frn}\_\text{reflns} \_\text{number} \quad \text{(numb)}

The total number of measured intensities, excluding reflections that are classed as systematically absent arising from translational symmetry in the crystal unit cell.

The permitted range is \(0 \rightarrow \infty\).

_\text{diff} \text{frn}\_\text{reflns} \_\text{reduction} \_\text{process} \quad \text{(char)}

A description of the process used to reduce the intensities into structure-factor magnitudes.

Example: 'data averaged using Fisher test'.

_\text{diff} \text{frn}\_\text{reflns} \_\text{resolution} \_\text{full} \quad \text{(numb)}

The resolution in reciprocal ångströms at which the measured reflection count is close to complete.

The permitted range is \(0 \rightarrow \infty\).

Related item _\text{diff} \text{frn}\_\text{reflns} \_\text{theta} \_\text{full} (alternate).

_\text{diff} \text{frn}\_\text{reflns} \_\text{resolution} \_\text{max} \quad \text{(numb)}

Maximum resolution in reciprocal ångströms of the measured diffraction pattern.

The permitted range is \(0 \rightarrow \infty\).

Related item _\text{diff} \text{frn}\_\text{reflns} \_\text{theta} \_\text{max} (alternate).

_\text{diff} \text{frn}\_\text{reflns} \_\text{theta} \_\text{full} \quad \text{(numb)}

The \(\theta\) angle (in degrees) at which the measured reflection count is close to complete. The fraction of unique reflections measured out to this angle is given by _\text{diff} \text{frn}\_\text{reflns} \_\text{theta} \_\text{full}.

The permitted range is \(0 \rightarrow 90.0\).

DIFFRN_REFIN_CLASS

Data items in the DIFFRN_REFIN_CLASS category record details about the classes of reflections measured in the diffraction experiment.

Example 1 – example corresponding to the one-dimensional incommensurately modulated structure of \(K2SeO4\).

Each reflection class is defined by the number \(m = \sum |m_i|\), where the \(m_i\) are the integer coefficients that, in addition to \(h, k, l\), index the corresponding diffraction vector in the basis defined for the reciprocal lattice.

\[
(h \ k \ l)_{\text{diffraction}} = (11 \ 12 \ 13) = (h' \ k' \ l').
\]

_\text{diff} \text{frn}\_\text{reflns} \_\text{class} \_\text{av} \_\text{R} \_\text{eq} \quad \text{(numb)}

For each reflection class, the residual \(\frac{\sum |\text{av}(I)|}{\sum |\text{av}(I)|}\) for symmetry-equivalent reflections used to calculate the average intensity \(\text{av}(I)\). The \(|\text{av}(I)|\) term is the average absolute difference between \(\text{av}(I)\) and the individual symmetry-equivalent intensities.

Appears in list containing _\text{diff} \text{frn}\_\text{reflns} \_\text{class} \_\text{code}.

The permitted range is \(0 \rightarrow \infty\).

_\text{diff} \text{frn}\_\text{reflns} \_\text{class} \_\text{av} \_\text{sigma}/\text{I} \quad \text{(numb)}

This definition has been superseded and is retained here only for archival purposes. Use instead _\text{diff} \text{frn}\_\text{reflns} \_\text{class} \_\text{av} \_\text{unetI}/\text{I}.

Measure \(\frac{\sum |\text{std}(I)|}{\sum |\text{netI}|}\) for all measured intensities in a reflection class.

Appears in list containing _\text{diff} \text{frn}\_\text{reflns} \_\text{class} \_\text{code}.

The permitted range is \(0 \rightarrow \infty\).
4.1. CORE DICTIONARY (coreCIF)

DIFFRN_SOURCE

Data items in the DIFFRN_SOURCE category record details of the source of radiation used in the diffraction experiment.

Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.

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<tr>
<th>Data item</th>
<th>Value</th>
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<td>_diffrn_source_type</td>
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</tr>
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<td>'8 mm x 0.4 mm broad focus'</td>
</tr>
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</table>

This definition has been superseded and is retained here only for archival purposes. Use instead _diffrn_source.

The source of radiation.

The general class of the source of radiation.

Related item: _diffrn_radiation_source(alternate).

Examples: 'sealed X-ray tube', 'nuclear reactor', 'spallation source', 'electron microscope', 'rotating-anode X-ray tube', 'synchrotron'.

The current in milliamperes at which the radiation source was operated.

The permitted range is 0.0 → ∞.

A description of special aspects of the source.

The power in kilowatts at which the radiation source was operated.

The permitted range is 0.0 → ∞.

The dimensions of the source as viewed from the sample.

Examples: '8 mm x 0.4 mm fine-focus', 'broad focus'.

DIFFRN_SCALE_GROUP

A description of the scaling factors applied to place all intensities in the reflection lists on a common scale. Scaling groups might, for instance, correspond to each film in a multi-film data set or each crystal in a multi-crystal data set.

Example 1 – hypothetical example.

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_cif_core_dic

_diffrrn_reflns_class_av_u1/I

Measure \( \sum w(netI)/\sum \left| netI \right| \) for all measured intensities in a reflection class.

The permitted range is 0 \( \rightarrow \infty \).

Appears in list containing _diffrrn_reflns_class_code.

Related item: _diffrrn_reflns_class_av_sgI/I(alternate).

Diffrrn_reflns_class_code

The code identifying a certain reflection class.

Appears in list as essential element of loop structure. May match child data name(s):

Examples: '1', 'm1', 's1', 'A', 'B', 'c1', 'c2', 'c3'.

related item: _diffrrn_reflns_class_code

Diffrrn_reflns_class_d_res_high

The smallest value in ångströms of the interplanar spacings of the reflections in each reflection class. This is called the highest resolution for this reflection class.

Appears in list containing _diffrrn_reflns_class_code.

The permitted range is 0 \( \rightarrow \infty \).

Diffrrn_reflns_class_d_res_low

The highest value in ångströms of the interplanar spacings of the reflections in each reflection class. This is called the lowest resolution for this reflection class.

Appears in list containing _diffrrn_reflns_class_code.

The permitted range is 0 \( \rightarrow \infty \).

Diffrrn_reflns_class_description

Description of each reflection class.

Appears in list containing _diffrrn_reflns_class_code.

Examples: 'm=1 first order satellites', 'H0L0 common projection reflections'.

Diffrrn_reflns_class_number

The total number of measured intensities for each reflection class, excluding the systematic absences arising from centring translations.

Appears in list containing _diffrrn_reflns_class_code.

The permitted range is 0 \( \rightarrow \infty \).
DIFFRN_SOURCE

_diffrn_source_take-off_angle (numb)
The complement of the angle in degrees between the normal to the surface of the X-ray tube target and the primary X-ray beam for beams generated by traditional X-ray tubes. The permitted range is 0 → 90.
Example: ‘1.53’.

_diffrn_source_target (char)
The chemical element symbol for the X-ray target (usually the anode) used to generate X-rays. This can also be used for spallation sources. The value must be one of the following: H He Li Be B C N O F Ne Na Mg Al Si P S Cl Ar K Ca Sc Ti V Cr Mn Fe Co Ni Cu Zn Ga Ge As Se Br Kr Rb Sr Y Zr Nb Mo Tc Ru Rh Pd Ag Cd In Sn Sb Te I Xe Cs Ba La Ce Pr Nd Pm Sm Eu Gd Tb Dy Ho Er Tm Yb Lu Hf Ta W Re Os Ir Pt Au Hg Tl Pb Bi Po At Rn Fr Ra Ac Th Pa U Np Pu Am Cm Bk Cf Es Fm Md No Lr

_diffrn_source_type (char)
The make, model or name of the source of radiation. Examples: ‘NSLS beamline X8C’, ‘Rigaku RU200’.

_diffrn_source_voltage (numb)
The voltage in kilovolts at which the radiation source was operated. The permitted range is 0.0 → ∞.

DIFFRN_STANDARD_REFLN

_data items in the DIFFRN_STANDARD_REFLN category record details about the reflections treated as standards during the measurement of the diffraction intensities. Note that these are the individual standard reflections, not the standard reflections themselves. These records describe properties common to the set of standard reflections, not the standard reflections themselves.


loop
_diffrn_standard_refln_index_h
diffrn_standard_refln_index_k
diffrn_standard_refln_index_l
3 2 4 1 9 1 3 0 1 0

_diffrn_standard_refln_code (char)
The code identifying a reflection measured as a standard reflection with the indices _diffrn_standard_refln_index_. This is the same code as the _diffrn_refln_standard_code_. Appears in list containing _diffrn_refln_standard_code_. May match child data name(s) _diffrn_refln_standard_code_. Examples: ‘1’, ‘2’, ‘3’, ‘a1’, ‘A’, ‘B’.

DIFFRN_STANDARDS

Data items in the DIFFRN_STANDARDS category record details about the set of standard reflections used to monitor intensity stability during the measurement of diffraction intensities. Note that these records describe properties common to the set of standard reflections, not the standard reflections themselves.


_diffrn_standards_number 3
diffrn_standards_interval_count 120
diffrn_standards_interval_time 120

_diffrn_standards_decay_% (numb, su)
The percentage decrease in the mean of the intensities for the set of standard reflections from the start of the measurement process to the end. This value usually affords a measure of the overall decay in crystal quality during the diffraction measurement process. Negative values are used in exceptional instances where the final intensities are greater than the initial ones. The permitted range is −∞ → 100.

_diffrn_standards_interval_count (numb)
The number of reflection intensities, or the time in minutes, between the measurement of standard reflection intensities. The permitted range is 0 → ∞.

_diffrn_standards_interval_time (numb)
The number of unique standard reflections used during the measurement of the diffraction intensities. The permitted range is 0 → ∞.

_diffrn_standards_number (numb)
The number of unique standard reflections used during the measurement of the diffraction intensities. The permitted range is 0 → ∞.

_diffrn_standards_scale_sigma (numb)
The standard uncertainty (e.s.d.) of the individual mean standard scales applied to the intensity data. The permitted range is 0 → ∞.
EXPTL

Data items in the EXPTL category record details about the experimental work prior to the intensity measurements and details about the absorption-correction technique employed.


| _exptl_absorpt_coefficient_mu | 0.962 |
| _exptl_absorpt_correction_process_details | ‘North, Phillips & Mathews (1968)’ |
| _exptl_absorpt_correction_T_min | 0.929 |
| _exptl_absorpt_correction_T_max | 0.957 |

_**exptl_absorpt_coefficient_mu** (numb)

The absorption coefficient $\mu$ in reciprocal millimetres calculated from the atomic content of the cell, the density and the radiation wavelength.

The permitted range is $0 \rightarrow \infty$.

_**exptl_absorpt_correction_T_max** and _**exptl_absorpt_correction_T_min** (numb)

The maximum and minimum transmission factors for the crystal and radiation. These factors are also referred to as the absorption correction $A$ or $1/A$.

The permitted range is $0 \rightarrow 1.0$.

_**exptl_absorpt_correction_type** (char)

The absorption-correction type and method. The value ‘empirical’ should not be used unless more detailed information is not available.

The data value must be one of the following:

- analytical
- cylinder
- empirical
- gaussian
- integration
- multi-scan
- none
- numerical
- psi-scan
- refdelf
- sphere

_**exptl_absorpt_correction_process_details** (char)

Description of the absorption process applied to the intensities. A literature reference should be supplied for ψ-scan techniques.


_**exptl_crystals_number** (numb)

The total number of crystals used for the measurement of intensities.

The permitted range is $1 \rightarrow \infty$.

EXPTLCRYSTAL

Data items in the EXPTLCRYSTAL category record details about experimental measurements on the crystal or crystals used, such as shape, size or density.


| _exptl_crystal_description | prism |
| _exptl_crystal_colour | colourless |
| _exptl_crystal_size_max | 0.32 |
| _exptl_crystal_size_mid | 0.27 |
| _exptl_crystal_size_min | 0.10 |
| _exptl_crystal_density_diffrn | 1.146 |
| _exptl_crystal_density_meas | ? |
| _exptl_crystal_density_method | ‘not measured’ |
| _exptl_crystal_F_000 | 656 |

Example 2 – using separate items to define upper and lower limits for a value.

| _exptl_crystal_density_meas_gt | 2.5 |
| _exptl_crystal_density_meas_lt | 5.0 |

Example 3 – here the density was measured at some unspecified temperature below room temperature.

| _exptl_crystal_density_meas_temp_lt | 300 |

_**exptl_crystal_colour** (char)

The colour of the crystal.

May appear in list containing _exptl_crystal_id.

Related items: _exptl_crystal_colour_lustre(alternate), _exptl_crystal_colour_modifier(alternate), _exptl_crystal_colour_primary(alternate).

Example: ‘dark green’.

_**exptl_crystal_colour_lustre** (char)

The enumeration list of standardized names developed for the International Centre for Diffraction Data. The colour of a crystal is given by the combination of _exptl_crystal_colour_modifier with _exptl_crystal_colour_primary, as in ‘dark-green’ or ‘bluish-violet’, if necessary combined with _exptl_crystal_colour_lustre, as in ‘metallic-green’.

