4.1. Core dictionary (coreCIF)

BY S. R. HALL, F. H. ALLEN AND I. D. BROWN

This is version 2.4.2 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-diffusion 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 using a rigorously relational data model that expresses dependencies and inheritances between individual items. The macromolecular CIF (mmCIF) dictionary described in Chapter 3.6 and given in Chapter 4.5 provides a complete set of data items within this model, including the content of the core CIF dictionary in a modified formalism.

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

**ATOM_SITE**

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_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_label
  #----- data truncated for brevity -----
  C1 1 . . # . | .
  H11A .5 M A # . . .
  H11B .5 M A # / . \ # . .
  H12A .5 M A # / . \ # . .
  H12B .5 M B # / . \ # . .
  H13A .5 M B # H12A H12B H13B
```


```
loop
  _atom_site_label
  _atom_site_aniso_label
  _atom_site_aniso_B_11
  _atom_site_aniso_B_12
  _atom_site_aniso_B_13
  _atom_site_aniso_B_22
  _atom_site_aniso_B_33
  _atom_site_U_iso_or_equiv
  _atom_site_label
  #----- data truncated for brevity -----
  C1 1 . . # . | .
  H11A .5 M A # . . .
  H11B .5 M A # / . \ # . .
  H12A .5 M A # / . \ # . .
  H12B .5 M B # / . \ # . .
  H13A .5 M B # H12A H12B H13B
```


```
loop
  _atom_site_label
  _atom_site_chemical_comp_name
  _atom_site_calc_phase_number
  _atom_site_calc_flag
  _atom_site_occupancy
  _atom_site_label
  #----- data truncated for brevity -----
  C1 1 . . # . | .
  H11A .5 M A # . . .
  H11B .5 M A # / . \ # . .
  H12A .5 M A # / . \ # . .
  H12B .5 M B # / . \ # . .
  H13A .5 M B # H12A H12B H13B
```

**Example 4** – hypothetical example to illustrate the description of a disordered methyl group.

```
loop
  _atom_site_label
  _atom_site_disorder_assembly
  _atom_site_disorder_group
  #----- data truncated for brevity -----
  C1 1 . . # . | .
  H11A .5 M A # . . .
  H11B .5 M A # / . \ # . .
  H12A .5 M A # / . \ # . .
  H12B .5 M B # / . \ # . .
  H13A .5 M B # H12A H12B H13B
```