May appear in list containing _exptl_crystal_id.

Related item: _exptl_crystal_colour(alternate).

The data value must be one of the following:

- metallic
- dull
- clear

_**exptl_crystal_colour_modifier** (char)

The enumeration list of standardized names developed for the International Centre for Diffraction Data. The colour of a crystal is given by the combination of _exptl_crystal_colour_modifier with _exptl_crystal_colour_primary, as in ‘dark-green’.
or ‘bluish-violet’, if necessary combined with _exptl_crystal_colour_lustre, as in ‘metallic-green’.

May appear in list containing _exptl_crystal_id.

The data value must be one of the following:

- light
- dark
- whitish
- blackish
- grayish
- brownish
- reddish
- pinkish
- orangish
- yellowish
- greenish
- bluish

May appear in list containing _exptl_crystal_id.

The data value must be one of the following:

- colourless
- white
- black
- gray
- brown
- red
- pink
- orange
- yellow
- green
- blue
- violet

May appear in list containing _exptl_crystal_id.

The data value must be one of the following:

- 0
- 1.0
- 2.0
- 3.0
- 4.0
- 5.0
- 234

May appear in list containing _exptl_crystal_id.

The data value must be one of the following:

- Temperature in kelvins at which _exptl_crystal_density_meas was determined.

May appear in list containing _exptl_crystal_id.

The permitted range is 0.0 → ∞.

_\text{\texttt{exptl\_crystal\_colour\_primary}}\ (\text{char})_

The enumeration list of standardized names developed for the International Centre for Diffraction Data. The colour of a crystal is given by the combination of _exptl\_crystal\_colour\_modifier_, with _exptl\_crystal\_colour\_primary_, as in ‘dark-green’ or ‘bluish-violet’, if necessary combined with _exptl\_crystal\_colour\_lustre_, as in ‘metallic-green’.

May appear in list containing _exptl\_crystal_id.

The data value must be one of the following:

- colourless
- white
- black
- gray
- brown
- red
- pink
- orange
- yellow
- green
- blue
- violet

May appear in list containing _exptl\_crystal_id.

The data value must be one of the following:

- Density values calculated from the crystal cell and contents. The units are megagrams per cubic metre (grams per cubic centimetre).

May appear in list containing _exptl\_crystal_id.

The permitted range is 0.0 → ∞.

_\text{\texttt{exptl\_crystal\_density\_diffrn}}\ (\text{numb})_

Density values calculated from the crystal cell and contents. The units are megagrams per cubic metre (grams per cubic centimetre).

May appear in list containing _exptl\_crystal_id.

The permitted range is 0.0 → ∞.

_\text{\texttt{exptl\_crystal\_density\_meas}}\ (\text{numb, su})_

Density values measured using standard chemical and physical methods. The units are megagrams per cubic metre (grams per cubic centimetre).

May appear in list containing _exptl\_crystal_id.

The permitted range is 0.0 → ∞.

_\text{\texttt{exptl\_crystal\_density\_meas\_lt}}\ (\text{numb})_

The value below which the density measured using standard chemical and physical methods lies. The units are megagrams per cubic metre (grams per cubic centimetre). _exptl\_crystal\_density\_meas\_gt_ and _exptl\_crystal\_density\_meas\_lt_ should not be used to report new experimental work, for which _exptl\_crystal\_density\_meas_ should be used. These items are intended for use in reporting information in existing databases and archives which would be misleading if reported under _exptl\_crystal\_density\_meas_.

May appear in list containing _exptl\_crystal_id.

The permitted range is 0.0 → ∞.

_\text{\texttt{exptl\_crystal\_density\_meas\_temp}}\ (\text{numb, su})_

Temperature in kelvins at which _exptl\_crystal\_density\_meas_ was determined.

May appear in list containing _exptl\_crystal_id.

The permitted range is 0.0 → ∞.

_\text{\texttt{exptl\_crystal\_density\_meas\_temp\_gt}}\ (\text{numb})_

Temperature in kelvins above which _exptl\_crystal\_density\_meas_ was determined. _exptl\_crystal\_density\_meas\_temp\_gt_ and _exptl\_crystal\_density\_meas\_temp\_lt_ should not be used for reporting new work, for which _exptl\_crystal\_density\_meas_ should be used. These items are intended for use in reporting information in existing databases and archives which would be misleading if reported under _exptl\_crystal\_density\_meas_.

May appear in list containing _exptl\_crystal_id.

The permitted range is 0.0 → ∞.

_\text{\texttt{exptl\_crystal\_density\_meas\_temp\_lt}}\ (\text{numb})_

Temperature in kelvins below which _exptl\_crystal\_density\_meas_ was determined. _exptl\_crystal\_density\_meas\_temp\_gt_ and _exptl\_crystal\_density\_meas\_temp\_lt_ should not be used for reporting new work, for which _exptl\_crystal\_density\_meas_ should be used. These items are intended for use in reporting information in existing databases and archives which would be misleading if reported under _exptl\_crystal\_density\_meas_.

May appear in list containing _exptl\_crystal_id.

The permitted range is 0.0 → ∞.

_\text{\texttt{exptl\_crystal\_density\_meas\_temp\_gt}}\ (\text{numb})_

Temperature in kelvins above which _exptl\_crystal\_density\_meas_ was determined. _exptl\_crystal\_density\_meas\_temp\_gt_ and _exptl\_crystal\_density\_meas\_temp\_lt_ should not be used for reporting new work, for which the correct temperature of measurement should be given. These items are intended for use in reporting information in existing databases and archives which would be misleading if reported under _exptl\_crystal\_density\_meas_.

May appear in list containing _exptl\_crystal_id.

The permitted range is 0.0 → ∞.

_\text{\texttt{exptl\_crystal\_density\_meas\_temp\_lt}}\ (\text{numb})_

Temperature in kelvins below which _exptl\_crystal\_density\_meas_ was determined. _exptl\_crystal\_density\_meas\_temp\_gt_ and _exptl\_crystal\_density\_meas\_temp\_lt_ should not be used for reporting new work, for which the correct temperature of measurement should be given. These items are intended for use in reporting information in existing databases and archives which would be misleading if reported under _exptl\_crystal\_density\_meas_.

May appear in list containing _exptl\_crystal_id.

The permitted range is 0.0 → ∞.

_\text{\texttt{exptl\_crystal\_density\_meas\_temp\_lt}}\ (\text{numb})_

Temperature in kelvins below which _exptl\_crystal\_density\_meas_ was determined. _exptl\_crystal\_density\_meas\_temp\_gt_ and _exptl\_crystal\_density\_meas\_temp\_lt_ should not be used for reporting new work, for which the correct temperature of measurement should be given. These items are intended for use in reporting information in existing databases and archives which would be misleading if reported under _exptl\_crystal\_density\_meas_.

May appear in list containing _exptl\_crystal_id.

The permitted range is 0.0 → ∞.
4.1. CORE DICTIONARY (coreCIF)

**_exptl_crystal_density_method_**

The method used to measure _exptl_crystal_density_meas_.
May appear in list containing _exptl_crystal_id_.

**_exptl_crystal_description_**

A description of the quality and habit of the crystal. The crystal dimensions should not normally be reported here; use instead _exptl_crystal_size_ for the gross dimensions of the crystal and _exptl_crystal_face_ to describe the relationship between individual faces.
May appear in list containing _exptl_crystal_id_.

**_exptl_crystal_F_000_**

The effective number of electrons in the crystal unit cell contributing to \( F(000) \). This may contain dispersion contributions and is calculated as

\[
F(000) = \left[ \left( \sum f_i \right)^2 + \left( \sum f_i \right)^2 \right]^{1/2},
\]

where \( f_i \) = real part of the scattering factors at \( \theta = 0^\circ \), \( f_i \) = imaginary part of the scattering factors at \( \theta = 0^\circ \) and the sum is taken over each atom in the unit cell.
May appear in list containing _exptl_crystal_id_.
The permitted range is 0 → ∞.

**_exptl_crystal_id_**

Code identifying each crystal if multiple crystals are used. It is used to link with _diffn_refln_crystal_id_ in the intensity measurements and with _refln_crystal_id_ in the _refln_list_.
Appears in list as essential element of loop structure. May match child data name(s): _diffn_refln_crystal_id_ _refln_crystal_id_.

**_exptl_crystal_preparation_**

Details of crystal growth and preparation of the crystal (e.g. mounting) prior to the intensity measurements.
May appear in list containing _exptl_crystal_id_.
Example: ‘mounted in an argon-filled quartz capillary’.

**_exptl_crystal_pressure_history_**

Relevant details concerning the pressure history of the sample.
May appear in list containing _exptl_crystal_id_.

**_exptl_crystal_recrysallization_method_**

Describes the method used to recrystallize the sample. Sufficient details should be given for the procedure to be repeated. The temperature or temperatures should be given as well as details of the solvent, flux or carrier gas with concentrations or pressures and ambient atmosphere.

---

**EXPTL.CRYSTAL_FACE**

Data items in the EXPTL.CRYSTAL_FACE category record details of the crystal faces.


```
loop_
  _exptl_crystal_face_index_h
  _exptl_crystal_face_index_k
  _exptl_crystal_face_index_l
  _exptl_crystal_face_perp_dist
  0  -1  -2  0.19688
  1   0  -2  0.23571
 -1   1  -2  0.18849
 -2   1   0  0.21010
-1   0   2  0.20450
 1  -1   2  0.26860
-1  -2   0  0.21988
 0  -1   2  0.15206
```

---

**_exptl_crystal_face_diffr_chi_**

**_exptl_crystal_face_diffr_kappa_**

**_exptl_crystal_face_diffr_phi_**

**_exptl_crystal_face_diffr_psi_**

The goniometer angle settings in degrees when the perpendicular to the specified crystal face is aligned along a specified direction (e.g. the bisector of the incident and reflected beams in an optical goniometer).
Appears in list containing _exptl_crystal_face_index_.

**_exptl_crystal_face_index_h_**

**_exptl_crystal_face_index_k_**

**_exptl_crystal_face_index_l_**

Miller indices of the crystal face associated with the value _exptl_crystal_face_perp_dist_.
Appears in list as essential element of loop structure.

**_exptl_crystal_face_perp_dist_**

The perpendicular distance in millimetres from the face to the centre of rotation of the crystal.
Appears in list containing _exptl_crystal_face_index_.
The permitted range is 0 → ∞.
**GEOM**

Data items in the GEOM and related (GEOM_ANGLE, GEOM_BOND, GEOM_CONTACT, GEOM_HBOND and GEOM_TORSION) categories record details about the molecular and crystal geometry as calculated from the ATOM, CELL and SYMMETRY data.

Geometry data are usually redundant, in that they can be calculated from other more fundamental quantities in the data block. However, they serve the dual purposes of providing a check on the correctness of both sets of data and of enabling the most important geometric data to be identified for publication by setting the appropriate publication flag.


<table>
<thead>
<tr>
<th>_geom_angle_atom_site_label_1</th>
<th>_geom_angle_atom_site_label_2</th>
<th>_geom_angle_atom_site_label_3</th>
</tr>
</thead>
<tbody>
<tr>
<td>C2 O1 C3 111.6(2) 1 555 1 555 1 555 yes</td>
<td>C1 O2 110.9(2) 1 555 1 555 1 555 yes</td>
<td>C2 O1 C2 122.2(3) 1 555 1 555 1 555 yes</td>
</tr>
<tr>
<td>C2 C1 O2 122.2(3) 1 555 1 555 1 555 yes</td>
<td>C3 C2 O1 127.0(3) 1 555 1 555 1 555 yes</td>
<td>C2 C3 H3 107.1(2) 1 555 1 555 1 555 no</td>
</tr>
<tr>
<td>C2 C3 N4 103.2(3) 1 555 1 555 1 555 yes</td>
<td>C2 C3 C1 111.3(2) 1 555 1 555 1 555 yes</td>
<td>N4 C3 C1 116.7(2) 1 555 1 555 1 555 yes</td>
</tr>
</tbody>
</table>

# - - - - data truncated for brevity - - - -

**GEOM_ANGLE**

Data items in the GEOM_ANGLE category record details about the bond angles as calculated from the ATOM, CELL and SYMMETRY data.


<table>
<thead>
<tr>
<th>_geom_angle_atom_site_label_1</th>
<th>_geom_angle_atom_site_label_2</th>
<th>_geom_angle_atom_site_label_3</th>
</tr>
</thead>
<tbody>
<tr>
<td>C2 O1 C3 111.6(2) 1 555 1 555 1 555 yes</td>
<td>C1 O2 110.9(2) 1 555 1 555 1 555 yes</td>
<td>C2 O1 C2 122.2(3) 1 555 1 555 1 555 yes</td>
</tr>
<tr>
<td>C2 C1 O2 122.2(3) 1 555 1 555 1 555 yes</td>
<td>C3 C2 O1 127.0(3) 1 555 1 555 1 555 yes</td>
<td>C2 C3 H3 107.1(2) 1 555 1 555 1 555 no</td>
</tr>
<tr>
<td>C2 C3 N4 103.2(3) 1 555 1 555 1 555 yes</td>
<td>C2 C3 C1 111.3(2) 1 555 1 555 1 555 yes</td>
<td>N4 C3 C1 116.7(2) 1 555 1 555 1 555 yes</td>
</tr>
</tbody>
</table>

_geom_angle

Angle in degrees defined by the three sites _geom_angle_atom_site_label_1, _geom_angle_atom_site_label_2 and _geom_angle_atom_site_label_3. The site at _geom_angle_atom_site_label_2 is at the apex of the angle.

Appears in list containing _geom_angle_atom_site_label_. [geom_angle]

_geom_angle_atom_site_label_1

_geom_angle_atom_site_label_2

_geom_angle_atom_site_label_3

The labels of the three atom sites which define the angle given by _geom_angle. These must match labels specified as

**GEOM_BOND**

Data items in the GEOM_BOND category record details about bonds as calculated from the ATOM, CELL and SYMMETRY data.


<table>
<thead>
<tr>
<th>_geom_bond_atom_site_label_1</th>
<th>_geom_bond_atom_site_label_2</th>
<th>_geom_bond_distance</th>
</tr>
</thead>
<tbody>
<tr>
<td>C2 C1 1.342(4) 1 555 1 555 1 555 yes</td>
<td>C5 C1 1.439(3) 1 555 1 555 1 555 yes</td>
<td>C2 C3 1.512(4) 1 555 1 555 1 555 yes</td>
</tr>
<tr>
<td>C2 C3 1.465(3) 1 555 1 555 1 555 yes</td>
<td>C3 C1 1.472(3) 1 555 1 555 1 555 yes</td>
<td>C3 C1 1.537(4) 1 555 1 555 1 555 yes</td>
</tr>
<tr>
<td>C3 C1 1.00(3) 1 555 1 555 1 555 no</td>
<td>C3 C1 1.00(3) 1 555 1 555 1 555 no</td>
<td>N4 C5 1.472(3) 1 555 1 555 1 555 yes</td>
</tr>
</tbody>
</table>

# - - - - data truncated for brevity - - - -

_geom_bond_atom_site_label_1

_geom_bond_atom_site_label_2

_geom_bond_distance

The labels of two atom sites that form a bond. These must match labels specified as _atom_site_label_ in the atom list.

Appears in list as essential element of loop structure. Must match parent data name _atom_site_label_. [geom_bond]

_geom_bond_publ_flag

The intramolecular bond distance in angstroms.

The permitted range is 0.0 → ∞.

Appears in list containing _geom_bond_atom_site_label_. [geom_bond]
4.1. CORE DICTIONARY (coreCIF)

**GEOM.HBOND**

Data items in the GEOM.HBOND category record details about hydrogen bonds as calculated from the ATOM, CELL and SYM-
MERTY data.

Example 1 – based on C14H13ClN2O.H2O, reported by Palmer, Puddle & Lisle-

```
loop
  _geom hbond_atom site label D
  _geom hbond_atom site label H
  _geom hbond_atom site label A
  _geom hbond_distance DH
  _geom hbond_distance HA
  _geom hbond_distance DA
  _geom hbond_angle DHA
  _geom hbond_publ flag
H6  HN6  OW  0.888(8)  1.921(12)  2.801(8)  169.6(8) yes
OW  HO2  O7  0.917(6)  1.923(12)  2.793(8)  153.5(8) yes
OW  HO1  N10  0.894(8)  1.866(12)  2.642(8)  179.7(5) yes
```

```
_geom hbond_angle DHA  (numb, su)
Angle in degrees defined by the three sites _geom hbond_atom
site label D, * H and * A. The site at * H (the hydrogen atom
participating in the interaction) is at the apex of the angle.
Appears in list containing _geom hbond_atom site label_.
```

```
_geom hbond_atom site label D
_geom hbond_atom site label H
_geom hbond_atom site label A  (char)
The labels of three atom sites (respectively, the donor atom, hydro-
gen atom and acceptor atom) participating in a hydrogen bond. These
must match labels specified as _atom site label_ in the atom list.
Appears in list as essential element of loop structure. Must match parent
data name
_atom site label_. [geom hbond]
```

```
_geom hbond_distance DH
_geom hbond_distance HA
_geom hbond_distance DA
```

}``
**GEOM_HBOND**

<table>
<thead>
<tr>
<th>Field</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>_geom_hbond_distance_DH</td>
<td>Distances in ångströms between the donor and hydrogen (* DH)</td>
</tr>
<tr>
<td>_geom_hbond_distance_HA</td>
<td>Hydrogen and acceptor (* HA)</td>
</tr>
<tr>
<td>_geom_hbond_distance_DA</td>
<td>Donor and acceptor (* DA) sites in a hydrogen bond.</td>
</tr>
</tbody>
</table>

These numbers are combined to form the code 'klm'. These must match codes specified in the atom list. The torsion-angle definition should be that of Klyne and Prelog. Reference: Klyne, W. & Prelog, V. (1960). Experientia, 16, 521–523.

**_geom_hbond_publ_flag**

This code signals whether the hydrogen-bond information is referred to in a publication or should be placed in a table of significant hydrogen-bond geometry.

**_geom_hbond_site_symmetry_D**

The symmetry code of each atom site as the symmetry-equivalent position number 'n' and the cell translation number 'klm'. These numbers are combined to form the code 'n klm' or n klm. The character string n klm is composed as follows:

- n refers to the symmetry operation that is applied to the coordinates stored in _atom_site_x, _atom_site_y, and _atom_site_z. It must match a number given in _space_group_symop_id. k, l and m refer to the translations that are subsequently applied to the symmetry-transformed coordinates to generate the atom used in calculating the hydrogen bond. These translations (x, y, z) are related to (k, l, m) by the relations k = 5 + x, l = 5 + y, m = 5 + z. By adding 5 to the translations, the use of negative numbers is avoided.

**_geom_torsion**

The torsion angle in degrees bounded by the four atom sites identified by the _geom_torsion_atom_site_label_ codes. These must match labels specified as _atom_site_label_ in the atom list. The torsion-angle definition should be that of Klyne and Prelog.


**_geom_torsion_publ_flag**

This code signals whether the torsion angle is referred to in a publication or should be placed in a table of significant torsion angles.

**_geom_torsion_site_symmetry_1**

The symmetry code of each atom site as the symmetry-equivalent position number 'n' and the cell translation number 'klm'. These numbers are combined to form the code 'n klm' or n klm. The character string n klm is composed as follows:

- n refers to the symmetry operation that is applied to the coordinates stored in _atom_site_x, _atom_site_y, and _atom_site_z. It must match a number given in _space_group_symop_id. k, l and m refer to the translations that are subsequently applied to the symmetry-transformed coordinates to generate the atom used in calculating the angle. These translations (x, y, z) are related to (k, l, m) by the relations k = 5 + x, l = 5 + y, m = 5 + z. By adding 5 to the translations, the use of negative numbers is avoided.
4.1. CORE DICTIONARY (coreCIF)

JOURNAL

Data items in the JOURNAL category record details about the book-keeping by the journal staff when processing a CIF submitted for publication. The creator of a CIF will not normally specify these data items. The data names are not defined in the dictionary because they are for journal use only.


<table>
<thead>
<tr>
<th>Data Item</th>
<th>Value</th>
</tr>
</thead>
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<td>journal_page_last</td>
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</table>

JOURNAL_INDEX

Data items in the JOURNAL_INDEX category are used to list terms used to generate the journal indexes. The creator of a CIF will not normally specify these data items.


<table>
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<tr>
<th>Data Item</th>
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<td>journal_index_subterm</td>
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<td></td>
</tr>
</tbody>
</table>

PUBL

Data items in the PUBL category are used when submitting a manuscript for publication. They refer either to the paper as a whole, or to specific named elements within a paper (such as the title and abstract, or the Comment and Experimental sections of Acta Crystallographica Section C). The data items in the PUBL_BODY category should be used for the text of other submissions. Typically, each journal will supply a list of the specific items it requires in its Notes for Authors.


<table>
<thead>
<tr>
<th>Data Item</th>
<th>Value</th>
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<tbody>
<tr>
<td>publ_section_title</td>
<td>trans-3-Benzoyl-2-(tert-butyl)-4- (iso-butyl)-1,3-oxazolidin-5-one</td>
</tr>
<tr>
<td>publ_section_abstract</td>
<td>The oxazolidone ring is a shallow envelope conformation with the tert-butyl and iso-butyl groups occupying trans-positions with respect to the ring. The angles at the N atom sum to 356.2°, indicating a very small degree of pyramidalization at this atom. This is consistent with electron delocalization between the N atom and the carbonyl centre [N-C=O = 1.374(3) Å].</td>
</tr>
</tbody>
</table>


<table>
<thead>
<tr>
<th>Data Item</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>publ_section_title</td>
<td>Hemiasterlin methyl ester</td>
</tr>
<tr>
<td>publ_section_title_footnote</td>
<td>IUPAC name: methyl 2,5-dimethyl-4-2-[3-methyl-2-methylamino-3-(N-methylbenzo[b]pyrrol-3-yl)butanamido]-3,3-dimethyl-N-methyl-butananmido-2-hexenoate.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Data Item</th>
<th>Value</th>
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<tr>
<td>publ_contact_author</td>
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</tr>
<tr>
<td>[publ]</td>
<td></td>
</tr>
</tbody>
</table>
4. DATA DICTIONARIES

_publ_contact_author_address (char)
The address of the author submitting the manuscript and data block. This is the person contacted by the journal editorial staff.

Example:
; Department of Chemistry and Biochemistry
University of Guelph
Ontario
Canada
N1G 2W1
;

_publ_contact_author_email (char)
E-mail address in a form recognizable to international networks. The format of e-mail addresses is given in Section 3.4, Address Specification, of Internet Message Format, RFC 2822, P. Resnick (Editor), Network Standards Group, April 2001.

Example: 'name@host.domain.country'.'bm@iucr.org'.

_publ_contact_author_fax (char)
Facsimile telephone number of the author submitting the manuscript and data block. The recommended style is the international dialing prefix, followed by the area code in parentheses, followed by the local number with no spaces. The earlier convention of including the international dialing prefix in parentheses is no longer recommended.

Examples: '12()349477334', '12(34)9477334'.

_publ_contact_author_id_iucr (char)
Identifier in the IUCr contact database of the author submitting the manuscript and data block. This identifier may be available from the World Directory of Crystallographers (http://wdc.iucr.org).

Example: '2985'.

_publ_contact_author_name (char)
The name of the author submitting the manuscript and data block. This is the person contacted by the journal editorial staff.

Example: 'Professor George Ferguson'.

_publ_contact_phone (char)
Telephone number of the author submitting the manuscript and data block. The recommended style is the international dialing prefix, followed by the area code in parentheses, followed by the local number and any extension number prefixed by 'x', with no spaces. The earlier convention of including the international dialing prefix in parentheses is no longer recommended.

Examples: '12(34)9477330', '12()349477330', '12(34)9477330x5543'.

_publ_contact_letter (char)
A letter submitted to the journal editor by the contact author.

_publ_manuscript_creation (char)
A description of the word-processor package and computer used to create the word-processed manuscript stored as _publ_manuscript_processed.

Example: 'Tex file created by FrameMaker on a Sun 3/280'.

_publ_manuscript_processed (char)
The full manuscript of a paper (excluding possibly the figures and the tables) output in ASCII characters from a word processor. Information about the generation of this data item must be specified in the data item _publ_manuscript_creation.

_publ_manuscript_text (char)
The full manuscript of a paper (excluding figures and possibly the tables) output as standard ASCII text.

_publ_requested_category (char)
The category of paper submitted. For submission to Acta Crystallographica Section C or Acta Crystallographica Section E, only the codes indicated for use with these journals should be used. The data value must be one of the following:

FA  Full article
FI  Full submission – inorganic (Acta C)
FO  Full submission – organic (Acta C)
FM  Full submission – metal-organic (Acta C)
CI  CIF-access paper – inorganic (Acta C) (no longer in use)
CO  CIF-access paper – organic (Acta C) (no longer in use)
CM  CIF-access paper – metal-organic (Acta C) (no longer in use)
EI  Electronic submission – inorganic (Acta E)
EO  Electronic submission – organic (Acta E)
EM  Electronic submission – metal-organic (Acta E)
AD  Addenda and Errata (Acta C, Acta E)
SC  Short communication

Where no value is given, the assumed value is 'FA'.

_publ_requested_coeditor_name (char)
The name of the co-editor whom the authors would like to handle the submitted manuscript.

_publ_requested_journal (char)
The name of the journal to which the manuscript is being submitted.