```
loop
  _atom_site_label
  _atom_site_chemical_comp_name
  _atom_site_calc_phase_number
  _atom_site_calc_flag
  _atom_site_occupancy
  _atom_site_label
  #----- data truncated for brevity -----
  C1 1 . . # . | .
  H11A .5 M A # . . .
  H11B .5 M A # / . \ # . .
  H12A .5 M A # / . \ # . .
  H12B .5 M B # / . \ # . .
  H13A .5 M B # H12A H12B H13B
```

**ATOM_SITE**

A standard code used to describe the type of atomic displacement parameters used for the site.

The data value must be one of the following:

- Uani: anisotropic
- Uiso: isotropic
- Uovl: overall
- Umpe: multipole expansion
- Bani: anisotropic
- Biso: isotropic
- Bovl: overall

Appears in list containing _atom_site_label

Related item: _atom_site_chemical_comp_name

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4. DATA DICTIONARIES

_atom_site_attached_hydrogens (numb)
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).

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

$$B_{\text{eqv}} = (B_{11}B_{22}B_{33})^{1/3},$$

where $B_{jj}$ are the principal components of the orthogonalized $B_{ij}$.

The IUCr Commission on Nomenclature recommends against the use of $B$ for reporting atomic displacement parameters. $\mathbf{U}$, being directly proportional to $B$, is preferred. Appears in list containing _atom_site_label.
The permitted range is 0.0 → $\infty$.

Related items: _atom_site_B_iso_or_equiv(alternate), _atom_site_U_iso_or_equiv(alternate), _atom_site_U_equiv_geom_mean(alternate), _atom_site_U_iso_or_equiv(alternate), _atom_site_U_equiv_geom_mean(alternate), _atom_site_label.

_atom_site_B_iso_or_equiv (numb, su)
Isotropic atomic displacement parameter, or equivalent isotropic atomic displacement parameter, $B_{\text{eqv}}$, in ångströms squared, calculated from anisotropic displacement parameters.

$$B_{\text{eqv}} = (1/3) \sum_i \sum_j (B_{ij} + 2B_{ij})^{1/2},$$

where $A$ are the real-space cell lengths and $a^* = \text{reciprocal-space cell lengths}$; $B_{ij}$ is the anisotropic $U_{ij}$.


The IUCr Commission on Nomenclature recommends against the use of $B$ for reporting atomic displacement parameters. $\mathbf{U}$, being directly proportional to $B$, is preferred. Appears in list containing _atom_site_label.
The permitted range is 0.0 → $\infty$.

Related items: _atom_site_B_equiv_geom_mean(alternate), _atom_site_U_iso_or_equiv(alternate), _atom_site_U_equiv_geom_mean(alternate), _atom_site_U_iso_or_equiv(alternate), _atom_site_U_equiv_geom_mean(alternate), _atom_site_label.

_atom_site_calc_attached_atom (char)
The _atom_site_label of 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 ‘.’.

_atom_site_calc_flag (char)
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’.

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’.

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

$$T = \exp\left\{-2\pi^2 \sum_i \sum_j (U_{ij} + 2U_{ij})\right\},$$

where $h$ are the Miller indices and $a^* = \text{reciprocal-space cell lengths}$.

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

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

$$T = \exp\left\{-2\pi^2 \sum_i \sum_j (U_{ij} + 2U_{ij})\right\},$$

where $h$ are the Miller indices and $a^* = \text{reciprocal-space cell lengths}$.

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

$\mathbf{B}$ being directly proportional to $\mathbf{U}$, for reporting atomic displacement parameters.
4.1. CORE DICTIONARY (CORECIF)

**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,...’ is acceptable and represents the components C, 233, ‘...’ and ‘...’. Different labels may have a different number of components.

Appears in list as essential element of loop structure. May match child name(s): **atom_site_aniso_label**, **atom_angle_atom_site_label_1**, **atom_angle_atom_site_label_2**, **atom_angle_atom_site_label_3**, **atom_bond_atom_site_label_1**, **atom_bond_atom_site_label_2**, **atom_contact_atom_site_label_1**, **atom_contact_atom_site_label_2**, **atom_hbond_atom_site_label_1**, **atom_hbond_atom_site_label_2**, **atom_hbond_atom_site_label_3**, **atom_hbond_atom_site_label_4**, **atom_torsion_atom_site_label_1**, **atom_torsion_atom_site_label_2**, **atom_torsion_atom_site_label_3**, **atom_torsion_atom_site_label_4**.

Example: 'C12', 'Ca3g28', 'Fe3+17', 'Hx251', 'boron2a', 'C,phe_83_p,0', 'Zn,Zn,301,A,0'.

- **atom_site_occupancy** (numb, su)
  
  The **atom_site_occupancy** is the fraction of the atom type present at this site. The sum of the occupancies of all the atom types at this site may not significantly exceed 1.0 unless it is a dummy site. The value must lie in the 99.97% Gaussian confidence interval $-3 \sigma \leq x \leq 1 + 3 \sigma$. The **enumeration range** of 0.0 → 1.0 is thus correctly interpreted as meaning $0.0 - 3 \sigma \leq x \leq 1.0 + 3 \sigma$.

Appears in list containing **atom_site_label**.

The permitted range is 0.0 → 1.0. Where no value is given, the assumed value is ‘1.0’. **atom_site_label**

- **atom_site_cartn_x**
  
  Atom-site coordinates in Ångström specified according to a set of orthogonal Cartesian axes related to the cell axes as specified by _atom_sites_cartn_transform_axes_ description. The permitted range is 0 ≤ x ≤ 1.0. Where no value is given, the assumed value is ‘1.0’. **atom_site_label**

- **atom_site_cartn_y**
  
  Related item: **atom_site_cartn_z** (alternate).

- **atom_site_cartn_z**
  
  Related item: **atom_site_cartn_x** (alternate).
**atom_site_refinement_flags** (char)
This definition has been superseded and is retained here only for archival purposes. Use instead **atom_site_refinement_flags_adp**, **atom_site_refinement_flags_occupancy**.

A concatenated series of single-letter codes which indicate the refinement restraints or constraints applied to this site. This item should not be used. It has been replaced by **atom_site_refinement_flags_adp** and **atom_site_refinement_flags_occupancy**. It is retained in this dictionary only to provide compatibility with legacy CIFs.

Appears in list containing **atom_site_label**.

The data value must be one of the following:
- no refinement constraints
- special-position constraint on site
- rigid-group refinement of site
- riding-atom site attached to non-riding atom
- distance or angle restraint on site
- thermal displacement constraints
- Uiso or U^1\textsuperscript{1/2} restraint (rigid bond)
- partial occupancy constraint

**atom_site_refinement_flags_adp** (char)
A code which indicates the refinement restraints or constraints applied to the atomic displacement parameters of this site.

Appears in list containing **atom_site_label**.

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

The data value must be one of the following:
- no constraints on atomic displacement parameters
- special-position constraints on atomic displacement parameters
- Uiso or U^1\textsuperscript{1/2} restraint (rigid bond)
- both constraints applied

**atom_site_refinement_flags_occupancy** (char)
A code which indicates that refinement restraints or constraints were applied to the occupancy of this site.

Appears in list containing **atom_site_label**.

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

The data value must be one of the following:
- no constraints on site-occupancy parameters
- site-occupancy constraint

**atom_site_refinement_flags_posn** (char)
A code which indicates the refinement restraints or constraints applied to the positional coordinates of this site.

Appears in list containing **atom_site_label**.

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

The data value must be one of the following:
- no constraints on positional coordinates
- rigid-group refinement of positional coordinates
- riding-atom site attached to non-riding atom
- special-position constraint on positional coordinates
- combination of the above constraints
- combination of the above constraints
- combination of the above constraints
- combination of the above constraints
- combination of the above constraints
- combination of the above constraints
- combination of the above constraints

**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’.

**atom_site_symmetry_multiplicity** (numb)

Appears in list containing **atom_site_label**.

The permitted range is 1 → 192.

**atom_site_thermal_displace_type** (char)
A code to identify 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**.

The data value must be one of the following:
- Uani: anisotropic U\textsuperscript{1/2}
- Uiso: isotropic U
- Uo particulate U\textsuperscript{1/2}
- Uovl: overall U
- Ump: overall U
- Bani: anisotropic B\textsuperscript{1/2}
- Biso: isotropic B
- Boyl: overall B

**atom_site_U_equiv_geom_mean** (numb, su)
Equivalent isotropic atomic displacement parameter, U\textsubscript{eqv}, in ångströms squared, calculated as the geometric mean of the anisotropic atomic displacement parameters.

\[ U_{\text{eqv}} = (U_{\text{ij}})^{1/3} \]

where \( U_{\text{ij}} \) is the principal components of the orthogonalized U\textsuperscript{ij}.

Appears in list containing **atom_site_label**.

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

**atom_site_U_iso_or_equiv** (numb, su)
Isotopic atomic displacement parameter, or equivalent isotropic atomic displacement parameter, U\textsubscript{eqv}, in ångströms squared, calculated from anisotropic atomic displacement parameters.

\[ U_{\text{eqv}} = (1/3) \sum_i \left[ \sum_{j} (U_{ij}A_iA_ja^*_ia^*_j) \right] \]

where A = the real-space cell lengths and a\textsuperscript{*} = the reciprocal-space cell lengths.


Appears in list containing **atom_site_label**.

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

**atomSiteWyckoffSymbol** (char)

Appears in list containing **atom_site_label**.
Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.

Example: "Cartesian orthogonal axes as applied in the transformation matrix A description of the relative alignment of the crystal cell axes to the...

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

Example: "A description of the relative alignment of the crystal cell axes to the Cartesian orthogonal axes as applied in the transformation matrix A description of the relative alignment of the crystal cell axes to the...

Matrix elements used to transform 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 × 1 translation is defined in _atom_sites_Cartn_transform_axes.

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

Elements of a 3 × 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.

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

Codes 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 notdet coordinates were not determined dual dual-space method (Sheldrick et al., 2001) iterative iterative algorithm, e.g. charge flipping (Oszlányi, G. and Sütő, A. (2004). *Acta Cryst. A* 60, 134-141) other a method not included elsewhere in this list
4. DATA DICTIONARIES

_atom_sites_solution_secondary (char)
Codes 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
dispers anomalous-dispersion techniques
isomor isomorphous structure methods
notdet coordinates were not determined
dual dual-space method (Sheldrick et al., 2001)
dual iterative iterative algorithm, e.g. charge flipping [Oszlányi, G.
other a method not included elsewhere in this list

_atom_sites_solution_secondary

_atom_sites_solution_hydrogens (char)
Codes 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
gam anomalous-dispersion techniques
isomor isomorphous structure methods
notdet coordinates were not determined
dual dual-space method (Sheldrick et al., 2001)
dual iterative iterative algorithm, e.g. charge flipping [Oszlányi, G.
other a method not included elsewhere in this list

_atom_sites_solution_hydrogens

_atom_sites_special_details (char)
Additional information about the atomic coordinates not coded elsewhere in the CIF.

_atom_sites_special_details
---

**_atom_type_scat_dispersion_img** (char)
The imaginary and real components of the anomalous-dispersion scattering factor, f'/ and f'', in electrons for this atom type and the radiation given in _diffrn_radiation_wavelength_.

Appears in list containing _atom_type_symbol_. Where no value is given, the assumed value is '0.0'.

**_atom_type_scat_dispersion_source** (char)
Reference to source of real and imaginary dispersion corrections for scattering factors used for this atom type.

Appears in list containing _atom_type_symbol_.

Example: 'International Tables Vol. IV Table 2.3.1'.

**_atom_type_scat_length_neutron** (numb)
The bound coherent scattering length in femtometres for the atom type at the isotopic composition used for the diffraction experiment.

Appears in list containing _atom_type_symbol_. Where no value is given, the assumed value is '0.0'.

**_atom_type_scat_source** (char)
Reference to source of scattering factors or scattering lengths used for this atom type.

Appears in list containing _atom_type_symbol_.

Example: 'International Tables Vol. IV Table 2.4.6B'.

**_atom_type_scat_versus_stol_list** (char)
A table of scattering factors as a function of \(\sin \theta/\lambda\). This table should be well commented to indicate the items present. Regularly formatted lists are strongly recommended.

Appears in list containing _atom_type_symbol_.

**_atom_type_symbol** (char)
The code used to identify the atom species (singular or plural) representing this atom type. Normally this code is the element symbol. The code may be composed of any character except an underscore with the additional proviso that digits designate an oxidation state and must be followed by a + or - character.

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

Examples: 'C', 'Cl2+', 'H(RDS)', 'dummy', 'FeNi'.

---

**AUDIT**

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


---

**_audit_block_code**

A code intended to identify uniquely the current data block.

Example: 'TOZ_1991-03-20'.

---

**_audit_creation_date**

The date that the data block was created. The date format is yyyy-mm-dd.

Example: '1990-07-12'.

---

**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.

---

**_audit_author_address**

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
Street
City and postcode
COUNTRY

---

**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.

---

**_audit_creation_method**

A description of how data were entered into the data block.

Example: 'Spawned by the program QBEE'.

---

**_audit_update_record**

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.

Example: '1990-07-15 Updated by the Co-editor'.
AUDIT_CONFORM

_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]

_audit_conform_dict_version (char)
The version number of the dictionary to which the current data block conforms.
May appear in list containing _audit_conform_dict_name. [audit_conform]

AUDIT_CONTACT_AUTHOR

Data items in the AUDIT_CONTACT_AUTHOR category record details about the name and address of the author to be contacted concerning the contents of this data block.

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

<table>
<thead>
<tr>
<th>loop</th>
<th>audit_contact_author_name</th>
<th>audit_contact_author_address</th>
<th>audit_contact_author_email</th>
<th>audit_contact_author_phone</th>
</tr>
</thead>
<tbody>
<tr>
<td>'Fitzgerald, Paula M. D.'</td>
<td>Department of Biophysical Chemistry</td>
<td>Merck Research Laboratories</td>
<td>PO Box 2000, 8y9M203</td>
<td>New Jersey 07045 USA</td>
</tr>
<tr>
<td>12(34)9477330</td>
<td>'<a href="mailto:paula_fitzgerald@merck.com">paula_fitzgerald@merck.com</a>'</td>
<td>'1(908)5945510'</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>loop</th>
<th>audit_contact_author_name</th>
<th>audit_contact_author_address</th>
<th>audit_contact_author_email</th>
<th>audit_contact_author_phone</th>
</tr>
</thead>
<tbody>
<tr>
<td>'Yang, D.-L.'</td>
<td>'Simonov, Yu.A.'</td>
<td>'uller, H.A.'</td>
<td>'ross II, C.R.'</td>
<td></td>
</tr>
</tbody>
</table>

AUDIT_LINK

Data items in the AUDIT_LINK category record details about the relationships between data blocks in the current CIF.

Example 1 – multiple structure paper, as illustrated in A Guide to CIF for Authors (1995), IUCr: Chester.

<table>
<thead>
<tr>
<th>loop</th>
<th>audit_link_block_code</th>
<th>audit_link_block_description</th>
</tr>
</thead>
<tbody>
<tr>
<td>'publication details'</td>
<td>KSE_MOD 'modulated structure'</td>
<td></td>
</tr>
<tr>
<td>'discursive text of paper with two structures'</td>
<td>KSE_REF 'reference structure'</td>
<td></td>
</tr>
<tr>
<td>'structure 1 of 2'</td>
<td>KSE_COM 'experimental data common to ref./mod. structures'</td>
<td></td>
</tr>
<tr>
<td>'structure 2 of 2'</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>loop</th>
<th>audit_link_block_code</th>
<th>audit_link_block_description</th>
</tr>
</thead>
<tbody>
<tr>
<td>'modulated structure'</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

CELL

Data items in the CELL category record details about the crystallographic cell parameters and their measurement.


<table>
<thead>
<tr>
<th>cell_length_a</th>
<th>cell_length_b</th>
<th>cell_length_c</th>
<th>cell_angle_alpha</th>
<th>cell_angle_beta</th>
<th>cell_angle_gamma</th>
<th>cell_volume</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.959(1)</td>
<td>14.956(1)</td>
<td>19.737(3)</td>
<td>90</td>
<td>90</td>
<td>90</td>
<td>1759.0(3)</td>
</tr>
<tr>
<td>cell_measurement_temperature</td>
<td>cell_measurement_refns_used</td>
<td>cell_measurement_theta_min</td>
<td>cell_measurement_theta_max</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>293</td>
<td>25</td>
<td>25</td>
<td>31</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
4.1. CORE DICTIONARY (CORECIF)

**_cell_angle_alpha_**

**_cell_angle_beta_**

**_cell_angle_gamma_** *(numb, su)*

Unit-cell angles of the reported structure in degrees. The values of _refln_index_h_ , _k_ , _l_ must correspond to the cell defined by these values and _cell_length_a_ , _b_ and _c_. 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_refln_transf_matrix_.

The permitted range is 0.0 → 180.0. Where no value is given, the assumed value is ‘90.0’.

**_cell_formula_units_Z_** *(numb)*

The number of the formula units in the unit cell as specified by _chemical_formula_structural_ , _chemical_formula_moiety_ or _chemical_formula_sum_.

The permitted range is 1 → ∞.

**_cell_length_a_**

**_cell_length_b_**

**_cell_length_c_** *(numb, su)*

Unit-cell lengths in ångströms corresponding to the structure reported. The values of _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_refln_transf_matrix_.

The permitted range is 0.0 → ∞.

**_cell_measurement_pressure_** *(numb, su)*

The pressure in kilopascals at which the unit-cell parameters were measured (not the pressure at which the sample was synthesized).

The permitted range is 0.0 → ∞.

**_cell_measurement_radiation_** *(char)*

Description of the radiation used to measure the unit-cell data. See also _cell_measurement_wavelength_.


**_cell_measurement_reflns_used_** *(numb)*

The total number of reflections used to determine the unit cell. These reflections may be specified as _cell_measurement_refln_data_items_.

**_cell_measurement_temperature_** *(numb, su)*

The temperature in kelvins at which the unit-cell parameters were measured (not the temperature of synthesis).

The permitted range is 0.0 → ∞.

**_cell_measurement_theta_max_**

**_cell_measurement_theta_min_** *(numb)*

The maximum and minimum θ angles of reflections used to measure the unit cell in degrees.

The permitted range is 0.0 → 90.0.

**_cell_measurement_wavelength_** *(numb)*

The wavelength in ångströms of the radiation used to measure the unit cell. If this is not specified, the wavelength is assumed to be the same as that given in _diffrn_radiation_wavelength_.

The permitted range is 0.0 → ∞.

### CELL_MEASUREMENT_REFLN

Data items in the CELL_MEASUREMENT_REFLN category record details about the reflections used in the determination of the crystallographic cell parameters. The _cell_measurement_refln_data_items_ would in general be used only for diffractometer measurements.

Example 1 – extracted from the CAD-4 listing for Rb₂S₂O₆ at room temperature (unpublished).