_publ_section_title (char)
_publ_section_title_footnote (char)
_publ_section Synopsis (char)
_publ_section Abstract (char)
_publ_section_comment (char)
_publ_section_introduction (char)
_publ_section experimental (char)
_publ_section_exptl_prep (char)
_publ_section_exptl_refinement (char)
_publ_section_exptl_solution (char)
_publ_section_discussion (char)
_publ_section_acknowledgements (char)
_publ_section References (char)
_publ_section_figure captions (char)
_publ_section_table_legends (char)

The sections of a manuscript if submitted in parts. As an alternative, see _publ_manuscript_text and _publ_manuscript_processed. The _publ_section_exptl_prep, _publ_section_exptl_refinement and _publ_section_exptl_solution items are preferred for separating the chemical preparation, refinement and structure solution aspects of the experimental description.
The data items in the PUBL_AUTHOR category record details of the authors of a manuscript submitted for publication. Example 1 – based on Willis, Beckwith & Tezer [Acta Cryst. (1991), C47, 2276-2277].

<table>
<thead>
<tr>
<th>Loop</th>
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<th>publ_auth_address</th>
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</thead>
<tbody>
<tr>
<td>'Willis, Anthony C.'</td>
<td>Research School of Chemistry</td>
<td>Australian National University</td>
</tr>
<tr>
<td></td>
<td>GPO Box 4</td>
<td>Canberra, ACT</td>
</tr>
<tr>
<td></td>
<td>Australia 2601</td>
<td></td>
</tr>
</tbody>
</table>

The address of a publication author. If there is more than one author, this will be looped with _publ_author_name_. May appear in list containing _publ_author_name_. Example:

```
; Department
; Institute
; Street
; City and postcode
; COUNTRY

[publ_author]
```

The e-mail address of a publication author. If there is more than one author, this will be looped with _publ_author_name_. The format of e-mail addresses is given in Section 3.4, Address Specification, of Internet Message Format, RFC 2822, P. Resnick (Editor), Network Standards Group, April 2001. May appear in list containing _publ_author_name_. Examples: 'name@host.domain.country', 'dm@iucr.org'.

```
[publ_author]
```

A footnote accompanying an author’s name in the list of authors of a paper. Typically indicates sabbatical address, additional affiliations or date of decease. May appear in list containing _publ_author_name_. Examples: 'On leave from U. Western Australia', 'Also at Department of Biophysics'.

```
[publ_author]
```

Identifier in the IUCr contact database of a publication author. This identifier may be available from the World Directory of Crystallographers (http://wdc.iucr.org). May appear in list. Example: '2985'.

```
[publ_author]
```

The name of a publication author. If there are multiple authors, this will be looped with _publ_author_name_. The family name(s), followed by a comma and including any dynastic components, precedes the first names or initials. May appear in list as essential element of loop structure. Examples: 'Bleary, Percival R.', 'O’Neil, P.K.', 'Van den Bossche, G.', 'Yang, D.-L.', 'Simonov, Yu.A.', 'Muller, H.A.', 'Ross II, C.R.'

```
[publ_author]
```

The data items in the PUBL_BODY category permit the labelling of different text sections within the body of a paper. Note that these should not be used in a paper which has a standard format with sections tagged by specific data names (such as in Acta Crystallographica Section C). Typically, each journal will supply a list of the specific items it requires in its Notes for Authors.


```
loop
_publ_body_element
_publ_body_label
_publ_body_title
_publ_body_format
_publ_body_contents

; section 1
;
; Introduction
cif
;
; X-ray diffraction from a crystalline material provides
;
; information on the thermally and spatially averaged
electron density in the crystal...

; section 2
tex
;
; In the rigid-atom approximation, the dynamic electron
density of an atom is described by the convolution
product of the static atomic density and a probability density function,
$\rho_{\text{dyn}}(\mathbf{r}) = \rho_{\text{stat}}(\mathbf{r}) \ast P(\mathbf{r})$.

; section 3
tex
;
; The two-channel method for retrieval of the deformation
electron density...

; subsection 3.1
;
; 'The two-channel entropy $S[D(\sigma)]$'
;
; As the wide dynamic range involved in the total electron
density...

; subsection 3.2
;
; 'Uniform vs informative prior model densities'
;
; subsection 3.2.1
;
; 'Use of uniform models'
;
; Straightforward algebra leads to expressions analogous to...

[publ_body]
```

The data value must be one of the following:

- section
- subsection
- appendix
- footnote

[publ_body]
4. DATA DICTIONARIES

PUBL_BODY

_publ_body_format (char)
Code indicating the appropriate typesetting conventions for accented characters and special symbols in the text section.
Appears in list containing _publ_body_label.
The data value must be one of the following:
ascii no coding for special symbols
cif CIF convention
latex \LaTeX
rtf Rich Text Format
gsml SGML (ISO 8879)
tex \TeX
troff troff or nroff
Where no value is given, the assumed value is ‘cif’.

_publ_body_label (char)
Code identifying the section of text. The combination of this with _publ_body_element must be unique.
Appears in list as essential element of loop structure.
Examples: ‘1’, ‘1.1’, ‘2.1.3’.

_publ_body_title (char)
Title of the associated section of text.
Appears in list containing _publ_body_label.

PUBL_MANUSCRIPT_INCL

Data items in the PUBL_MANUSCRIPT_INCL category allow the authors of a manuscript submitted for publication to list data names that should be added to the standard request list used by the journal printing software. Although these fields are primarily intended to identify CIF data items that the author wishes to include in a published paper, they can also be used to identify data names created so that non-CIF items can be included in the publication. Note that *_item names must be enclosed in single quotes.

Example 1 – directive to include a hydrogen-bonding table, including cosmetic headings in comments.

_\_publ_manuscript_incl_extra_defn
\_publ_manuscript_incl_extra_info
\_publ_manuscript_incl_extra_item
# Include Hydrogen Bonding Geometry Description
# _________________________________
# Name explanation standard?
# _________________________________
‘_geom_hbond_atom_site_label_D’ ‘H-bond donor’ yes
‘_geom_hbond_atom_site_label_H’ ‘H-bond hydrogen’ yes
‘_geom_hbond_atom_site_label_A’ ‘H-bond acceptor’ yes
‘_geom_hbond_distance_DH’ ‘H-bond D-H’ yes
‘_geom_hbond_distance_HA’ ‘H-bond H...A’ yes
‘_geom_hbond_distance_DA’ ‘H-bond D...A’ yes
‘_geom_hbond_angle_DHA’ ‘H-bond D-H...A’ yes

Example 2 – hypothetical example including both standard CIF data items and a non-CIF quantity which the author wishes to list.

_\_refine_special_details
\_refine_is_structure_factor_coef F
\_refine_is_matrix_type full
\_refine_is_weighting_scheme calc
\_refine_is_weighting_details ‘w=1/(uˆ2ˆ(F)+0.0004Fˆ2ˆ)’
\_refine_is_hydrogen_treatment refxyz
\_refine_is_extinction_method Zachariasen
\_refine_is_extinction_coef 3514(42)
\_refine_is_extinction_expression
\_refine_is_abs_structure_details
\_refine_is_abs_structure_details
\_refine_is_abs_structure_details

REFINE

Data items in the REFINE category record details about the structure-refinement parameters.


\_refine_is_number_reflns 1408
\_refine_is_number_parameters 272
\_refine_is_number_restraints 0
\_refine_is_number_constraints 0
\_refine_is_W_factor_all .038
\_refine_is_R_factor_all .034
\_refine_is_W_factor_gt .042
\_refine_is_goodness_of_fit_all 1.462
\_refine_is_goodness_of_fit_gt 1.515
The largest and smallest values and the root-mean-square deviation, in electrons per ångström cubed, of the final difference electron density. The \( \ast \) \_diffrms value is measured with respect to the arithmetic mean density and is derived from summations over each grid point in the asymmetric unit of the cell. This quantity is useful for assessing the significance of \( \ast \) \_min and \( \ast \) \_max values, and also for defining suitable contour levels.

The measure of absolute structure as defined by Flack (1983). For centrosymmetric structures, the only permitted value, if the data name is present, is ‘inapplicable’, represented by ‘.’. For noncentrosymmetric structures, the value must lie in the 99.97% Gaussian confidence interval \(-3\sigma \leq \eta \leq 3\sigma\) and a standard uncertainty (e.s.d.) \(u\) must be supplied. The \_enumeration_range of \(1.0 \rightarrow 0.1\) is correctly interpreted as meaning \((0.0-3\sigma) \leq \eta \leq (1.0+3\sigma)\).


The permitted range is \(1.0 \rightarrow 0.1\).

The measure of the absolute structure as defined by Rogers (1981). The value must lie in the 99.97% Gaussian confidence interval \(-3\sigma \leq \eta \leq 3\sigma\) and a standard uncertainty (e.s.d.) \(u\) must be supplied. The \_enumeration_range of \(-1.0 \rightarrow 1.0\) is correctly interpreted as meaning \((-1.0-3\sigma) \leq \eta \leq (1.0+3\sigma)\).


The permitted range is \(-1.0 \rightarrow 1.0\).

The smallest value in ångströms of the interplanar spacings of the reflections used in the refinement. This is called the highest resolution.

The permitted range is \(0.0 \rightarrow \infty\).

The largest value in ångströms of the interplanar spacings of the reflections used in the refinement. This is called the lowest resolution.

The permitted range is \(0.0 \rightarrow \infty\).

The extinction coefficient used to calculate the correction factor applied to the structure-factor data. The nature of the extinction coefficient is given in the definitions of \_refine\_ls\_extinction\_expression and \_refine\_ls\_extinction\_method. For the ‘Zachariasen’ method it is the \(r^2\) value; for the ‘Becker–Coppens type 1 isotropic’ method it is the \(\eta^\prime\) value and for ‘Becker–Coppens type 2 isotropic’ corrections it is the \(\rho^\prime\) value. Note that the magnitude of these values is usually of the order of 10,000.


Example: ‘3472 (52)’ (Zachariasen coefficient \(r^2 = 0.347(5)\) E04).

The least-squares goodness-of-fit parameter \(S\) for all reflections after the final cycle of refinement. Ideally, account should be taken of parameters restrained in the least-squares refinement. See also \_refine\_ls\_restrained\_S\_definitions.

\[
S = \left( \frac{\sum |w(Y_{\text{obs}} - Y_{\text{calc}})|^2}{N_{\text{ref}} - N_{\text{param}}} \right)^{1/2},
\]

where \(Y_{\text{obs}}\) = the observed coefficients (see \_refine\_ls\_structure\_factor\_coefs), \(Y_{\text{calc}}\) = the calculated coefficients (see \_refine\_ls\_structure\_factor\_coefs), \(w\) = the least-squares reflection weight \(1/\sigma^2\), \(u\) = the standard uncertainty, \(N_{\text{ref}}\) = the number of reflections used in the refinement, \(N_{\text{param}}\) = the number of refined parameters and the sum is taken over the specified reflections.

The permitted range is \(0.0 \rightarrow \infty\).
**4. DATA DICTIONARIES**

**_refine_ls_goodness_of_fit_gt_**

The least-squares goodness-of-fit parameter $S$ for significantly intense reflections (see _refinls_threshold_expression_) after the final cycle of refinement. Ideally, account should be taken of parameters restrained in the least-squares refinement. See also _refine_ls_restrained_S_ definitions.

$$S = \left( \frac{\sum |w(Y_{\text{obs}} - Y_{\text{calc}})|^2}{N_{\text{ref}} - N_{\text{param}}} \right)^{1/2},$$

where $Y_{\text{obs}}$ = the observed coefficients (see _refine_ls_structure_factor_coef_), $Y_{\text{calc}}$ = the calculated coefficients (see _refine_ls_structure_factor_coef_), $w$ = the least-squares reflection weight ($1/u^2$), $u$ = the standard uncertainty, $N_{\text{ref}}$ = the number of reflections used in the refinement, $N_{\text{param}}$ = the number of refined parameters; the sum is taken over all the specified reflections.

The permitted range is $0.0 \rightarrow \infty$.

Related item: _refine_ls_goodness_of_fit_obs_ (alternate).

**_refine_ls_goodness_of_fit_obs_**

This definition has been superseded and is retained here only for archival purposes. Use instead _refine_ls_goodness_of_fit_gt_.

The least-squares goodness-of-fit parameter $S$ for observed reflections (see _reflns_observed_criterion_) after the final cycle of refinement. Ideally, account should be taken of parameters restrained in the least-squares refinement. See also _refine_ls_restrained_S_ definitions.

$$S = \left( \frac{\sum |w(Y_{\text{obs}} - Y_{\text{calc}})|^2}{N_{\text{ref}} - N_{\text{param}}} \right)^{1/2},$$

where $Y_{\text{obs}}$ = the observed coefficients (see _refine_ls_structure_factor_coef_), $Y_{\text{calc}}$ = the calculated coefficients (see _refine_ls_structure_factor_coef_), $w$ = the least-squares reflection weight ($1/u^2$), $u$ = the standard uncertainty, $N_{\text{ref}}$ = the number of reflections used in the refinement, $N_{\text{param}}$ = the number of refined parameters; the sum is taken over all the specified reflections.

The permitted range is $0.0 \rightarrow \infty$.

**_refine_ls_goodness_of_fit_ref_**

The least-squares goodness-of-fit parameter $S$ for all reflections included in the refinement after the final cycle of refinement. Ideally, account should be taken of parameters restrained in the least-squares refinement. See also _refine_ls_restrained_S_ definitions.

$$S = \left( \frac{\sum |w(Y_{\text{obs}} - Y_{\text{calc}})|^2}{N_{\text{ref}} - N_{\text{param}}} \right)^{1/2},$$

where $Y_{\text{obs}}$ = the observed coefficients (see _refine_ls_structure_factor_coef_), $Y_{\text{calc}}$ = the calculated coefficients (see _refine_ls_structure_factor_coef_), $w$ = the least-squares reflection weight ($1/u^2$), $u$ = the standard uncertainty, $N_{\text{ref}}$ = the number of reflections used in the refinement, $N_{\text{param}}$ = the number of refined parameters; the sum is taken over all the specified reflections.

The permitted range is $0.0 \rightarrow \infty$.

**_refine_ls_matrix_type_**

The number of constrained (non-refined or dependent) parameters in the least-squares process. These may be due to symmetry or any other constraint process (e.g. rigid-body refinement). See also _atom_site_constraints_ definitions. A general description of constraints may appear in _refine_special_details_.

The data value must be one of the following:

- full
- fullcycle
- atomblock
- userblock
- diagonal
- sparse

The permitted range is $0 \rightarrow \infty$. Where no value is given, the assumed value is 'full'.

**_refine_ls_number_constraints_**

The number of constrained (non-refined or dependent) parameters refined in the least-squares process. If possible, this number should include some contribution from the restrained parameters. The restrained parameters are distinct from the constrained parameters (where one or more parameters are linearly dependent on the refined value of another). Least-squares restraints often depend on geometry or energy considerations and this makes their direct contribution to this number, and to the goodness-of-fit calculation, difficult to assess.

The permitted range is $0 \rightarrow \infty$.

**_refine_ls_number_parameters_**

The number of unique reflections contributing to the least-squares refinement calculation.

The permitted range is $0 \rightarrow \infty$.

**_refine_ls_number_reflns_**

The number of reflections used in the least-squares refinement calculation.

The permitted range is $0 \rightarrow \infty$.

**_refine_ls_number_restraints_**

The number of restrained parameters. These are parameters which are not directly dependent on another refined parameter. Restricted parameters often involve geometry or energy dependencies. See also _atom_site_constraints_ and _atom_site_refinement_flags_. A general description of refinement constraints may appear in _refine_special_details_.

The permitted range is $0 \rightarrow \infty$.

**_refine_ls_R_factor_all_**

Residual factor for all reflections satisfying the resolution limits established by _refine_ls_d_res_high_ and _refine_ls_d_res_low_. This is the conventional $R$ factor. See also _refine_ls_wR_factor_ definitions.
4.1. CORE DICTIONARY (coreCIF)  

**_refine_ls_R_factor_gt_** *(numb)*  
Residual factor for the reflections (with number given by _refine_number_gt_) judged significantly intense (i.e. satisfying the threshold specified by _reflns_threshold_expression) and included in the refinement. The reflections also satisfy the resolution limits established by _refine_ls_d_res_high and _refine_ls_d_res_low. This is the conventional R factor. See also _refine_ls_wR_factor_definitions.*

\[ R = \frac{\sum |F_{\text{obs}} - F_{\text{calc}}|}{\sum |F_{\text{obs}}|}, \]

where \( F_{\text{obs}} \) = the observed structure-factor amplitudes, \( F_{\text{calc}} \) = the calculated structure-factor amplitudes and the sum is taken over the specified reflections.

The permitted range is \( 0.0 \rightarrow \infty \).

**Related item: _refine_ls_R_factor_obs_(alternate).**

**_refine_ls_R_factor_obs_** *(numb)*  
This definition has been superseded and is retained here only for archival purposes. Use instead _refine_ls_R_factor_gt_.

Residual factor for the reflections classified as ‘observed’ (see _reflns_observed_criterion) and included in the refinement. The reflections also satisfy the resolution limits established by _refine_ls_d_res_high and _refine_ls_d_res_low. This is the conventional R factor. See also _refine_ls_wR_factor_definitions.*

\[ R = \frac{\sum |F_{\text{obs}} - F_{\text{calc}}|}{\sum |F_{\text{obs}}|}, \]

where \( F_{\text{obs}} \) = the observed structure-factor amplitudes, \( F_{\text{calc}} \) = the calculated structure-factor amplitudes and the sum is taken over the specified reflections.

The permitted range is \( 0.0 \rightarrow \infty \).

**Related item: _refine_ls_R_Fsqd_factor_(alternate).**

**_refine_ls_R_Fsqd_factor_** *(numb)*  
Residual factor \( R(F^2) \), calculated on the squared amplitudes of the observed and calculated structure factors, for significantly intense reflections (satisfying _reflns_threshold_expression) and included in the refinement. The reflections also satisfy the resolution limits established by _refine_ls_d_res_high and _refine_ls_d_res_low.

\[ R(F^2) = \frac{\sum F_{\text{obs}}^2 - F_{\text{calc}}^2}{\sum F_{\text{obs}}^2}, \]

where \( F_{\text{obs}}^2 \) = squares of the observed structure-factor amplitudes, \( F_{\text{calc}}^2 \) = squares of the calculated structure-factor amplitudes and the sum is taken over the specified reflections.

The permitted range is \( 0.0 \rightarrow \infty \).

**Related item: _refine_ls_restrained_S_all_(alternate).**
**REFINE**

_**_refine_ls_restrained_S_obs_ (numb)

This definition has been superseded and is retained here only for archival purposes. Use instead _refine_ls_restrained_S_gt_.

The least-squares goodness-of-fit parameter \( S \) for observed reflections after the final cycle of least-squares refinement. This parameter explicitly includes the restraints applied in the least-squares process. See also _refine_ls_goodness_of_fit_definitions_.

\[
S = \left( \frac{\sum |w(Y_{obs} - Y_{calc})|^2}{N_{red} + N_{rest} - N_{param}} \right)^{1/2},
\]

where \( Y_{obs} \) = the observed coefficients (see _refine_ls_structure_factor_coef_), \( Y_{calc} \) = the calculated coefficients (see _refine_ls_structure_factor_coef_), \( w \) = the least-squares reflection weight (/square of standard uncertainty (e.s.d.)), \( P_{red} \) = the calculated restraint values, \( P_{rest} \) = the target restraint values, \( w_{red} \) = the restraint weight, \( N_{red} \) = the number of reflections used in the refinement (see _refine_ls_number_reflns_obs_), \( N_{rest} \) = the number of restraints (see _refine_ls_number_restraints_) and \( N_{param} \) = the number of refined parameters (see _refine_ls_number_parameters_); the sum \( \sum \) is taken over the specified reflections and the sum \( \sum \) is taken over the restraints.

The permitted range is 0 \( \rightarrow \infty \). [refine]

_**_refine_ls_shift/su max_ (numb)

This definition has been superseded and is retained here only for archival purposes. Use instead _refine_ls_shift/su mean_.

The largest ratio of the final least-squares parameter shift to the final standard uncertainty (s.u., formerly described as estimated standard deviation, e.s.d.).

The permitted range is 0 \( \rightarrow \infty \). [refine]

_**_refine_ls_shift/su mean_ (numb)

The largest ratio of the final least-squares parameter shift to the final standard uncertainty. The permitted range is 0 \( \rightarrow \infty \).

Related item: _refine_ls_shift/su_max_(alternate). [refine]

_**_refine_ls_shift/su max_lt_ (numb)

An upper limit for the largest ratio of the final least-squares parameter shift to the final standard uncertainty. This item is used when the average value of the shift divided by the final standard uncertainty is too small to measure.

The permitted range is 0 \( \rightarrow \infty \).

Related item: _refine_ls_shift/su_max_(alternate). [refine]

_**_refine_ls_shift/su mean_ (numb)

The average ratio of the final least-squares parameter shift to the final standard uncertainty.

The permitted range is 0 \( \rightarrow \infty \).

Related item: _refine_ls_shift/su_max_(alternate). [refine]

**4. DATA DICTIONARIES**

_**cif_core_dic_**

_**_refine_ls_restrained_S_obs_**

An upper limit for the average ratio of the final least-squares parameter shift to the final standard uncertainty. This item is used when the average value of the shift divided by the final standard uncertainty is too small to measure.

The permitted range is 0 \( \rightarrow \infty \).

Related item: _refine_ls_shift/su_mean_(alternate). [refine]

_**_refine_ls_structure_factor_coef_**

Structure-factor coefficient \( |F| \), \( F^2 \) or \( f \) used in the least-squares refinement process.

The data value must be one of the following:

- \( F \) structure-factor magnitude
- \( F_{sqd} \) structure factor squared
- \( \text{Inet} \) net intensity

Where no value is given, the assumed value is ‘0’. [refine]

_**_refine_ls_weighting_details_**

A description of special aspects of the weighting scheme used in the least-squares refinement. Used to describe the weighting when the value of _refine_ls_weighting_scheme_ is specified as ‘calc’.

Example:

; Sigdel model of Konnert-Hendrickson:

Sigdel = \( Afsig = \{ Bfsig \} \cdot \sin(\theta) / \\lambda - 1/6 \) 

\( Afsig = 22.0 \), \( Bfsig = 150.0 \) at the beginning of refinement.

\( Afsig = 16.0 \), \( Bfsig = 60.0 \) at the end of refinement.

; [refine]

_**_refine_ls_weighting_scheme_**

The weighting scheme applied in the least-squares process. The standard code may be followed by a description of the weight (but see _refine_ls_weighting_details_ for a preferred approach).

The data value must be one of the following:

- \( \text{sigma} \) based on measured s.u.’s
- \( \text{unit} \) unit or no weights applied
- \( \text{calc} \) calculated weights applied

Where no value is given, the assumed value is ‘sigma’. [refine]

_**_refine_ls_WR_factor_all_**

Weighted residual factors for all reflections. The reflections also satisfy the resolution limits established by _refine_ls_d_res_high_ and _refine_ls_d_res_low_. See also the _refine_ls_R_factor_definitions._

\[
wR = \left( \frac{\sum |w(Y_{obs} - Y_{calc})|^2}{\sum |wY_{obs}|^2} \right)^{1/2},
\]

where \( Y_{obs} \) = the observed amplitude specified by _refine_ls_structure_factor_coef_, \( Y_{calc} \) = the calculated amplitude specified by _refine_ls_structure_factor_coef_, \( w \) = the least-squares weight and the sum is taken over the specified reflections.

The permitted range is 0 \( \rightarrow \infty \). [refine]

_**_refine_ls_WR_factor_gt_**

Weighted residual factors for significantly intense reflections (satisfying _refine_threshold_expression_) included in the refinement. The reflections also satisfy the resolution limits established by _refine_ls_d_res_high_ and _refine_ls_d_res_low_. See also the _refine_ls_R_factor_definitions._

246
wR = \left( \frac{\sum |Y_{\text{obs}} - Y_{\text{calc}}|^2}{\sum |Y_{\text{obs}}|^2} \right)^{1/2},

where \( Y_{\text{obs}} \) = the observed amplitude specified by \texttt{_reflns_class_code}, \( Y_{\text{calc}} \) = the calculated amplitude specified by \texttt{_reflns_class_code}, \( w \) = the least-squares weight and the sum is taken over the specified reflections. The permitted range is \( 0 \rightarrow \infty \).

The reflection class limits are established by \texttt{_reflns_class_d_res_low} and \texttt{_reflns_class_d_res_high}. See also the \texttt{_reflns_class_code} definitions.

\texttt{_reflns_class_code} (char)
The code identifying a certain reflection class. This code must match \texttt{_reflns_class_code}.

Appears in list. Must match parent data name \texttt{_reflns_class_code}.

Examples: ‘1’, ‘m1’, ‘a2’.

\texttt{_reflns_class_d_res_high} (numb)
For each reflection class, the highest resolution in Ångström for the reflections used in the refinement. This is the lowest \( d \) value in a reflection class.

Appears in list containing \texttt{_reflns_class_code}.
The permitted range is \( 0 \rightarrow \infty \).

\texttt{_reflns_class_d_res_low} (numb)
For each reflection class, the lowest resolution in Ångström for the reflections used in the refinement. This is the highest \( d \) value in a reflection class.

Appears in list containing \texttt{_reflns_class_code}.
The permitted range is \( 0 \rightarrow \infty \).