```plaintext
#---- data truncated for brevity ----
```


The permitted range is 0.0 → 180.0. Where no value is given, the assumed value is ‘90.0’.

**_cell_reciprocal_angle_alpha_**

**_cell_reciprocal_angle_beta_**

**_cell_reciprocal_angle_gamma_** *(numb, su)*

The angles defining the reciprocal cell in degrees. These are related to those in the real cell by

\[
\begin{align*}
\cos \alpha^* &= (\cos \beta \cos \gamma - \cos \alpha)/(\sin \beta \sin \gamma), \\
\cos \beta^* &= (\cos \gamma \cos \alpha - \cos \beta)/(\sin \gamma \sin \alpha), \\
\cos \gamma^* &= (\cos \alpha \cos \beta - \cos \gamma)/(\sin \alpha \sin \beta).
\end{align*}
\]


The permitted range is 0.0 → ∞.

**_cell_reciprocal_length_a_**

**_cell_reciprocal_length_b_**

**_cell_reciprocal_length_c_** *(numb, su)*

The reciprocal-cell lengths in inverse ångströms. These are related to the real cell by

\[
\begin{align*}
\alpha &= b c \sin \alpha/V, \\
\beta &= a c \sin \beta/V, \\
\gamma &= a b \sin \gamma/V,
\end{align*}
\]

where V is the cell volume.


The permitted range is 0.0 → ∞.

**_cell_special_details_** *(char)*

A description of special aspects of the cell choice, noting possible alternative settings.

Examples: ‘pseudo-orthorhombic’, ‘standard setting from 45 deg rotation around c’.

**_cell_volume_** *(numb, su)*

Cell volume V in ångströms cubed.

\[
V = abc(1 - \cos^2 \alpha - \cos^2 \beta - \cos^2 \gamma + 2 \cos \alpha \cos \beta \cos \gamma)^{1/2},
\]

where \(a = _cell_length_a, b = _cell_length_b, c = _cell_length_c, \alpha = _cell_angle_alpha, \beta = _cell_angle_beta\) and \(\gamma = _cell_angle_gamma\).

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

**_chemical_name_common_** (char)
Trivial name by which the compound is commonly known.
Example: '1-bromoestradiol'.

**_chemical_name_mineral_** (char)
Mineral name accepted by the International Mineralogical Association. Use only for natural minerals. See also _chemical_compound_source_.
Example: 'chalcopyrite'.

**_chemical_name_structure_type_** (char)
Commonly used structure-type name. Usually only applied to minerals or inorganic compounds.
Examples: 'perovskite', 'ephalerite', 'A1S'.

**_chemical_name_systematic_** (char)
IUPAC or Chemical Abstracts full name of the compound.
Example: '1-bromoestr-1,3,5(10)-triene-3,17\-b-diol'.

**_chemical_optical_rotation_** (char)
The optical rotation in solution of the compound is specified in the following format:

\[ \alpha^{TEMP}_{D,WAVE} = SORT (c = CONC, SOLV), \]

where TEMP is the temperature of the measurement in degrees Celsius, WAVE is an indication of the wavelength of the light used for the measurement, CONC is the concentration of the solution given as the mass of the substance in g per 100 ml of solution, SORT is the signed value (preceded by a + or a - sign) of 100α/(lc), where α is the signed optical rotation in degrees measured in a cell of length l in dm and c is the value of CONC as defined above, and SOLV is the chemical formula of the solvent.
Example: '[(α)25°]D = +108 (c = 3.42, CHCl3-3').

**_chemical_properties_biological_** (char)
A free-text description of the biological properties of the material.
Examples:
- diverse biological activities including use as a laxative and strong antibacterial activity against S. aureus and weak activity against cyclooxygenase-1 (Cox-1);
- antibiotic activity against Bacillus subtilis (ATCC 6051) but no significant activity against Candida albicans (ATCC 14053), Aspergillus flavus (NRRL 6544) and Fusarium verticillioides (NRRL 6545);
- weakly potent lipoxygenase nonredox inhibitor;
- no influenza A virus sialidase inhibitory and plaque reduction activities;
- low toxicity against Drosophila melanogaster;

**_chemical_properties_physical_** (char)
A free-text description of the physical properties of the material.
Examples: 'air-sensitive, moisture-sensitive, hygroscopic, deliquescent, oxygen-sensitive, photo-sensitive, pyrophoric, semiconductor, ferromagnetic at low temperature, paramagnetic and thermochromic'.

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

**_chemical_temperature_sublimation_** (numb, su)
The temperature in kelvins at which the solid sublimes.
The permitted range is 0 → ∞.
Example: '350'.

**_chemical_temperature_decomposition_alt_** (numb, su)
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).
Example: '350'.

**_chemical_temperature_sublimation_alt_** (numb, su)
The temperature in kelvins below which (*_lt_*) or above which (_gt_) the solid is known to sublime. 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).
Example: '350'.

---

**CHEMICAL_CONN_ATOM**

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_atom_ data items provide information about the chemical properties of the atoms in the structure. In cases where crystallographic and molecular symmetry elements coincide, they must also contain symmetry-generated atoms, so that the _chemical_conn_atom_ and chemical_conn_bond data items will always describe a complete chemical entity.


loop
  _chemical_conn_atom_number
  _chemical_conn_atom_type_symbol
  _chemical_conn_atom_display_x
  _chemical_conn_atom_display_y
  _chemical_conn_atom_MCA
  _chemical_conn_atom_NR
  1 S .39 .81 1 0
  2 S .39 .96 2 0
  3 N .14 .88 3 0
  4 C .33 .88 3 0
  5 C .11 .96 2 2
  6 C .03 .96 2 2
  7 C .03 .96 2 2
  8 C .11 .96 2 2
  9 S .54 .81 1 0
  10 S .54 .96 2 0
  11 N .80 .88 3 0
  12 C .80 .88 3 0
  13 C .80 .96 2 2
decomp
  15 C .91 .80 2 2
  16 C .84 .80 2 2

**_chemical_conn_atom_charge_** (numb)
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 -6 → 6. Where no value is given, the assumed value is '0'.
Examples: '1' (for an ammonium nitrogen), '-1' (for a chloride ion).

Example: '1' (for an ammonium nitrogen), '-1' (for a chloride ion).
CHEMICAL_CONN_ATOM

_chemical_conn_atom_display_x (numb)
The 2D Cartesian coordinates \((x, y)\) of the position of this atom in a recognizable chemical diagram. The coordinate origin is at the lower left corner, the \(x\) axis is horizontal and the \(y\) axis is vertical. The coordinates must lie in the range 0.0 to 1.0. These coordinates can be obtained from projections of a suitable uncluttered view of the molecular structure.

Appears in list containing _chemical_conn_atom_type_symbol.
The permitted range is 0.0 → 1.0. [chemical_conn_atom]

_chemical_conn_atom_NCA (numb)
The number of connected atoms excluding terminal hydrogen atoms.

Appears in list containing _chemical_conn_atom_type_symbol.
The permitted range is 0 → \(\infty\). [chemical_conn_atom]

_chemical_conn_atom_NH (numb)
The total number of hydrogen atoms attached to this atom, regardless of whether they are included in the refinement or the _atom_site_list. This number will be the same as _atom_site_attached_hydrogens only if none of the hydrogen atoms appear in the _atom_site_list.

Appears in list containing _chemical_conn_atom_type_symbol.
The permitted range is 0 → \(\infty\). [chemical_conn_atom]

_chemical_conn_atom_number (numb)
The chemical sequence number to be associated with this atom.

Appears in list containing _chemical_conn_atom_type_symbol. May match child data name(s) _atom_site_chemical_conn_number.

_chemical_conn_bond_atom_1, _chemical_conn_bond_atom_2

The chemical bond type associated with the connection between the two sites _chemical_conn_bond_atom_1 and _chemical_conn_bond_atom_2.

Appears in list containing _chemical_conn_bond_atom.
The data value must be one of the following:
sing single bond
doub double bond
trip triple bond
quad quadruple bond
atom aromatic bond
poly polymeric bond
delo delocalized double bond
pi π bond

Where no value is given, the assumed value is ‘sing’. [chemical_conn_bond]

CHEMICAL_FORMULA

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.


loop
_chemical_conn_bond_atom_1
_chemical_conn_bond_atom_2
_chemical_conn_bond_type
4 1 doub 4 3 sing
4 2 sing 5 3 sing
6 3 sing 7 6 sing
8 7 sing 8 3 sing
10 2 sing 12 9 doub
12 11 sing 12 10 sing
13 11 sing 14 13 sing
14 15 sing 16 15 sing
16 13 sing 17 5 sing
18 5 sing 19 6 sing
20 6 sing 21 7 sing
22 7 sing 23 8 sing
24 8 sing 25 13 sing
26 13 sing 27 14 sing
28 14 sing 29 15 sing
30 15 sing 31 16 sing
32 16 sing


_chemical_formula_sum 'C18 H25 N O3'
_chemical_formula_moiety 'C18 H25 N O3'
_chemical_formula_weight 303.40


_chemical_formula_moiety 'C18 H25 N O3'
_chemical_formula_sum 'C18 H25 N O3'
_chemical_formula_weight 303.40

_chemical_formula_1upac 'Mo [C (O) 4] (C18 H33 P) 2'
_chemical_formula_1upac 'C40 H66 Mo O4 P2'
_chemical_formula_1upac '(C1 O) (P (C6 H11) 3.) 2 Mo'
4.1. CORE DICTIONARY (CORECIF)  

### _chemical_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.\text{.}s.\text{.}d\text{.})

Example: 'Fe2.45(2) Ni1.69(3) S4'. [chemical_formula]

### _chemical_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 _chemical_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 _chemical_formula_data_ names.


Example: 'Co Re (Cl2 H22 P)2 (C O)6].0.5C H3 O H'. [chemical_formula]

### _chemical_formula_moiety_ (char)

Formula with each discrete bonded residue or ion shown as a separate moiety. See the `CHEMICAL_FORMULA` category description for rules for writing chemical formulae. In addition to the general formulae requirements, the following rules apply: (1) Moieties are separated by commas ',', (2) The order of elements within a moiety follows general rule (5) in the `CHEMICAL_FORMULA` category description. (3) Parentheses are not used within moieties but may surround a moiety. Parentheses may not be nested. (4) Charges should be placed at the end of the moiety. The charge '+' or '-' may be preceded by a numerical multiplier and should be separated from the last (element symbol + count) by a space. Pre- or post-multipliers may be used for individual moieties.

Examples: 'C7 H4 Cl 19g N 03 S', 'C12 H17 N4 O S 1-', 'C6 H2 N3 O7 1-', 'C12 H16 N6 O5 (H2 O)1', 'C8 H4 Cl Hg N O3 S 1+, C6 H2 N3 O7 1-'. [chemical_formula]

### _chemical_formula_structural_ (char)

See the `CHEMICAL_FORMULA` category description for the rules for writing chemical formulae for inorganics, organonutrients, metal complexes *etc.*, in which bonded groups are preserved as discrete entities within parentheses, with post-multipliers as required. The order of the elements should give as much information as possible about the chemical structure. Parentheses may be used and nested as required. This formula should correspond to the structure as actually reported, *i.e.* trace elements not included in atom-type and atom-site lists should not be included in this formula (see also _chemical_formula_analytical_).

Examples: 'Ca (|Cl H3)2 O2 (H2 O)4', 'P 1(1) (N H3)2 (C N O3)2 (C1 O4)2'. [chemical_formula]

### _chemical_formula_sum_ (char)

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: 'C18 H19 N7 O8 S'. [chemical_formula]

### _chemical_formula_weight_ (numb)

Formula mass in daltons. This mass should correspond to the formulae given under _chemical_formula_structural_, *iupac_, *moiety* or *sum* find, together with the Z value and cell parameters, should yield the density given as _exptl_crytad_density_.

The permitted range is $1.0 \rightarrow \infty$. [chemical_formula]

### _chemical_formula_weight_meas_ (numb)

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

The permitted range is $1.0 \rightarrow \infty$. [chemical_formula]

### CITATION

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.

```
loop
   _citation_id
   _citation_coordinate_linkage
   _citation_title
   _citation_country
   _citation_page_first
   _citation_page_last
   _citation_year
   _citation_journal_abbr
   _citation_journal_volume
   _citation_journal_issue
   _citation_journal_id_AST
   _citation_journal_id_ISSN
   _citation_book_title
   _citation_book_publisher
   _citation_book_id_ISSN
   _citation_special_details
   primary yes
   citation
   Crystallographic analysis of a complex between human immunodeficiency virus type 1 protease and acetyl-peptatin at 2.0-Angstroms resolution.
   HBCHA3 0021-9258 . . .
   The publication that directly relates to this coordinate set.
   .
   no
   Three-dimensional structure of aspartyl-protease from human immunodeficiency virus HIV-1.
   NATAS 0028-0836 . . .
   Determination of the structure of the unliganded enzyme.
   .
   no
   Crystallization of the aspartylprotease from human immunodeficiency virus, HIV-1.
   HBCHA3 0021-9258 . . .
   Crystallization of the unliganded enzyme.
   .
```

### _citation_abstract_ (char)

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

Appears in list containing _citation_id  [citation]

### _citation_abstract_id_CAS_ (char)

The *Chemical Abstracts* Service (CAS) abstract identifier; relevant for journal articles.

Appears in list containing _citation_id  [citation]

### _citation_book_id_ISSN_ (char)


Appears in list containing _citation_id  [citation]

### _citation_book_publisher_ (char)

The name of the publisher of the citation; relevant for books or book chapters.

Appears in list containing _citation_id  [citation]

### _citation_book_publisher_city_ (char)

The location of the publisher of the citation; relevant for books or book chapters.

Appears in list containing _citation_id  [citation]
4. DATA DICTIONARIES

_citation_book_title

The title of the book in which the citation appeared; relevant for books or book chapters.

Appears in list containing _citation_id

Example: 'Structure of Diferric Duck Ovo transferrin at 2.35 Å Resolution'.

_citation_coordinate_linkage

_abbreviation for 'yes'

_abbreviation for 'no'

The data value must be one of the following:

yes citation related to current coordinates
no abbreviation for 'no'

Appears in list containing _citation_id

_citation_id

The value of _citation_id must uniquely identify a record in the _citation_list. The _citation_id 'primary' should be used to indicate the citation that the author(s) consider to be the most pertinent to the contents of the data block. Note that this item need not be a number; it can be any unique identifier.

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

Example: 'primary', '1', '2', '3'.

_citation_language

Language in which the cited article is written.

Appears in list containing _citation_id

Example: 'German'.

_citation_year

The year of the citation; relevant for journal articles, books and book chapters.

Appears in list containing _citation_id

Example: '1984'.

_citation_journal_full

Full name of the journal cited; relevant for journal articles.

Appears in list containing _citation_id

Example: 'Journal of Molecular Biology'.

_citation_journal_id

_abbreviation for 'yes'

_abbreviation for 'no'

The year of the citation; relevant for journal articles, books and book chapters.

Appears in list containing _citation_id

Example: '1984'.

_citation_journal_id_CSD

The Cambridge Structural Database (CSD) code assigned to the journal cited; relevant for journal articles. This is also the system used at the Protein Data Bank (PDB).

Appears in list containing _citation_id

Example: '0070'.

_citation_journal_id_ISSN

The International Standard Serial Number (ISSN) code assigned to the journal cited; relevant for journal articles.

Appears in list containing _citation_id

Example: '174'.

_citation_journal_issue

Issue number of the journal cited; relevant for journal articles.

Appears in list containing _citation_id

Example: '2'.

_citation_journal_volume

Volume number of the journal cited; relevant for journal articles.

Appears in list containing _citation_id

Example: 'Volume 174'.

_citation_country

The country of publication; relevant for books and book chapters.

Appears in list containing _citation_id

Example: 'LIBRDB'.

_citation_database_id_CSD

Identifier ('recode') of the database record in the Cambridge Structural Database that contains details of the cited structure.

Appears in list containing _citation_id

Example: 'LIBRDB'.

_citation_database_id_Medline

Accession number used by Medline to categorize a specific bibliographic entry.

Appears in list containing _citation_id

The permitted range is 1 → ∞.

Example: '89064067'.

_citation_author_citation_id

Examples: 'primary', '1', '2', '3'.

_citation_editor_citation_id

Used at the Protein Data Bank (PDB).
**CITATION_AUTHOR**

Data items in the CITATION_AUTHOR category record details about the authors associated with the citations in the _citation_list_.

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

<table>
<thead>
<tr>
<th>_citation_author_citation_id</th>
<th>(char)</th>
</tr>
</thead>
<tbody>
<tr>
<td>_citation_author_name</td>
<td>(char)</td>
</tr>
<tr>
<td>_citation_author_ordinal</td>
<td>(char)</td>
</tr>
</tbody>
</table>

The value of _citation_author_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_author]

Name of an author of the citation; relevant for journal articles, 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.


 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.

<table>
<thead>
<tr>
<th>_citation_editor_citation_id</th>
<th>(char)</th>
</tr>
</thead>
<tbody>
<tr>
<td>_citation_editor_name</td>
<td>(char)</td>
</tr>
<tr>
<td>_citation_editor_ordinal</td>
<td>(char)</td>
</tr>
</tbody>
</table>

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 | 'VOBYUG' |
| _database_code_COD | |
| _database_code_MDF | |
| _database_code_ICSD | |
| _database_code_CAS | |
| _database_code_PDB | |
| _database_code_NBS | |
| _database_code_PDF | |

The codes are assigned by databases: Chemical Abstracts; Crystallography Open Database (COD); Cambridge Structural Database
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).

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

_ddatabase_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).

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

_database_CSD_history (char)
A history of changes made by the Cambridge Crystallographic Data Centre and incorporated into the Cambridge Structural Database (CSD).

_database_journal_ASTM_ddatabase_journal_CSD (char)
The ASTM CODEN designator for a journal as given in the Chemical Source List maintained by the Chemical Abstracts Service, and the journal code used in the Cambridge Structural Database.

DIFFRN

Data items in the DIFFRN category record details about the intensity measurements.


_diffrn_special_details
; q scan width (1.00 + 0.14\tan(q))\%/ q scan rate
1.2%/min”^{-1”}. Background counts for 5 s on each side
of every scan.
;
_diffrn_environment

The gas or liquid surrounding the sample, if not air.


_diffrn_pressure

The mean hydrostatic pressure in kilopascals at which the intensities were measured.

The permitted range is 0 \rightarrow \infty.

_diffrn_pressure_gt
_diffrn_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_pressure should always be used in preference to these items whenever possible.

The permitted range is 0 \rightarrow \infty.

_diffrn_temperature

The mean temperature in Kelvins at which the intensities were measured.

The permitted range is 0 \rightarrow \infty.

DIFFRN_ATTENUATOR

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

Example 1 – hypothetical example.

loop_
_diffrn_attenuator_code
_diffrn_attenuator_scale
0 1.00
1 16.97
2 33.89

_diffrn_attenuator_code

A code associated with a particular attenuator setting. This code is referenced by the _diffrn_reflns_attenuator_code which is stored with the intensities. See _diffrn_attenuator_scale.

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

_diffrn_attenuator_material

Material from which the attenuator is made.

Appears in list containing _diffrn_attenuator_code.  

_diffrn_attenuator_scale

The scale factor applied when an intensity measurement is reduced to the same scale as unattenuated intensities. 

Appears in list containing _diffrn_attenuator_code.  

The permitted range is 1.0 \rightarrow \infty.
**DIFFRN_DETECTOR**

Data items in the DIFFRN_DETECTOR category describe the 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:

<table>
<thead>
<tr>
<th>diffrn_detector</th>
<th>'multiwire'</th>
</tr>
</thead>
<tbody>
<tr>
<td>diffrn_detector_type</td>
<td>'Siemens'</td>
</tr>
</tbody>
</table>

**d2frrn_detector**

The general class of the radiation detector.

Related item: _diffrn_radiation_detector (alternate).

Example: 'photographic film', 'scintillation counter', 'CCD plate', 'BF-3' counter'.

<table>
<thead>
<tr>
<th>diffrn_detector_area_resol_mean</th>
<th>(numb)</th>
</tr>
</thead>
<tbody>
<tr>
<td>The resolution of an area detector, in pixels mm(^{-1}).</td>
<td></td>
</tr>
<tr>
<td>The permitted range is 0 (\rightarrow) (\infty).</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>diffrn_detector_details</th>
<th>(char)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A description of special aspects of the radiation detector.</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>diffrn_detector_dtime</th>
<th>(numb)</th>
</tr>
</thead>
<tbody>
<tr>
<td>The deadtime in microseconds of the detector used to measure the diffraction intensities.</td>
<td></td>
</tr>
<tr>
<td>The permitted range is 0 (\rightarrow) (\infty).</td>
<td></td>
</tr>
</tbody>
</table>

Related item: _diffrn_radiation_detector_dtime (alternate).

**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>diffrn_measurement_device_type</th>
<th>'Philips PW1100/20 diffractometer'</th>
</tr>
</thead>
<tbody>
<tr>
<td>diffrn_measurement_method</td>
<td>(\langle q/2q \rangle) scans.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>diffrn_measurement_details</th>
<th>(char)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A description of special aspects of the intensity measurement.</td>
<td></td>
</tr>
<tr>
<td>Example: 440 frames of 0.25%</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>diffrn_measurement_device</th>
<th>(char)</th>
</tr>
</thead>
<tbody>
<tr>
<td>The general class of goniometer or device used to support and orient the specimen.</td>
<td></td>
</tr>
<tr>
<td>Examples: 'three-circle diffractometer', 'four-circle diffractometer', '(\langle k \rangle)-geometry diffractometer', 'oscillation camera', 'precession camera'.</td>
<td></td>
</tr>
</tbody>
</table>

**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.


<table>
<thead>
<tr>
<th>diffrn_orient_matrix UB_11</th>
<th>-0.04170</th>
</tr>
</thead>
<tbody>
<tr>
<td>diffrn_orient_matrix UB_12</td>
<td>-0.01429</td>
</tr>
<tr>
<td>diffrn_orient_matrix UB_13</td>
<td>-0.02226</td>
</tr>
<tr>
<td>diffrn_orient_matrix UB_21</td>
<td>-0.00380</td>
</tr>
<tr>
<td>diffrn_orient_matrix UB_22</td>
<td>-0.05578</td>
</tr>
<tr>
<td>diffrn_orient_matrix UB_23</td>
<td>-0.05681</td>
</tr>
<tr>
<td>diffrn_orient_matrix UB_31</td>
<td>0.00587</td>
</tr>
<tr>
<td>diffrn_orient_matrix UB_32</td>
<td>-0.13766</td>
</tr>
<tr>
<td>diffrn_orient_matrix UB_33</td>
<td>0.02277</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>diffrn_orient_matrix_type</th>
<th>'TEXSAN convention (MSC, 1989)'</th>
</tr>
</thead>
</table>

**d2frrn_orient_matrix_type**

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.

<table>
<thead>
<tr>
<th>diffrn_orient_matrix UB_11</th>
</tr>
</thead>
<tbody>
<tr>
<td>diffrn_orient_matrix UB_12</td>
</tr>
<tr>
<td>diffrn_orient_matrix UB_13</td>
</tr>
<tr>
<td>diffrn_orient_matrix UB_21</td>
</tr>
<tr>
<td>diffrn_orient_matrix UB_22</td>
</tr>
<tr>
<td>diffrn_orient_matrix UB_23</td>
</tr>
<tr>
<td>diffrn_orient_matrix UB_31</td>
</tr>
<tr>
<td>diffrn_orient_matrix UB_32</td>
</tr>
<tr>
<td>diffrn_orient_matrix UB_33</td>
</tr>
<tr>
<td>The elements of the diffractometer orientation matrix. These define the dimensions of the reciprocal cell and its orientation to the local diffractometer axes. See _diffrn_orient_matrix_type.</td>
</tr>
</tbody>
</table>
DIFFRN_ORIENTATION

Data items in the DIFFRN_ORIENTATION 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.