\texttt{_reflns_class_R_factor_all} (numb)
For each reflection class, the residual factors for all reflections, and for significantly intense reflections (see \texttt{_reflns_threshold_expression}), included in the refinement. The reflections also satisfy the resolution limits established by \texttt{_reflns_class_d_res_high} and \texttt{_reflns_class_d_res_low}. This is the conventional \( R \) factor.

\begin{equation}
R = \frac{\sum |F_{\text{obs}} - F_{\text{calc}}|}{\sum |F_{\text{obs}}|},
\end{equation}

where \( F_{\text{obs}} \) = the observed structure-factor amplitudes, \( F_{\text{calc}} \) = the calculated structure-factor amplitudes and the sum is taken over the specified reflections. See also \texttt{_reflns_class_code}.

Appears in list containing \texttt{_reflns_class_code}.
The permitted range is \( 0 \rightarrow \infty \).

\texttt{_reflns_class_R_Fsqd_factor} (numb)
For each reflection class, the residual factor \( R(F^2) \) calculated on the squared amplitudes of the observed and calculated structure factors for the reflections judged significantly intense (i.e. satisfying the threshold specified by \texttt{_reflns_threshold_expression}) and included in the refinement. The reflections also satisfy the resolution limits established by \texttt{_reflns_class_d_res_high} and \texttt{_reflns_class_d_res_low}.

\begin{equation}
R(F^2) = \frac{\sum |F_{\text{obs}}^2 - F_{\text{calc}}^2|}{\sum |F_{\text{obs}}^2|},
\end{equation}

where \( F_{\text{obs}}^2 \) = squares of the observed structure-factor amplitudes, \( F_{\text{calc}}^2 \) = squares of the calculated structure-factor amplitudes and the sum is taken over the specified reflections.

Appears in list containing \texttt{_reflns_class_code}.
The permitted range is \( 0 \rightarrow \infty \).
**REFINE.LS.CLASS**

**_refine_ls_class_R_I_factor_** *(numb)*

For each reflection class, the residual factor \( R(I) \) for the reflections judged significantly intense (i.e. satisfying the threshold specified by _refines_threshold_expression_ and included in the refinement. This is most often calculated in Rietveld refinements against powder data, where it is referred to as \( R_B \) or \( R_{Bragg} \).

\[
R(I) = \frac{\sum |I_{obs} - I_{calc}|}{\sum |I_{obs}|},
\]

where \( I_{obs} \) = the net observed intensities, \( I_{calc} \) = the net calculated intensities and the sum is taken over the specified reflections.

Appears in list containing _refine_ls_class_code_.
The permitted range is 0.0 → ∞.

**_refine_ls_class_wR_factor_all_** *(numb)*

For each reflection class, the weighted residual factors for all reflections included in the refinement. The reflections also satisfy the resolution limits established by _refine_ls_class_d_res_high_ and _refine_ls_class_d_res_low_.

\[
wR = \left( \frac{\sum |wY_{obs} - Y_{calc}|^2}{\sum |wY_{obs}|^2} \right)^{1/2},
\]

where \( Y_{obs} \) = the observed amplitudes specified by _refine_ls_structure_factor_coef_. \( Y_{calc} \) = the calculated amplitudes specified by _refine_ls_structure_factor_coef_. \( w \) = the least-squares weights and the sum is taken over the reflections of this class. See also _refine_ls_class_R_factor_ definitions.

Appears in list containing _refine_ls_class_code_.
The permitted range is 0.0 → ∞.

**REFLN**

Data items in the REF LN category record details about the reflections used to determine the ATOM_SITE data items. The REF LN data items refer to individual reflections and must be included in looped lists. The REF LN data items specify the parameters that apply to all reflections. The REF LN data items are not looped.


<table>
<thead>
<tr>
<th>Code</th>
<th>Value</th>
<th>Phase</th>
<th>Status</th>
</tr>
</thead>
<tbody>
<tr>
<td><em>refln_index_h</em></td>
<td>0 0 0 15718.18 15631.06 30.40 o</td>
<td></td>
<td></td>
</tr>
<tr>
<td><em>refln_index_k</em></td>
<td>0 0 0 55613.11 49840.09 61.86 o</td>
<td></td>
<td></td>
</tr>
<tr>
<td><em>refln_index_l</em></td>
<td>0 0 0 246.85 241.86 10.02 o</td>
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<td></td>
</tr>
<tr>
<td><em>refln_F_squared_calc</em></td>
<td>0 0 0 82.26 69.97 1.93 o</td>
<td></td>
<td></td>
</tr>
<tr>
<td><em>refln_F_squared_meas</em></td>
<td>0 0 0 1133.62 947.79 11.78 o</td>
<td></td>
<td></td>
</tr>
<tr>
<td><em>refln_F_squared_sigma</em></td>
<td>0 0 0 2558.04 2453.33 20.44 o</td>
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<td></td>
</tr>
<tr>
<td><em>refln_index</em></td>
<td>0 0 0 283.88 393.66 7.79 o</td>
<td></td>
<td></td>
</tr>
<tr>
<td><em>refln_d_spacing</em></td>
<td>0 0 0 283.70 171.98 4.26 o</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**4. DATA DICTIONARIES**

cif_core_dic


<table>
<thead>
<tr>
<th>Code</th>
<th>Value</th>
<th>Phase</th>
<th>Status</th>
</tr>
</thead>
<tbody>
<tr>
<td><em>refln_index_h</em></td>
<td>0 0 6 34.395 36.034 3.143 o</td>
<td></td>
<td></td>
</tr>
<tr>
<td><em>refln_index_k</em></td>
<td>0 0 12 42.599 40.855 2.131 o</td>
<td></td>
<td></td>
</tr>
<tr>
<td><em>refln_index_l</em></td>
<td>0 1 0 42.500 42.507 4.719 o</td>
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<td></td>
</tr>
<tr>
<td><em>refln_F_meas</em></td>
<td>0 1 1 59.272 57.976 4.719 o</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td><em>refln_F_calc</em></td>
<td>0 1 2 89.694 94.741 4.325 o</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td><em>refln_F_sigma</em></td>
<td>0 1 3 51.743 52.241 3.850 o</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td><em>refln_include_status</em></td>
<td>0 1 4 9.294 10.318 2.346 o</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td><em>refln_index</em></td>
<td>0 1 5 41.160 39.951 3.313 o</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td><em>refln_index</em></td>
<td>0 1 6 6.755 7.102 0.895 o</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td><em>refln_index</em></td>
<td>0 1 7 30.693 31.171 2.668 o</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td><em>refln_index</em></td>
<td>0 1 8 12.324 12.085 2.391 o</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td><em>refln_index</em></td>
<td>0 1 9 15.348 15.122 2.239 o</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td><em>refln_index</em></td>
<td>0 1 10 17.622 19.605 1.997 o</td>
<td>1</td>
<td></td>
</tr>
</tbody>
</table>

**_refln_A_calc_** *(numb)*

The calculated and measured structure-factor component \( A \) (in electrons for X-ray diffraction).

\[
A = |F| \cos(\text{phase}).
\]

Appears in list containing _refln_.

**_refln_B_calc_** *(numb)*

The calculated and measured structure-factor component \( B \) (in electrons for X-ray diffraction).

\[
B = |F| \sin(\text{phase}).
\]

Appears in list containing _refln_.

**_refln_class_code_** *(char)*

The code identifying the class to which this reflection has been assigned. This code must match a value of _refln_class_code_. Reflections may be grouped into classes for a variety of purposes. For example, for modulated structures each reflection class may be defined by the number \( m = \sum |m_i| \), where the \( m_i \) are the integer coefficients that, in addition to \( h,k,l \) index the corresponding diffraction vector in the basis defined for the reciprocal lattice.

Appears in list containing _refln_. Must match parent data name _refln_class_code_.

**_refln_crystal_id_** *(char)*

Code identifying each crystal if multiple crystals are used. Is used to link with _exptl_crystal_id_ in the _exptl_crystal_list_.

Appears in list containing _refln_. Must match parent data name _exptl_crystal_id_.

**_refln_d_spacing_** *(numb)*

The \( d \) spacing in ångströms for this reflection. This is related to the \( \sin(\theta)/\lambda \) value by the expression _refln_d_spacing_ = \( 2/(\text{_refln_sint/lambda}_) \).

Appears in list containing _refln_.

The permitted range is 0.0 → ∞.
4.1. CORE DICTIONARY (coreCIF)

**_refln_F_calc** (numb)

The calculated, measured and estimated standard uncertainty (derived from measurement) of the structure factors (in electrons for X-ray diffraction).

Appears in list containing _refln_index_.

**_refln_F_meas** (numb)

The calculated, measured and estimated standard uncertainty (derived from measurement) of the squared structure factors (in electrons for X-ray diffraction).

Appears in list containing _refln_index_.

**_refln_sint/lambda** (numb)

The (sinθ)/λ value in reciprocal ångströms for this reflection.

Appears in list containing _refln_index_.

The permitted range is 0.0 → ∞.

**_refln_symmetry_multiplicity** (numb)

The number of reflections symmetry-equivalent under the Laue symmetry to the present reflection. In the Laue symmetry, Friedel opposites (hkl and −h −k −l) are equivalent. Tables of symmetry-equivalent reflections are available in *International Tables for Crystallography* Volume A (2002), Chapter 10.1.

Appears in list containing _refln_index_.

The permitted range is 1 → 48.

**_refln_symmetry_omega** (numb)

The symmetry reinforcement factor corresponding to the number of times the reflection indices are generated identically from the space-group symmetry operations.

Appears in list containing _refln_index_.

The permitted range is 1 → ∞.

**_refln_index_** (numb)

Miller indices of the reflection. The values of the Miller indices in the REFLN category must correspond to the cell defined by the cell lengths and cell angles in the CELL category.

Appears in list as essential element of loop structure.

**_refln_phase_calc** (numb)

The calculated structure-factor phase in degrees.

Appears in list containing _refln_index_.

The calculated structure-factor phase in degrees.

Appears in list containing _refln_index_.

**_refln_phase_meas** (numb, su)

The measured structure-factor phase in degrees.

Appears in list containing _refln_index_.

**_reflns_scale_group_code** (char)

Code identifying the structure-factor scale. This code must correspond to one of the _reflns_scale_group_code values.

Appears in list containing _refln_index_. Must match parent data name _reflns_scale_group_code.


**_reflns_threshold_ expression** (char)

The permitted range is 1 → 48.

**_reflns_observed_criterion** (char)

The (sinθ)/λ value in reciprocal ångströms for this reflection.

Appears in list containing _refln_index_.

**_reflns_scale_group_code** (char)

Code identifying the structure-factor scale. This code must correspond to one of the _reflns_scale_group_code values.

Appears in list containing _refln_index_. Must match parent data name _reflns_scale_group_code.


**_reflns_threshold_ expression** (char)

The permitted range is 1 → 48.

**_reflns_observed_criterion** (char)

The (sinθ)/λ value in reciprocal ångströms for this reflection.

Appears in list containing _refln_index_.

**_refln_symmetry_omega** (numb)

The symmetry reinforcement factor corresponding to the number of times the reflection indices are generated identically from the space-group symmetry operations.

Appears in list containing _refln_index_.

The permitted range is 1 → ∞.

**_refln_symmetry_multiplicity** (numb)

The number of reflections symmetry-equivalent under the Laue symmetry to the present reflection. In the Laue symmetry, Friedel opposites (hkl and −h −k −l) are equivalent. Tables of symmetry-equivalent reflections are available in *International Tables for Crystallography* Volume A (2002), Chapter 10.1.

Appears in list containing _refln_index_.

The permitted range is 1 → 48.

**_refln_mean_path_length_tbar** (numb)

Mean path length in millimetres through the crystal for this reflection.

Appears in list containing _refln_index_.

The permitted range is 0.0 → ∞.

**_refln_F_squared_calc** (numb)

Calculated, measured and estimated standard uncertainty (derived from measurement) of the squared structure factors (in electrons for X-ray diffraction).

Appears in list containing _refln_index_.

**_refln_F_squared_meas** (numb)

Calculated, measured and estimated standard uncertainty (derived from measurement) of the squared structure factors (in electrons for X-ray diffraction).

Appears in list containing _refln_index_.

**_refln_F_squared_sigma** (numb)

Calculated, measured and estimated standard uncertainty (derived from measurement) of the squared structure factors (in electrons for X-ray diffraction).

Appears in list containing _refln_index_.

**_refln_intensity_meas** (numb)

Mean path length in millimetres through the crystal for this reflection.

Appears in list containing _refln_index_.

The permitted range is 0.0 → ∞.

**_refln_mean_path_length_tbar** (numb)

Mean path length in millimetres through the crystal for this reflection.
The mean wavelength in ångströms of the radiation used to measure this reflection. This is an important parameter for data collected using energy-dispersive detectors or the Laue method.

The permitted range is \(0.0 \rightarrow \infty\).

Code identifying the wavelength in the \_diffrn_radiation_list.

\_refln_wavelength (char)

Appears in list containing \_refln_index_.

The permitted range is \(0.0 \rightarrow \infty\).

The proportion of Friedel-related reflections present in the number of 'independent' reflections specified by the item \_reflns_number_total. This proportion is calculated as the ratio

\[
\frac{N(\text{crystal class}) - N(\text{Laue symmetry})}{N(\text{Laue symmetry})},
\]

where, working from the \_diffrn_refln_list, \(N(\text{crystal class})\) is the number of reflections obtained on averaging under the symmetry of the crystal class and \(N(\text{Laue symmetry})\) is the number of reflections obtained on averaging under the Laue symmetry.

Examples: \(a\) For centrosymmetric structures, \_reflns_Friedel_coverage is necessarily equal to 0.0 as the crystal class is identical to the Laue symmetry. \(b\) For whole-sphere data for a crystal in the space group \(P1\), \_reflns_Friedel_coverage is equal to 1.0, as no reflection \((hkl)\) is equivalent to \(-h -k -l\) in the crystal class and all Friedel pairs \((hkl); \ -h -k -l\) have been measured. \(c\) For whole-sphere data in space group \(Pmm2\), \_reflns_Friedel_coverage will be \(< 1.0\) because although reflections \(hkl\) and \(-h -k -l\) are not equivalent when \(hkl\) indices are nonzero, they are when \(l = 0\). \(d\) For a crystal in the space group \(Pmm2\), measurements of the two inequivalent octants \(h \geq 0, k \geq 0, l \geq 0\) lead to the same value as in \(c\), whereas measurements of the two equivalent octants \(h \geq 0, k \geq 0, l \geq 0\) will lead to a value of zero for \_reflns_Friedel_coverage.
Description of the properties of the reported reflection list that are not given in other data items. In particular, this should include information about the averaging (or not) of symmetry-equivalent reflections including Friedel pairs.

The permitted range is $0 \rightarrow \infty$.

**Related item: _reflns_observed_criterion (alternate).**

Example: 'I>2u(I)'.

**Data items in the REFLNS_CLASS category record details, for each reflection class, about the reflections used to determine the structural parameters.**

Example 1 – corresponding to the one-dimensional incommensurately modulated structure of $K_2SeO_4$.

loop

- _reflns_class_number_gt
- _reflns_class_code

<table>
<thead>
<tr>
<th>Number</th>
<th>Code</th>
</tr>
</thead>
<tbody>
<tr>
<td>584</td>
<td>'Main'</td>
</tr>
<tr>
<td>226</td>
<td>'Sat1'</td>
</tr>
<tr>
<td>50</td>
<td>'Sat2'</td>
</tr>
</tbody>
</table>

The code identifying a certain reflection class.

The permitted range is $0 \rightarrow \infty$.

**For each reflection class, the number of significantly intense reflections (see _reflns_threshold_expression) in the _refln_list (not the _diffrn_refln_list). This may include Friedel-equivalent reflections (i.e. those which are symmetry-equivalent under the Laue symmetry but inequivalent under the crystal class) according to the nature of the structure and the procedures used. Special characteristics of the reflections included in the _refln_list should be given in the item _reflns_special_details.**

Appears in list containing _reflns_class_code.

The permitted range is $0 \rightarrow \infty$.

**For each reflection class, the total number of reflections in the _refln_list (not the _diffrn_refln_list). This may include Friedel-equivalent reflections (i.e. those which are symmetry-equivalent under the Laue symmetry but inequivalent under the crystal class) according to the nature of the structure and the procedures used. Special characteristics of the reflections included in the _refln_list should be given in the item _reflns_special_details.**

Appears in list containing _reflns_class_code.

The permitted range is $0 \rightarrow \infty$.

**For each reflection class, the residual factors for all reflections, and for significantly intense reflections (see _reflns_threshold_expression), included in the refinement. The reflections also satisfy the resolution limits established by _reflns_class_d_res_high and _reflns_class_d_res_low. This is the conventional $R$ factor.**

$$R = \frac{\sum |F_{obs} - F_{calc}|}{\sum |F_{obs}|},$$

where $F_{obs}$ = the observed structure-factor amplitudes, $F_{calc}$ = the calculated structure-factor amplitudes and the sum is taken over the reflections of this class. See also _reflns_class_wR_factor_all definitions.

Appears in list containing _reflns_class_code.

The permitted range is $0 \rightarrow \infty$.

**For each reflection class, the residual factor for all reflections, and for significantly intense reflections (see _reflns_threshold_expression), included in the refinement. The reflections also satisfy the resolution limits established by _reflns_class_d_res_high and _reflns_class_d_res_low. This is the residual factor $R(F^2)$ calculated on the squared amplitudes of the observed and calculated structure factors, for the reflections judged significantly intense (i.e. satisfying the threshold specified by _reflns_threshold_expression) and included in the refinement. The reflections also satisfy the resolution limits established by _reflns_class_d_res_high and _reflns_class_d_res_low.**

$$R(F^2) = \frac{\sum |F_{obs}^2 - F_{calc}^2|}{\sum |F_{obs}^2|},$$

where $F_{obs}^2$ = squares of the observed structure-factor amplitudes, $F_{calc}^2$ = squares of the calculated structure-factor amplitudes and the sum is taken over the reflections of this class.

Appears in list containing _reflns_class_code.

The permitted range is $0 \rightarrow \infty$. 

**Description of each reflection class.**

Appears in list containing _reflns_class_code.

Examples: 'm=1 first order satellites', 'H0L0 common projection reflections'.

The permitted range is $0 \rightarrow \infty$. 

**Example:**

<table>
<thead>
<tr>
<th>Code</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>'Main'</td>
<td>The code identifying a certain reflection class.</td>
</tr>
<tr>
<td>'Sat1'</td>
<td>The code identifying a certain reflection class.</td>
</tr>
<tr>
<td>'Sat2'</td>
<td>The code identifying a certain reflection class.</td>
</tr>
</tbody>
</table>
REFLNS.CLASS

_reflns_class_R_I_factor (numb)
For each reflection class, the residual factor $R(I)$ for the reflections judged significantly intense (i.e. satisfying the threshold specified by _reflns_threshold_expression and included in the refinement. This is most often calculated in Rietveld refinements against powder data, where it is referred to as $R_B$ or $R_{\text{Bragg}}$.

$$R(I) = \frac{\sum |I_{\text{obs}} - I_{\text{calc}}|}{\sum |I_{\text{obs}}|},$$

where $I_{\text{obs}}$ = the net observed intensities, $I_{\text{calc}}$ = the net calculated intensities and the sum is taken over the reflections of this class.

Appears in list containing _reflns_class_code.
The permitted range is $0 \rightarrow \infty$.

_reflns_class_wR_factor_all (numb)
For each reflection class, the weighted residual factor for all reflections included in the refinement. The reflections also satisfy the resolution limits established by _reflns_class_d_res_high and _reflns_class_d_res_low.

$$wR = \left( \frac{\sum w|Y_{\text{obs}} - Y_{\text{calc}}|^2}{\sum w|Y_{\text{obs}}|^2} \right)^{1/2},$$

where $Y_{\text{obs}}$ = the observed amplitudes specified by _reflns_class_d_res_high, $Y_{\text{calc}}$ = the calculated amplitudes specified by _reflns_class_d_res_low, $w$ = the least-squares weights and the sum is taken over the reflections of this class. See also _reflns_class_w_factor definitions.

Appears in list containing _reflns_class_code.
The permitted range is $0 \rightarrow \infty$.

REFLNS.SCALE

Data items in the REFLNS.SCALE category record details about the structure-factor scales. They are referenced from within the REFLNS.list through _reflns_scale_group_code.


loop
_reflns_scale_group_code
_reflns_scale_group_code_Maas_F
  1 .895447
  2 .912743

_reflns_scale_group_code (char)
The code identifying a scale _reflns_scale_meas. These are linked to the _reflns_list by the _reflns_scale_group_code. These codes need not correspond to those in the _diffrn_scale_list.

Appears in list as essential element of loop structure. May match child data name(s):
_reflns_scale_group_code

_reflns_scale_meas_F
_reflns_scale_meas_F_squared
_reflns_scale_meas_intensity (numb, su)
Scales associated with _reflns_scale_group_code.

Appears in list containing _reflns_scale_group_code.
The permitted range is $0 \rightarrow \infty$.
4.1. CORE DICTIONARY (coreCIF)

**_reflns_shell_meanI_over_UI_all** (numb)
The ratio of the mean of the intensities of all reflections in this shell to the mean of the standard uncertainties of the intensities of all reflections in the resolution shell.

Appears in list.

Related item: _reflns_shell_meanI_over_sigI_all (alternate). [reflns_shell]

**_reflns_shell_meanI_over_UI_gt** (numb)
The ratio of the mean of the intensities of the significantly intense reflections (see _reflns_threshold_expression) in this shell to the mean of the standard uncertainties of the intensities of the significantly intense reflections in the resolution shell.

Appears in list.

Related items: _reflns_shell_meanI_over_sigI_gt (alternate), _reflns_shell_meanI_over_sigI_obs (alternate). [reflns_shell]

**_reflns_shell_number_measured_all** (numb)
The total number of reflections measured for this resolution shell.

Appears in list.

The permitted range is $0 \rightarrow \infty$. [reflns_shell]

**_reflns_shell_number_measured_gt** (numb)
The number of significantly intense reflections (see _reflns_threshold_expression) measured for this resolution shell.

Appears in list.

The permitted range is $0 \rightarrow \infty$.

Related item: _reflns_shell_number_measured_obs (alternate). [reflns_shell]

**_reflns_shell_number_possible** (numb)
This definition has been superseded and is retained here only for archival purposes. Use instead _reflns_shell_number_unique_gt.

The number of unique reflections it is possible to measure in this reflection shell.

Appears in list.

The permitted range is $0 \rightarrow \infty$. [reflns_shell]

**_reflns_shell_number_unique_all** (numb)
The total number of measured reflections resulting from merging measured symmetry-equivalent reflections for this resolution shell.

Appears in list.

The permitted range is $0 \rightarrow \infty$. [reflns_shell]

**_reflns_shell_number_unique_gt** (numb)
The total number of significantly intense reflections (see _reflns_threshold_expression) resulting from merging measured symmetry-equivalent reflections for this resolution shell.

Appears in list.

The permitted range is $0 \rightarrow \infty$.

Related item: _reflns_shell_number_unique_obs (alternate). [reflns_shell]

**_reflns_shell_number_unique_obs** (numb)
This definition has been superseded and is retained here only for archival purposes. Use instead _reflns_shell_number_unique_gt.

The total number of reflections classified as ‘observed’ (see _reflns_observed_criterion) resulting from merging measured symmetry-equivalent reflections for this resolution shell.

Appears in list.

The permitted range is $0 \rightarrow \infty$. [reflns_shell]

**_reflns_shell_number_unique_obs** (numb)
This definition has been superseded and is retained here only for archival purposes. Use instead _reflns_shell_number_unique_gt.

The total number of measured symmetry-equivalent reflections for this resolution shell.

The total number of measured reflections resulting from merging measured symmetry-equivalent reflections for this resolution shell.

The number of unique reflections it is possible to measure in this resolution shell.

The number of significantly intense reflections (see _reflns_threshold_expression) measured for this resolution shell.

The number of reflections classified as ‘observed’ (see _reflns_observed_criterion) resulting from merging measured symmetry-equivalent reflections for this resolution shell.

The ratio of the mean of the intensities of all reflections in this shell to the mean of the standard uncertainties of the intensities of all reflections in the resolution shell.

The permitted range is $0 \rightarrow \infty$.

Related item: _reflns_shell_meanI_over_sigI_all (alternate). [reflns_shell]

**_reflns_shell_percent_possible_all** (numb)
The percentage of geometrically possible reflections represented by all reflections measured for this resolution shell.

Appears in list.

The permitted range is $0 \rightarrow 100.0$. [reflns_shell]

**_reflns_shell_percent_possible_gt** (numb)
The percentage of geometrically possible reflections represented by significantly intense reflections (see _reflns_threshold_expression) measured for this resolution shell.

Appears in list.

The permitted range is $0 \rightarrow 100.0$.

Related item: _reflns_shell_percent_possible_obs (alternate). [reflns_shell]

**_reflns_shell_percent_possible_obs** (numb)
This definition has been superseded and is retained here only for archival purposes. Use instead _reflns_shell_percent_possible_gt.

The percentage of geometrically possible reflections represented by all reflections measured for this resolution shell.

Appears in list.

The permitted range is $0 \rightarrow 100.0$. [reflns_shell]

**_reflns_shell_Rmerge_F_all** (numb)
The value of $R_{merge}(F)$ for all reflections in a given shell.

$$ R_{merge} = \frac{\sum_i (|F_i| - \langle F \rangle)}{\sum_i |F_i|}, $$

where $F_i$ = the amplitude of the $i$th observation of reflection $j$, $\langle F \rangle$ = the mean of the amplitudes of all observations of reflection $j$, $\sum_i$ is taken over all reflections and $\sum_j$ is taken over all observations of each reflection.