```
loop
  _diffrn_orientation_refl_index_h
  _diffrn_orientation_refl_index_k
  _diffrn_orientation_refl_index_l
  _diffrn_orientation_refl_angle_theta
  _diffrn_orientation_refl_angle_phi
  _diffrn_orientation_refl_angle_omega
  _diffrn_orientation_refl_angle_kappa
-3 2 3 7.35 44.74 2.62 17.53
-4 1 0 5.26 83.27 8.06 5.79
  2 0 6 5.85 -43.93 -25.36 86.20
  2 1 3 7.36 -57.87 6.26 5.42
  0 0 -6 5.85 -161.59 36.96 -86.79
-3 1 0 6.74 80.28 5.87 2.60
  2 0 3 5.86 -76.86 -0.17 21.34
  0 0 12 11.78 -44.02 -19.51 86.41
  0 0 -12 11.78 -161.67 42.81 -86.61
-5 1 0 11.75 86.24 9.16 7.44
  4 6 12 11.82 -19.82 10.45 4.13
  5 0 6 14.13 -77.28 10.17 15.34
  8 0 0 20.79 -77.08 25.30 -13.96
```

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.


```
_diffrn_radiation_type 'Cu Kα'
_diffrn_radiation_monochromator 'graphite'
```

DIFFRN_RADIATION_WAVELENGTH

Data items in the DIFFRN_RADIATION_WAVELENGTH category describe the wavelength of the radiation used in measuring the diffraction intensities. Items may be looped to identify and assign weights to distinct wavelength components from a polychromatic beam.


```
_diffrn_radiation_wavelength 1.5418
```
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_REFLN data items specify the parameters that apply to all intensity measurements. The DIFFRN_REFLN data items are not looped.)

Example 1 — extracted from the CAD-4 listing for Tl2Cd2(SO4)3 at 85 K (unpublished).

loop
  _diffrn_refln_index_h
  _diffrn_refln_index_k
  _diffrn_refln_index_l
  _diffrn_refln_angle_ch
  _diffrn_refln_angle_kappa
  _diffrn_refln_angle_omega
  _diffrn_refln_angle_phi
  _diffrn_refln_angle_psi
  _diffrn_refln_angle_theta
  _diffrn_refln_counts_bg_1
  _diffrn_refln_counts_bg_2
  _diffrn_refln_counts_total
  _diffrn_refln_counts_peak
  _diffrn_refln_detector_slit_horiz
  _diffrn_refln_detector_slit_vert
  _diffrn_refln_transf_matrix
  _diffrn_refln_intensity_net

# - - - data truncated for brevity - - -
3 4 -4 1.03 95 459 73 30.72 .53.744 46.543 .47.552 1.516 2082.58
3 4 -5 1.03 101 95 75 31.407 .54.811 45.519 .42.705 1.516 2084.07
3 4 -6 1.03 95 459 73 30.72 .53.744 46.543 .47.552 1.516 2085.57
0 0 -16 0.412 28 127 36 .33.157 .75.846 .16.404
0 0 -15 0.412 38 143 28 .30.847 .75.846 .14.094
0 0 -14 2.03 142 742 130 .28.592 .75.846 .11.839
0 0 -13 0.412 12 26 137 37 .26.384 .75.846 .9.631
0 0 -12 0.412 12 26 137 37 .26.384 .75.846 .9.631
0 0 -11 0.412 33 107 38 .22.087 .75.846 .5.334
0 0 -10 0.412 37 146 33 .29.989 .75.846 .3.235
0 0 -9 0.412 10 32 137 37 .26.384 .75.846 .1.164
0 0 -8 0.412 12 26 137 37 .26.384 .75.846 .1.164
0 0 -7 0.412 40 169 19 .17.918 .75.846 .1.164
0 0 -6 0.412 28 127 36 .33.157 .75.846 .16.404
DIFFRN_REFLN

_**DIFFRN_REFLN**_

4. DATA DICTIONARIES

**_diffrn_refl_intensity_sigma_** *(numb)*

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

Standard uncertainty (e.s.d.) of the net intensity calculated from the diffraction counts after the attenuator and standard scales have been applied.

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

**_diffrn_refl_intensity_u_** *(numb)*

Standard uncertainty of the net intensity calculated from the diffraction counts after the attenuator and standard scales have been applied.

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

**_diffrn_refl_scale_group_code_** *(char)*

The code identifying the scale applicable to this reflection. This code must match with a specified _diffrn_scale_group_code_ value.

Appears in list containing _diffrn_refl_index_. Must match parent data name _diffrn_scale_group_code_.

**_diffrn_refl_scan_mode_** *(char)*

The code identifying the mode of scanning for measurements using a diffractometer. See _diffrn_refl_scan_width_ and _diffrn_refl_scan_mode_backgd_.

Appears in list containing _diffrn_refl_index_.
The data value must be one of the following:

- _om_ scan
- _ω_ scan
- _Q_ scans (arbitrary reciprocal directions)

**_diffrn_refl_scan_mode_backgd_** *(char)*

The code identifying the mode of scanning a reflection to measure the background intensity.

Appears in list containing _diffrn_refl_index_.
The data value must be one of the following:

- _nt_ stationary counter background
- _mo_ moving counter background

**_diffrn_refl_scan_rate_** *(numb)*

The rate of scanning a reflection in degrees per minute to measure the intensity.

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

**_diffrn_refl_scan_time_backgd_** *(numb)*

The time spent measuring each background in seconds.

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

**_diffrn_refl_scan_width_** *(numb)*

The scan width in degrees of the scan mode defined by the code _diffrn_refl_scan_mode_.

Appears in list containing _diffrn_refl_index_.
The permitted range is $0.0 \rightarrow 90.0$.

**_diffrn_refl_sint/lambda_** *(numb)*

The $(\sin \theta)/\lambda$ value in reciprocal angstroms for this reflection.

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

**_diffrn_refl_standard_code_** *(char)*

A code indicating that this reflection was measured as a standard reflection. The value must be ‘S’ or match one of the _diffrn_standard_code_ values.

Appears in list containing _diffrn_refl_index_. Must match parent data name _diffrn_standard_code_.


**_diffrn_refl_wavelength_** *(numb)*

The mean wavelength in angstroms of the radiation used to measure the intensity of this reflection. This is an important parameter for reflections measured using energy-dispersive detectors or the Laue method.

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

**_diffrn_refl_wavelength_id_** *(char)*

Code identifying the wavelength in the _diffrn_radiation_ list.

Appears in list containing _diffrn_refl_index_. Must match parent data name _diffrn_radiation_wavelength_id_.

Examples: ’x1’, ’x2’, ’nut’.

**_diffrn_refls_theta_full_** *(numb)*

The maximum allowed difference between the _diffrn_refls_theta_min_ and _diffrn_refls_theta_max_ values.

**_diffrn_refls_Laue_measured_fraction_full_** *(numb)*

The measured fraction of all reflections that have been measured.

**_diffrn_refls_theta_min_** *(numb)*

The minimum value given in _diffrn_refls_theta_full_.

**_diffrn_refls_theta_max_** *(numb)*

The maximum value given in _diffrn_refls_theta_full_.

**_diffrn_refls_limit_h_min_** *(numb)*

The minimum allowed value given in _diffrn_refls_limit_h_max_.

**_diffrn_refls_limit_h_max_** *(numb)*

The maximum allowed value given in _diffrn_refls_limit_h_min_.

**_diffrn_refls_limit_k_min_** *(numb)*

The minimum allowed value given in _diffrn_refls_limit_k_max_.

**_diffrn_refls_limit_k_max_** *(numb)*

The maximum allowed value given in _diffrn_refls_limit_k_min_.

**_diffrn_refls_limit_l_min_** *(numb)*

The minimum allowed value given in _diffrn_refls_limit_l_max_.

**_diffrn_refls_limit_l_max_** *(numb)*

The maximum allowed value given in _diffrn_refls_limit_l_min_.

**_diffrn_refls_av_unetI/netI_** *(numb)*

The standard uncertainty of the net intensity calculated from the diffraction counts after the attenuator and standard scales have been applied.

**_diffrn_refls_av_R_equivalents_** *(numb)*

The residual $[\sum |I(\Delta I)/\|I\|]$, for symmetry-equivalent reflections used to calculate the average intensity $\bar{I}$. The $\bar{I}/\|I\|$ term is the average absolute difference between $\bar{I}$ and the individual symmetry-equivalent intensities.

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

**_diffrn_refls_av_split_R_equivalents_** *(numb)*

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

Measure $\sum |I(\Delta I)/\|I\|\|$ for all measured reflections.

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

**_diffrn_refls㋡__split_R_equivalents_** *(numb)*

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

Measure $\sum |I(\Delta I)/\|I\|\|$ for all measured reflections.

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

**_diffrn_refls_av_sigmaI/netI_** *(numb)*

The standard deviation of the net intensity calculated from the diffraction counts after the attenuator and standard scales have been applied.

**_diffrn_refls_av_R_equivalents_** *(numb)*

The residual $[\sum |I(\Delta I)/\|I\|]$, for symmetry-equivalent reflections used to calculate the average intensity $\bar{I}$. The $\bar{I}/\|I\|$ term is the average absolute difference between $\bar{I}$ and the individual symmetry-equivalent intensities.

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

**_diffrn_refls_av_sigmaI/netI_** *(numb)*

The standard deviation of the net intensity calculated from the diffraction counts after the attenuator and standard scales have been applied.

**_diffrn_refls_theta_min_** *(numb)*

The minimum value given in _diffrn_refls_theta_full_.

**_diffrn_refls_theta_max_** *(numb)*

The maximum value given in _diffrn_refls_theta_full_.

**_diffrn_refls_measured_fraction_theta_full_** *(numb)*

The measured fraction of the diffraction pattern that is essentially complete.


<table>
<thead>
<tr>
<th>Data item</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><em>diffrn_refls_number</em></td>
<td>1592</td>
</tr>
<tr>
<td><em>diffrn_refls_av_R_equivalents</em></td>
<td>0</td>
</tr>
<tr>
<td><em>diffrn_refls_av_unetI/netI</em></td>
<td>0.27</td>
</tr>
<tr>
<td><em>diffrn_refls_limit_h_min</em></td>
<td>0</td>
</tr>
<tr>
<td><em>diffrn_refls_limit_h_max</em></td>
<td>6</td>
</tr>
<tr>
<td><em>diffrn_refls_limit_k_min</em></td>
<td>-17</td>
</tr>
<tr>
<td><em>diffrn_refls_limit_k_max</em></td>
<td>0</td>
</tr>
<tr>
<td><em>diffrn_refls_limit_l_min</em></td>
<td>0</td>
</tr>
<tr>
<td><em>diffrn_refls_limit_l_max</em></td>
<td>22</td>
</tr>
<tr>
<td><em>diffrn_refls_theta_min</em></td>
<td>3.71</td>
</tr>
<tr>
<td><em>diffrn_refls_theta_max</em></td>
<td>61.97</td>
</tr>
</tbody>
</table>

**_diffrn_refls_theta_full_** *(numb)*

The measured fraction of reflections measured in the part of the diffraction pattern that is essentially complete.

The permitted range is $0.95 \rightarrow 1.0$.

**_diffrn_refls_fractional_fraction_theta_full_** *(numb)*

The fractional measured fraction of reflections measured in the part of the diffraction pattern that is essentially complete.

The permitted range is $0.00 \rightarrow 1.00$.

**_diffrn_refls_Laue_measured_fraction_full_** *(numb)*

The measured fraction of reflections measured in the part of the diffraction pattern that is essentially complete.

The permitted range is $0.00 \rightarrow 1.00$.

**_diffrn_refls_Laue_fractional_fraction_theta_full_** *(numb)*

The fractional measured fraction of reflections measured in the part of the diffraction pattern that is essentially complete.

The permitted range is $0.00 \rightarrow 1.00$.
4.1. CORE DICTIONARY (CORECIF)

**DIFFRN_REFLNS_CLASS**

**_diffrn_reflns_Laue_measured_fraction_max_** (numb)

Fraction of Laue unique reflections (symmetry-independent in the Laue group) measured out to the resolution given in _diffrn_reflns_resolution_max or _diffrn_reflns_theta_max. The Laue group always contains a centre of symmetry so that the reflection \(h, k, l\) is always equivalent to the reflection \(-h, -k, -l\) even in space groups without a centre of symmetry.

The permitted range is \(0 \rightarrow 1.0\).

Related item: _diffrn_measured_fraction_theta_max (alternate).

**_diffrn_reflns_limit_h_max_**

**_diffrn_reflns_limit_h_min_**

**_diffrn_reflns_limit_k_max_**

**_diffrn_reflns_limit_k_min_**

**_diffrn_reflns_limit_l_max_**

**_diffrn_reflns_limit_l_min_** (numb)

The limits on the Miller indices of the intensities specified by _diffrn_refln_index_h, *_k, *_l_.

**_diffrn_reflns_number_** (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 \(0 \rightarrow \infty\).

**_diffrn_reflns_point_group_measured_fraction_full_** (numb)

Fraction of crystal point-group unique reflections (i.e., symmetry-independent in the crystal point group) measured out to the resolution given in _diffrn_reflns_resolution_full or _diffrn_reflns_theta_full. For space groups that do not contain a centre of symmetry the reflections \(h, k, l\) and \(-h, -k, -l\) are independent. This number should not be less than 0.95, since it represents the fraction of reflections measured in the part of the diffraction pattern that is essentially complete.

The permitted range is \(0.95 \rightarrow 1.0\).

Related item: _diffrn_measured_fraction_theta_full (alternate).

**_diffrn_reflns_reduction_process_** (char)

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

Example: ‘data averaged using Fisher test’.

**_diffrn_reflns_resolution_full_** (numb)

The resolution in reciprocal Ångströms at which the measured reflecttion count is close to complete. The fraction of unique reflections measured out to this angle is given by _diffrn_measured_fraction_theta_full.

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

Related item: _diffrn_reflns_theta_full (alternate).

**_diffrn_reflns_resolution_max_** (numb)

Maximum resolution in reciprocal Ångströms of the measured diffraction pattern. The fraction of unique reflections measured out to this angle is given by _diffrn_measured_fraction_theta_max.

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

Related item: _diffrn_reflns_theta_max (alternate).

**_diffrn_reflns_theta_full_** (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 _diffrn_measured_fraction_theta_full.

The permitted range is \(0.0 \rightarrow 90.0\).

**_diffrn_reflns_theta_max_** (numb)

Maximum \(\theta\) angle in degrees for the measured intensities. The fraction of unique reflections measured out to this angle is given by _diffrn_measured_fraction_theta_max.

The permitted range is \(0.0 \rightarrow 90.0\).

**_diffrn_reflns_transf_matrix_11_**

**_diffrn_reflns_transf_matrix_12_**

**_diffrn_reflns_transf_matrix_13_**

**_diffrn_reflns_transf_matrix_21_**

**_diffrn_reflns_transf_matrix_22_**

**_diffrn_reflns_transf_matrix_23_**

**_diffrn_reflns_transf_matrix_31_**

**_diffrn_reflns_transf_matrix_32_**

**_diffrn_reflns_transf_matrix_33_** (numb)

Elements of the matrix used to transform the diffraction reflection indices _diffrn_refln_index_h, *_k, *_l_ into the _refln_index_h, *_k, *_l_ indices.

\[
\begin{pmatrix}
11 & 12 & 13 \\
21 & 22 & 23 \\
31 & 32 & 33
\end{pmatrix}
= \begin{pmatrix}
h & k & l \\
h' & k' & l'
\end{pmatrix}.
\]

**DIFFRN_REFLNS_CLASS**

Data items in the DIFFRN_REFLNS_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.

\[
\begin{align*}
\text{loop} & : \_\text{diffrn_reflns_class_number} \\
& : \_\text{diffrn_reflns_class_d_res_low} \\
& : \_\text{diffrn_reflns_class_d_res_high} \\
& : \_\text{diffrn_reflns_class_avg_R_eq} \\
& : \_\text{diffrn_reflns_class_av_R} \\
& : \_\text{diffrn_reflns_class_code} \\
& : \_\text{diffrn_reflns_class_description} \\
& : 1580 0.551 6.136 0.015 'Main' 'main reflections' \\
& : 1045 0.551 6.136 0.010 'Satl' 'swl, first-order satellites'
\end{align*}
\]

**_diffrn_reflns_class_av_R_eq_** (numb)

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

Appears in list containing _diffrn_reflns_class_code.

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

**_diffrn_reflns_class_av_R_** (numb)

This definition has been superseded and is retained here only for archival purposes. Use instead _diffrn_reflns_class_av_ul/1_.

Measure \(\sum |u(\text{net})|/\sum |\text{net}|\) for all measured intensities in a reflection class.

Appears in list containing _diffrn_reflns_class_code.

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

4. DATA DICTIONARIES

diffreflns_class_av_uI/I (numb)
Measure $\frac{\sum |a|}{\sum |I|}$ for all measured intensities in a reflection class.
Appears in list containing **diffreflns_class_code**.
The permitted range is 0 → ∞.
Related item: **diffreflns_class_av_sgI/I** (alternate).

**diffreflns_class_code** (char)
The code identifying a certain reflection class.
Appears in list as an essential element of loop structure. May match child data name(s):

Example: 'l', 'm1', 'm2'.

**diffreflns_class_d_res_high** (numb)
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 **diffreflns_class_code**.
The permitted range is 0 → ∞.

**diffreflns_class_d_res_low** (numb)
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 **diffreflns_class_code**.
The permitted range is 0 → ∞.

**diffreflns_class_description** (char)
Description of each reflection class.
Appears in list containing **diffreflns_class_code**.
Examples: 'm1' first order satellites', '400 common projection reflections'.

**diffreflns_class_number** (numb)
The total number of measured intensities for each reflection class, excluding the systematic absences arising from centring translations.
Appears in list containing **diffreflns_class_code**.
The permitted range is 0 → ∞.

**DIFFRN_SCALE_GROUP**

Data items in the DIFFRN_SCALE_GROUP category record details 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.