Appears in list.

The permitted range is $0 \rightarrow \infty$. [reflns_shell]

**_reflns_shell_Rmerge_F_gt** (numb)
The value of $R_{merge}(F)$ for significantly intense reflections (see _reflns_threshold_expression) in a given shell.

$$ R_{merge} = \frac{\sum_i (|F_i| - \langle F \rangle)}{\sum_i |F_i|}, $$

where $F_i$ = the amplitude of the $i$th observation of reflection $j$, $\langle F \rangle$ = the mean of the amplitudes of all observations of reflection $j$, $\sum_i$ is taken over all reflections and $\sum_j$ is taken over all observations of each reflection.

Appears in list.

The permitted range is $0 \rightarrow \infty$. [reflns_shell]
The value of \( R_{\text{merge}}(F) \) for reflections classified as ‘observed’ (see \_reflns_observedCriterion) in a given shell.

\[
R_{\text{merge}}(F) = \frac{\sum_{i,j} |F_i - (\langle F \rangle)|}{\sum_{i,j} |\langle F \rangle|},
\]

where \( F_i \) is the amplitude of the \( j \)th observation of reflection \( i \), \( (\langle F \rangle) \) is the mean of the amplitudes of all observations of reflection \( i \), \( \sum_{i} \) is taken over all reflections and \( \sum_{j} \) is taken over all observations of each reflection.

Appears in list.
The permitted range is \( 0 \rightarrow \infty \).

The value of \( R_{\text{merge}}(I) \) for significantly intense reflections (see \_reflns_thresholdExpression) in a given shell.

\[
R_{\text{merge}}(I) = \frac{\sum_{i,j} |I_i - (\langle I \rangle)|}{\sum_{i,j} |(\langle I \rangle)|},
\]

where \( I_i \) is the intensity of the \( j \)th observation of reflection \( i \), \( (\langle I \rangle) \) is the mean of the intensities of all observations of reflection \( i \), \( \sum_{i} \) is taken over all reflections and \( \sum_{j} \) is taken over all observations of each reflection.

Appears in list.
The permitted range is \( 0 \rightarrow \infty \).

This definition has been superseded and is retained here only for archival purposes. Use instead \_reflns_shell_Rmerge_F_gt.

The value of \( R_{\text{merge}}(I) \) for reflections classified as ‘observed’ (see \_reflns_observedCriterion) in a given shell.

\[
R_{\text{merge}}(I) = \frac{\sum_{i,j} |I_i - (\langle I \rangle)|}{\sum_{i,j} |\langle I \rangle|},
\]

where \( I_i \) is the intensity of the \( j \)th observation of reflection \( i \), \( (\langle I \rangle) \) is the mean of the intensities of all observations of reflection \( i \), \( \sum_{i} \) is taken over all reflections and \( \sum_{j} \) is taken over all observations of each reflection.

Appears in list.
The permitted range is \( 0 \rightarrow \infty \).

This definition has been superseded and is retained here only for archival purposes. Use instead \_reflns_shell_Rmerge_F_gt.

The value of \( R_{\text{merge}}(F) \) for reflections classified as ‘observed’ (see \_reflns_observedCriterion) in a given shell.

\[
R_{\text{merge}}(F) = \frac{\sum_{i,j} |F_i - (\langle F \rangle)|}{\sum_{i,j} |\langle F \rangle|},
\]

The permitted range is \( 0 \rightarrow \infty \).
of International Tables for Crystallography Vol. A (2002) or a Hermann–Mauguin symbol for a conventional or unconventional setting. Each component of the space-group name is separated by a space or an underscore. The use of a space is strongly recommended. The underscore is only retained because it was used in older files. It should not be used in new CIFs. Subscripts should appear without special symbols. Bars should be given as negative signs before the numbers to which they apply. The commonly used Hermann–Mauguin symbol determines the space-group type uniquely but a given space-group type may be described by more than one Hermann–Mauguin symbol. The space-group type is best described using _space_group_symop_operation_xyz. The Hermann–Mauguin symbol may contain information on the choice of basis, but not on the choice of origin. To define the setting uniquely, use _space_group_name_Hall or list the symmetry operations.

May appear in list containing _space_group_id.

Related item: _symmetry_equiv_pos_site_id

Example:

<table>
<thead>
<tr>
<th>_space_group_id</th>
<th>_space_group_name_Hall</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 'c m c m'</td>
<td>c2/c 2/m 21/m</td>
</tr>
<tr>
<td>2 'c 2/c 2/m 21/m'</td>
<td>c2/c 2/m 21/m</td>
</tr>
<tr>
<td>3 'A n a m'</td>
<td>c2/c 2/m 21/m</td>
</tr>
<tr>
<td>(three examples for space group No. 63)</td>
<td></td>
</tr>
</tbody>
</table>

[space_group]

_Symmetry

A parsable string giving one of the symmetry operations of the space group in algebraic form. If W is a matrix representation of the rotational part of the symmetry operation defined by the positions and signs of x, y and z, and w is a column of translations defined by fractions, an equivalent position x' is generated from a given position x by

\[ x' = Wx + w. \]

When a list of symmetry operations is given, it must contain a complete set of coordinate representatives which generates all the operations of the space group by the addition of all primitive translations of the space group. Such representatives are to be found as the coordinates of the general-equivalent position in International Tables for Crystallography Vol. A (2002), to which it is necessary to add any centring translations shown above the general-equivalent position. That is to say, it is necessary to list explicitly all the symmetry operations required to generate all the atoms in the unit cell defined by the setting used.

May appear in list containing _space_group_id.

Related item: _symmetry_equiv_pos_as_xyz

Example:

<table>
<thead>
<tr>
<th>_space_group_symop_operation_xyz</th>
<th>(char)</th>
</tr>
</thead>
<tbody>
<tr>
<td>x,1/2-y,1/2+z</td>
<td>(glide reflection through the plane (1/2, 1/2, z), with glide vector (1/2, 0, 1/2).)</td>
</tr>
</tbody>
</table>

[space_group]

_Space_group_symop_sg_id

(char)

This must match a particular value of _space_group_id, allowing the symmetry operation to be identified with a particular space group.

May appear in list containing _space_group_id. Must match parent data name _space_group_id.


<table>
<thead>
<tr>
<th>_symmetry_cell_setting</th>
<th>orthorhombic</th>
</tr>
</thead>
<tbody>
<tr>
<td>_symmetry_space_group_name_H-M</td>
<td>'P 21 21 21'</td>
</tr>
<tr>
<td>_symmetry_space_group_name_Hall</td>
<td>'P 2ac 2ab'</td>
</tr>
</tbody>
</table>

[space_group]

_Symmetry_cell_setting

(char)

This definition has been superseded and is retained here only for archival purposes. Use instead _space_group_crystal_system.

The cell settings for this space-group symmetry. The data value must be one of the following:

- triclinic
- monoclinic
- orthorhombic
- tetragonal
- rhombohedral
- trigonal
- hexagonal
- cubic

[space_group]

_Symmetry_Int_Tables_number

(num)

This definition has been superseded and is retained here only for archival purposes. Use instead _space_group_IT_number.


The permitted range is 1 → 230.
SYMMETRY

_4. DATA DICTIONARIES_

**SYMMETrY_EQUIV**

Data items in the SYMMETRY_EQUIV category list the symmetry-equivalent positions for the space group.


```
loop_
  symmetry_equiv_pos_as_xyz
    +x,y,z  1/2-x,-y,1/2+z  1/2+x,1/2-y,−z -x,1/2+y,1/2-z


Formally, the value of _symmetry_equiv_pos_site_id_ can be any unique character string: it is recommended that it be assigned the sequence number of the list of equivalent positions for compatibility with older files in which it did not appear.

```

```
loop_
  symmetry_equiv_pos_site_id
  symmetry_equiv_pos_as_xyz
  1  x,y,z
  2  1/2-x,-y,1/2+z
  3  1/2+x,1/2-y,−z
  4  -x,1/2+y,1/2-z

May appear in list.

Example: ‘-y,x,-z’.

**_symmetry_space_group_name_H-M_ (char)**

This definition has been superseded and is retained here only for archival purposes. Use instead _space_group_name_H-M_alt_.

Hermann–Mauguin space-group symbol. Note that the Hermann–Mauguin symbol does not necessarily contain complete information about the symmetry and the space-group origin. If used, always supply the full symbol from International Tables for Crystallography Vol. A (2002) and indicate the origin and the setting if it is not implicit. If there is any doubt that the equivalent positions can be uniquely deduced from this symbol, specify the _symmetry_equiv_pos_as_xyz_ or *_Hall_ data items as well. Leave spaces between symbols referring to different axes.

Examples: ‘P 1 1/2 1/2 1/2’, ‘P 2/n 2/n 2/n (origin at -1)’, ‘R 3 2/m’. [symmetry]

**_symmetry_space_group_name_Hall_ (char)**

This definition has been superseded and is retained here only for archival purposes. Use instead _space_group_name_Hall_.

Space-group symbol as described by Hall. This symbol gives the space-group setting explicitly. Leave spaces between the separate components of the symbol.


Examples: ‘P 2ac 2n’, ‘R 3 2’. [symmetry]

**VALENCE_PARAM**

Data items in the VALENCE_PARAM category define the parameters used for calculating bond valences from bond lengths. In addition to the parameters, a pointer is given to the reference (in VALENCE_REF) from which the bond-valence parameters were taken.

**Example 1** – a bond-valence parameter list with accompanying references.

```
loop_
  valence_param_id
  valence_param_atom_1
  valence_param_atom_1_valence
  valence_param_atom_2
  valence_param_atom_2_valence
  valence_param_details
  valence_param_ref_id
  valence_ref_reference


j ‘Liu & Thorp (1993), Inorg. Chem. 32, 4102-4205’

m ‘See, Krause & Strub (1998), Inorg. Chem. 37, 5369-5375’

```

```

VALENCE_PARAM

- _valence_param_atom_1_ (char)
  - The element symbol of the first atom forming the bond whose bond-valence parameters are given in this category.
  - Appears in list containing _valence_param_id_. [valence_param]

VALENCE_PARAM

- _valence_param_atom_2_ (char)
  - The element symbol of the second atom forming the bond whose bond-valence parameters are given in this category.
  - Appears in list containing _valence_param_id_. [valence_param]

VALENCE_PARAM

- _valence_param_atom_1_valence_ (numb)
  - The valence (formal charge) of the first atom whose bond-valence parameters are given in this category.
  - Appears in list containing _valence_param_id_. [valence_param]

VALENCE_PARAM

- _valence_param_atom_2_valence_ (numb)
  - The valence (formal charge) of the second atom whose bond-valence parameters are given in this category.
  - Appears in list containing _valence_param_id_. [valence_param]

VALENCE_PARAM

- _valence_param_details_ (char)
  - Details of or comments on the bond-valence parameters.
  - Appears in list containing _valence_param_id_. [valence_param]

VALENCE_PARAM

- _valence_param_ref_id_ (char)
  - A code identifying each entry in the _symmetry_equiv_pos_as_xyz_ list. It is normally the sequence number of the entry in that list, and should be identified with the code ‘n’ in _geom_*_symmetry_ codes of the form ‘n_klm’.
  - Appears in list containing _symmetry_equiv_pos_as_xyz_. [symmetry]

VALENCE_PARAM

- _valence_ref_reference_ (char)
  - Details of or comments on the bond-valence parameters.
  - Appears in list containing _valence_param_id_. [valence_param]
4.1. CORE DICTIONARY (coreCIF)

**VALENCE**

<table>
<thead>
<tr>
<th><strong>_valence_param_id</strong></th>
<th>(char)</th>
<th>An identifier for the valence parameters of a bond between the given atoms. Appears in list.</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>_valence_param_ref_id</strong></td>
<td>(char)</td>
<td>An identifier which links to the reference to the source from which the bond-valence parameters are taken. A child of _valence_ref_id, which it must match. Appears in list containing _valence_param_id. Must match parent data name _valence_ref_id.</td>
</tr>
<tr>
<td><strong>_valence_param_Ro</strong></td>
<td>(numb)</td>
<td>The bond-valence parameter $R_o$ used in the expression $s = \exp[(R_o - R)/B]$, where $s$ is the valence of a bond of length $R$. Appears in list containing _valence_param_id.</td>
</tr>
</tbody>
</table>

**VALENCE_REF**

Data items in the VALENCE_REF category list the references from which the bond-valence parameters have been taken.

<table>
<thead>
<tr>
<th><strong>_valence_ref_id</strong></th>
<th>(char)</th>
<th>An identifier for items in this category. Parent of _valence_param_ref_id, which must have the same value. Appears in list containing _valence_ref_id. May match child data name(s): _valence_param_ref_id.</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>_valence_ref_reference</strong></td>
<td>(char)</td>
<td>Literature reference from which the valence parameters identified by _valence_param_id were taken. Appears in list containing _valence_ref_id.</td>
</tr>
</tbody>
</table>

257