```
loop
diffscale_group_code
diffscale_group_scale_I_net
1 1.36473
2 1.0654
```

**diffscale_group_code** (char)
The code identifying a specific measurement group (e.g. for multi-film or multi-crystal data). The code must match a **diffreflns_group_scale_group_code** in the reflection list.
Appears in list as an essential element of loop structure. May match child data name(s):

Example: 'l', 'm1', 'm2', 'A', 'B', 'c1', 'c2', 'c3'.

**diffscale_group_scale_I_net** (numb)
The scale for a specific measurement group which is to be multiplied with the net intensity to place all intensities in the **diffreflns_scale_group_code** on a common scale.
Appears in list containing **diffscale_group_code**.
The permitted range is 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 results of the analysis of the standard reflections.


<table>
<thead>
<tr>
<th>_diffrn_standard_refln_index_h</th>
<th>_diffrn_standard_refln_index_k</th>
<th>_diffrn_standard_refln_index_l</th>
</tr>
</thead>
<tbody>
<tr>
<td>3 2 4</td>
<td>1 9 1</td>
<td>3 0 10</td>
</tr>
</tbody>
</table>

**_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_standard_code in the DIFFRN list.

Appears in list containing _diffrn_standard_refln_index_. May match child data name(s) _diffrn_standard_code. Examples: ‘h1’, ‘h2’, ‘h3’, ‘h4’, ‘k1’, ‘k2’. [diffrn_standard_refln]

**_diffrn_standard_refln_index_h** (numb)

Miller indices of standard reflections used in the diffraction measurement process.

Appears in list as essential element of loop structure. [diffrn_standard_refln]

**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.


<table>
<thead>
<tr>
<th>_diffrn_standards_number</th>
<th>_diffrn_standards_interval_time</th>
<th><em>diffrn_standards_decay</em>%</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>120</td>
<td>0</td>
</tr>
</tbody>
</table>

**_diffrn_standards_decay_%** (numb, su)

The percentage decrease in the mean intensity of the set of standard reflections measured at the start of the measurement process and at the finish. 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. If no measurable decay has occurred, the standard uncertainty should be quoted to indicate the maximum possible value the decay might have. A range of 3 standard uncertainties is considered possible. Thus 0.0(1) would indicate a decay of less than 0.3% or an enhancement of less than 0.3%. The permitted range is $-\infty$ to $100$.

Examples: ‘0.5(1)’ (represents a decay between 0.2% and 0.8%), ‘1.1(1)’ (the change in the standards lies between a decay of 2% and an increase of 4%), ‘0.0(2)’ (the change in the standards lies between a decay of 0.6% and an increase of 0.6%).

**_diffrn_standards_interval_count**

The number of reflection intensities, or the time in minutes, between the measurement of standard reflection intensities.

The permitted range is $0$ to $\infty$. [diffrn_standards]

**_diffrn_standards_interval_time** (numb)

The number of reflection intensities, or the time in minutes, between the measurement of standard reflection intensities.

The permitted range is $0$ to $\infty$. [diffrn_standards]

**_diffrn_standards_number** (numb)

The number of unique standard reflections used during the measurement of the diffraction intensities.

The permitted range is $0$ to $\infty$. [diffrn_standards]

**_diffrn_standards_scale_u**

The standard uncertainty (e.s.d.) of the individual mean standard scales applied to the intensity data.

The permitted range is $0$ to $\infty$. [diffrn_standards]

**_diffrn_standards_scale_sigma**

The standard uncertainty (e.s.d.) of the individual mean standard scales applied to the intensity data.

The permitted range is $0$ to $\infty$. [diffrn_standards]

**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.


<table>
<thead>
<tr>
<th>_exptl_absorpt_coefficient_mu</th>
<th>_exptl_absorpt_correction_type</th>
<th>_exptl_absorpt_process_details</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.962</td>
<td>psi-scan</td>
<td>‘North, Phillips &amp; Mathews (1968)’</td>
</tr>
<tr>
<td>0.929</td>
<td>psi-scan</td>
<td>‘North, Phillips &amp; Mathews (1968)’</td>
</tr>
<tr>
<td>0.997</td>
<td>psi-scan</td>
<td>‘North, Phillips &amp; Mathews (1968)’</td>
</tr>
</tbody>
</table>

**_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 $0$ to $\infty$. [exptl]

**_exptl_absorpt_correction_type**

The absorption-correction type and method. The value ‘empirical’ should 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_process_details**

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


**_exptl_crystals_number**

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

The permitted range is $1$ to $\infty$. [exptl]
The data value must be one of the following:

- Related item: _exptl_crystal_colour
  - Given by the combination of _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:

- light
- dark
- whitish
- blackish
- grayish
- brownish
- reddish
- pinkish
- orangish
- yellowish
- greenish
- bluish
- (alternate).

The permitted range is 0 → ∞.

The calculated maximum value of the transmission factor for the specimen. Its value does not include the effects of absorption in the specimen mount. The presence of this item does not imply that the structure factors have been corrected for absorption. The applied correction should be given by _exptl_absorpt_correction_T_max.

The permitted range is 0.0 → 1.0.

The calculated minimum value of the transmission factor for the specimen. Its value does not include the effects of absorption in the specimen mount. The presence of this item does not imply that the structure factors have been corrected for absorption. The applied correction should be given by _exptl_absorpt_correction_T_min.

The permitted range is 0.0 → 1.0.

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


- Related items: _exptl_crystal_density_meas, _exptl_crystal_density_method, _exptl_crystal_density_diffrn
- The units are megagrams per cubic metre (grams per cubic centimetre).

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

- Related items: _exptl_crystal_density_meas

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

The colour of the crystal.

May appear in list containing _exptl_crystal_id

Examples: 'dark green'.

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

The permitted range is 0.0 → ∞.

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

Related item: _exptl_crystal_density_meas (alternate).

The data value must be one of the following:

- colourless
- white
- black
- gray
- brown
- red
- pink
- orange
- yellow
- green
- blue
- violet
- (alternate).

The permitted range is 0.0 → ∞.

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

Related item: _exptl_crystal_density_meas (alternate).

The data value must be one of the following:

- metallic
- dull
- clear

The permitted range is 0.0 → ∞.

Example: '2.5' (lower limit for the density (only the range within which the density lies was given in the original paper)).

The value above which the density measured using standard chemical and physical methods lies. The units are megagrams per cubic metre (grams per cubic centimetre).

May appear in list containing _exptl_crystal_id

Related item: _exptl_crystal_density_meas (alternate).

Example: '2.5' (lower limit for the density (only the range within which the density lies was given in the original paper)).
4.1. CORE DICTIONARY (CORECIF)

**_exptl_crystal_density_meas_lt_** *(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 → ∞.

Related item: _exptl_crystal_density_meas_ (alternate).

Examples: '1.0' (specimen floats in water), '5.0' (upper limit for the density (only the range within which the density lies was given in the original paper)).

**_exptl_crystal_density_meas_temp_** *(numb, sir)*
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 → ∞.

**_exptl_crystal_density_meas_temp_gt_** *(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 stored in databases or archives which would be misleading if reported under _exptl_crystal_density_meas_temp_.

May appear in list containing _exptl_crystal_id_.
The permitted range is 0.0 → ∞.

Related item: _exptl_crystal_density_meas_temp_ (alternate).

**_exptl_crystal_pressure_history_** *(char)*
Relevant details concerning the pressure history of the sample.

May appear in list containing _exptl_crystal_id_.

**_exptl_crystal_recrystallization_method_** *(char)*
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_size_length_** *(numb)*
The maximum, medial and minimum dimensions in millimetres of the crystal. If the crystal is a sphere, then the *rad* item is its radius. If the crystal is a cylinder, then the *length* item is its length. These may appear in a list with _exptl_crystal_id_ if multiple crystals are used in the experiment.

**_exptl_crystal_size_max_** *(numb)*
**_exptl_crystal_size_mid_** *(numb)*
**_exptl_crystal_size_min_** *(numb)*
**_exptl_crystal_size_rad_** *(numb)*

**_exptl_crystal_size_face_** *(char)*
The method used to measure 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_description_** *(char)*
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_.

Example: 'Flotation in aqueous KI, not measured', 'Berman density torsion balance'.

**_exptl_crystal_thermal_history_** *(char)*
Relevant details concerning the thermal history of the sample.

May appear in list containing _exptl_crystal_id_.

**_exptl_crystal_id_** *(char)*
Code identifying each crystal if multiple crystals are used. It is used to link with _diffrn_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): _diffrn_refln_crystal_id_, _refln_crystal_id_.

**_exptl_crystal_F_000_** *(numb)*
The effective number of electrons in the crystal unit cell contributing to $F(000)$. This may contain dispersion contributions and is calculated as

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

where $f_r = \text{real part of the scattering factors at } \theta = 0^\circ$, $f_i = \text{imaginary part of the scattering factors at } \theta = 0^\circ$ and the sum is taken over each atom in the unit cell.

May appear in list containing _exptl_crystal_id_.
The permitted range is 0.0 → ∞.
EXPTL.CRYSTAL

EXPTL.CRYSTAL_FACE

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


<table>
<thead>
<tr>
<th>loop</th>
<th>exptl_crystal_face_index_b</th>
<th>exptl_crystal_face_index_k</th>
<th>exptl_crystal_face_index_l</th>
<th>exptl_crystal_face_perp_dist</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>-2</td>
<td>0</td>
<td>1.10274</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>0</td>
<td>-2</td>
<td>1.17971</td>
</tr>
<tr>
<td>-1</td>
<td>0</td>
<td>1</td>
<td>-2</td>
<td>0.17845</td>
</tr>
<tr>
<td>-2</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>1.16849</td>
</tr>
<tr>
<td>-2</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>1.36065</td>
</tr>
<tr>
<td>-1</td>
<td>1</td>
<td>2</td>
<td>0</td>
<td>0.16888</td>
</tr>
<tr>
<td>0</td>
<td>1</td>
<td>2</td>
<td>1</td>
<td>0.12066</td>
</tr>
</tbody>
</table>

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_.

geom_special_details (char)
The description of geometrical information not covered by the existing data names in the geometry categories, such as least-squares planes.

GEOM

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


<table>
<thead>
<tr>
<th>loop</th>
<th>geom_angle_atom_site_label_1</th>
<th>geom_angle_atom_site_label_2</th>
<th>geom_angle_atom_site_label_3</th>
<th>geom_angle</th>
<th>geom_angle_site_symmetry_1</th>
<th>geom_angle_site_symmetry_2</th>
<th>geom_angle_site_symmetry_3</th>
<th>geom_angle_publ_flag</th>
</tr>
</thead>
<tbody>
<tr>
<td>C2</td>
<td>C1</td>
<td>C5</td>
<td>112.6(2)</td>
<td>1.555</td>
<td>1.555</td>
<td>1.555</td>
<td>yes</td>
<td></td>
</tr>
<tr>
<td>C3</td>
<td>C2</td>
<td>C3</td>
<td>110.9(2)</td>
<td>1.555</td>
<td>1.555</td>
<td>1.555</td>
<td>yes</td>
<td></td>
</tr>
<tr>
<td>O21</td>
<td>C3</td>
<td>C2</td>
<td>127.0(3)</td>
<td>1.555</td>
<td>1.555</td>
<td>1.555</td>
<td>yes</td>
<td></td>
</tr>
<tr>
<td>O1</td>
<td>C2</td>
<td>O21</td>
<td>122.2(3)</td>
<td>1.555</td>
<td>1.555</td>
<td>1.555</td>
<td>yes</td>
<td></td>
</tr>
<tr>
<td>C3</td>
<td>C2</td>
<td>G21</td>
<td>127.0(3)</td>
<td>1.555</td>
<td>1.555</td>
<td>1.555</td>
<td>yes</td>
<td></td>
</tr>
<tr>
<td>C2</td>
<td>C3</td>
<td>H4</td>
<td>101.3(2)</td>
<td>1.555</td>
<td>1.555</td>
<td>1.555</td>
<td>yes</td>
<td></td>
</tr>
<tr>
<td>C2</td>
<td>C3</td>
<td>C11</td>
<td>111.3(2)</td>
<td>1.555</td>
<td>1.555</td>
<td>1.555</td>
<td>yes</td>
<td></td>
</tr>
<tr>
<td>C3</td>
<td>C3</td>
<td>C11</td>
<td>111.3(2)</td>
<td>1.555</td>
<td>1.555</td>
<td>1.555</td>
<td>yes</td>
<td></td>
</tr>
</tbody>
</table>

Angle in degrees defined by the three sites geom_angle_atom_site_label_1, _2 and _3. The site at _2 is at the apex of the angle.

Appears in list containing _geom_angle_atom_site_label_.

geom_angle (numb, su)
The labels of the three atom sites which define the angle given by _geom_angle_. These must match labels specified as _atom_site_label_ in the atom list. Label 2 identifies the site at the apex of the angle.

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

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

Appears in list containing _geom_angle_atom_site_label_.

geom_angle (numb, su)
The data value must be one of the following:

| n   | do not include angle in special list |
| n   | abbreviation for ‘no’ |
| y   | do include angle in special list |
| y   | abbreviation for ‘yes’ |

Where no value is given, the assumed value is ‘no’.

geom_angle_site_symmetry_1 (char)
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_fract_x, _atom_site_fract_y_ and _atom_site_fract_z_. It must match a number given in _space_group_symop_id_. k, l and m refer to the translations that 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,
### 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>
<th>_geom_bond_multiplicity</th>
<th>_geom_bond_valence</th>
</tr>
</thead>
<tbody>
<tr>
<td>O1</td>
<td>C2</td>
<td>1.342</td>
<td>75</td>
<td>1.848</td>
</tr>
<tr>
<td>C5</td>
<td>C1</td>
<td>1.439</td>
<td>75</td>
<td>1.918</td>
</tr>
<tr>
<td>C2</td>
<td>C3</td>
<td>1.522</td>
<td>75</td>
<td>1.940</td>
</tr>
<tr>
<td>C2</td>
<td>C1</td>
<td>1.529</td>
<td>75</td>
<td>1.940</td>
</tr>
<tr>
<td>N4</td>
<td>C3</td>
<td>1.465</td>
<td>75</td>
<td>1.940</td>
</tr>
<tr>
<td>C3</td>
<td>C1</td>
<td>1.537</td>
<td>75</td>
<td>1.940</td>
</tr>
<tr>
<td>C3</td>
<td>H3</td>
<td>1.00</td>
<td>75</td>
<td>1.940</td>
</tr>
<tr>
<td>C4</td>
<td>C5</td>
<td>1.472</td>
<td>75</td>
<td>1.940</td>
</tr>
</tbody>
</table>

The intramolecular bond distance in ångströms. The permitted range is 0 → ∞.

**GEOM_CONTACT**

Data items in the GEOM_CONTACT category record details about interatomic contacts as calculated from the ATOM, CELL, and SYMMETRY data.


<table>
<thead>
<tr>
<th>_geom_contact_atom_site_label_1</th>
<th>_geom_contact_atom_site_label_2</th>
<th>_geom_contact_distance</th>
<th>_geom_contact_flag</th>
</tr>
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<tbody>
<tr>
<td>O1</td>
<td>O2</td>
<td>2.735</td>
<td>yes</td>
</tr>
<tr>
<td>H(O1)</td>
<td>O(2)</td>
<td>2.18</td>
<td>no</td>
</tr>
</tbody>
</table>

The bond valence calculated from _geom_bond_distance_. The bond valence is computed as the number of bonds to which the atom is connected. The permitted range is 0 → ∞.
GEOM_CONTACT

_geom_contact_distance

The interatomic contact distance in Ångström.
Appears in list containing _geom_contact_atom_site_label_A
The permitted range is 0.0 → ∞.

_geom_contact_publ_flag

This code signals whether the contact distance is referred to in a publication or should be placed in a list of significant contact distances.
Appears in list containing _geom_contact_atom_site_label_A
The data value must be one of the following:
- no do not include distance in special list
- n abbreviation for ‘no’
- yes do include distance in special list
- y abbreviation for ‘yes’
Where no value is given, the assumed value is ‘no’.

_geom_contact_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 ‘nk lm’ or ‘n l k m’. The character string nk lm is composed as follows: n refers to the symmetry operation that is applied to the coordinates stored in _atom_site_fract_x, _atom_site_fract_y and _atom_site_fract_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 contact. 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.
Appears in list containing _geom_contact_atom_site_label_A
Examples: ‘ ’ (no symmetry or translation to site), ‘4 ’ (4th symmetry operation applied), ‘7,6,45 ’ (7th symmetry position: +a on x, −b on y).

GEOM_HBOND

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


loop  
  _geom_hbond_atom_site_label_H  
  _geom_hbond_atom_site_label_A  
  _geom_hbond_distance_DA  
  _geom_hbond_distance_HA  
  _geom_hbond_angle_ABC  
  _geom_hbond_publ_flag

M8 BH6 OW 0.888(8) 1.921(12) 2.801(8) 169.6(8) yes
OW HO1 O7 0.917(6) 1.923(12) 2.793(8) 153.5(8) yes
OW HO1 H10 0.894(8) 1.886(11) 2.842(8) 179.7(9) yes

_geom_hbond_angle_DHA

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_A

_geom_hbond_atom_site_label_D  
_geom_hbond_atom_site_label_A

The labels of three atom sites (respectively, the donor atom, hydrogen atom and acceptor atom) participating in a hydrogen bond. These must match labels specified as _atom_site_label in the atom list.

GEOM_TORSION

Data items in the GEOM_TORSION category record details about interatomic torsion angles as calculated from the ATOM, CELL and SYMMETRY data.


loop  
  _geom_torsion_atom_site_label_D  
  _geom_torsion_atom_site_label_A  
  _geom_torsion_atom_site_label_4  
  _geom_torsion  
  _geom_torsion_site_symmetry_1  
  _geom_torsion_site_symmetry_2  
  _geom_torsion_site_symmetry_3  
  _geom_torsion_site_symmetry_4  
  _geom_torsion_publ_flag

C(9) O(2) C(7) C(12) 71.8(2) . . . yes
C(7) O(2) C(9) C(10) -168.3(3) . . . 2.666 yes
C(10) O(3) C(8) C(6) -167.7(3) . . . . yes
C(8) O(3) C(10) C(9) -69.7(2) . . . 2.666 yes
O(12) C(12) C(2) C(3) -175.5(4) . . . . no
O(12) C(12) C(2) C(7) -0.6(1) . . . . no
**4.1. CORE DICTIONARY (CORECIF)**

**JOURNAL_INDEX**

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.


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<tr>
<td>journal_date_from_coeditor</td>
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<tr>
<td>journal_date_accepted</td>
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<td>journal_coeditor_code</td>
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</table>

Data items specified by the journal staff.

**journal**


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<td>journal_volume</td>
<td></td>
</tr>
<tr>
<td>journal_year</td>
<td></td>
</tr>
</tbody>
</table>

Data items specified by the journal staff.

**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.


Appears in list containing _geom_torsion_atom_site_label_ [geom_torsion]

<table>
<thead>
<tr>
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<th>Value</th>
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<tr>
<td>geom_torsion_publ_flag_value</td>
<td></td>
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</tbody>
</table>

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

Appears in list containing _geom_torsion_atom_site_label_.

<table>
<thead>
<tr>
<th>Data Item</th>
<th>Value</th>
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<tbody>
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<td>geom_torsion_site_symmetry_2</td>
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<tr>
<td>geom_torsion_site_symmetry_3</td>
<td></td>
</tr>
<tr>
<td>geom_torsion_site_symmetry_4</td>
<td></td>
</tr>
</tbody>
</table>

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_fract_x, atom_site_fract_y_ and _atom_site_fract_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.

Appears in list containing _geom_torsion_atom_site_label_.

Examples: ‘.’ (no symmetry or translation to site), ‘4’ (4th symmetry operation applied), ‘7,6,45’ (7th symmetry position: +a on x, −b on y).
4. DATA DICTIONARIES

**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.

---


```
loop
  _journal_index_type
  _journal_index_term
  _journal_index_subterm
  0 C16H19NO4.
  S alcaloids (-)-norcocaine.
  S (-)-norcocaine.
  S;
  [2R,3S-(2\b,3\b)]-methyl
  3-(benzoxolyoxy)-6-asabicyclo[3.2.1]octane-2-carboxylate.
```

---


```
loop
  _publ_section_title
  trans-3-Benzoyl-2-(tert-butyl)-4-(iso-butyl)-1,3-oxazolidin-5-one.
  _publ_section_abstract
  The oxazolidinone 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)\AA].
  
  _publ_section_title
  Hemiasterlin methyl ester.
  _publ_section_abstract
  The oxazolidinone 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)\AA].
  
```

---

**_publ_contact_author**

The name and address of the author submitting the manuscript and data block. This is the person contacted by the journal editorial staff. It is preferable to use the separate data items _publ_contact_author_name and _publ_contact_author_address.

Example:

Professor George Ferguson
Department of Chemistry and Biochemistry
University of Guelph
Ontario
Canada
N1G 2W1

---

**_publ_contact_author_email**

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.

Examples: 'name@host.domain.country', 'bm@iucr.org'.

---

**_publ_contact_author_id_iucr**

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_phone**

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(34)9477334', '12(34)9477334'.

---

**_publ_contact_author_id_iucr**

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_letter**

A letter submitted to the journal editor by the contact author.

---

**_publ_manuscript_creation**

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**

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**

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

4.1. CORE DICTIONARY (CORECIF)

**_publ_requested_category**

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*)
- QI Inorganic compounds (*Acta E*)
- QO Organic compounds (*Acta E*)
- QM Metal-organic compounds (*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**

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

**_publ_requested_journal**

The name of the journal to which the manuscript is being submitted.

**_publ_author**

Data items in the _PUBL_AUTHOR category record details of the authors of a manuscript submitted for publication.

Example 1 – based on Willis, Beckwith & Tozer [*Acta Cryst.* (1991), C47, 2276-2277].

```plaintext
loop _publ_author_name _publ_author_address

'Willis, Anthony C.'
: Research School of Chemistry
Australian National University
GPO Box 4
Canberra, ACT
Australia 2601
,

 bliery, Percival R.
; Department
Institute
Street
City and postcode
COUNTRY

[publ_author]

[publ_author_email]

The e-mail 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]

[publ_author_footnote]

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]

[publ_author_id_iucr]

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]

[publ_author_name]

The name of a publication author. If there are multiple authors, this will be looped with _publ_author_address. 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.


[publ_author]
The data value must be one of the following:

Appears in list containing

The functional role of the associated text section.

Example 2 – hypothetical example including both standard CIF data items and a non-CIF quantity which 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.

### _publ_body_element

The functional role of the associated text section.

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


The largest and smallest values and the root-mean-square deviation, in electrons per ångström cubed, of the final difference electron density. The *rms 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 *min and *max values, and also for defining suitable contour levels.

4.1. CORE DICTIONARY (CORECIF)

**_refine_ls_abs_structure_details**

The nature of the absolute structure and how it was determined.

**_refine_ls_abs_structure_Flack**

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 $-3 \leq \eta \leq 3$ and a standard uncertainty (e.s.d.) $u$ must be supplied. The _enumeration range of $0.0 \rightarrow 1.0$ is correctly interpreted as meaning $(0.0 - 3u) \leq \eta \leq (1.0 + 3u)$.


The permitted range is $0.0 \rightarrow 1.0$.

**_refine_ls_abs_structure_Rogers**

The measure of absolute structure as defined by Rogers (1981). The value must lie in the 99.97% Gaussian confidence interval $-1 - 3u \leq \eta \leq 1 + 3u$ 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 $(-1.0 - 3u) \leq \eta \leq (1.0 + 3u)$.


The permitted range is $-1.0 \rightarrow 1.0$.

**_refine_ls_d_res_high**

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 $0.0 \rightarrow \infty$.

**_refine_ls_d_res_low**

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 $0.0 \rightarrow \infty$.

**_refine_ls_extinction_coef**

The extinction coefficient used to calculate the correction factor applied to the structure-factor data. The natural 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 $\varepsilon$ value; for the ‘Becker–Coppens type 1 isotropic’ method it is the $g$ value and for ‘Becker–Coppens type 2 isotropic’ corrections it is the $\rho$ value. Note that the magnitude of these values is usually of the order of 10000.


Example: ‘3.472(52)’ (Zachariasen coefficient $\varepsilon = 0.347(5) \times 10^4$).

**_refine_ls_extinction_expression**

A description of or reference to the extinction-correction equation used to apply the data item _refine_ls_extinction_coef. This information must be sufficient to reproduce the extinction-correction factors applied to the structure factors.

Example:


33
The least-squares goodness-of-fit parameter $S$ is defined in terms of the observed coefficients ($\text{obs}$) and the calculated coefficients ($\text{calc}$) as:

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

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

The permitted range is 0.0 → $\infty$.


Where no value is given, the assumed value is 'Zachariasen'.
Refinement Details

- **_refine_ls_number_constraints**  (numb)
  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 and _atom_site_refinement_flags. A general description of constraints may appear in _refine_special_details.

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

- **_refine_ls_number_parameters**  (numb)
  The number of 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 → ∞.

- **_refine_ls_number_reflns**  (numb)
  The number of unique reflections contributing to the least-squares refinement calculation.

  The permitted range is 0 → ∞.

- **_refine_ls_number_restraints**  (numb)
  The number of restrained parameters. These are parameters which are not directly dependent on another refined parameter. Restained 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 → ∞.

- **_refine_ls_R_factor_all**  (numb)
  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.

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

  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 → ∞.

- **_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 _refl_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 → ∞.

- **_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 _refl_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 \(F_{\text{obs}}\) = 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 → ∞.

- **_refine_ls_R_I_factor**  (numb)
  Residual factor \(RI\) for significantly intense reflections (satisfying _refl_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 \(R_Bragg\).

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

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

  The permitted range is 0.0 → ∞.

- **_refine_ls_restrained_S_all**  (numb)
  The least-squares goodness-of-fit parameter \(S'\) for all 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.

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

  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/square of standard uncertainty (e.s.d.)], \(P_{\text{calc}}\) = the calculated restraint values, \(P_{\text{param}}\) = the target restraint values, \(w_r\) = the restraint weight, \(N_{\text{ref}}\) = the number of reflections used in the refinement (see _refine_ls_number_reflns), \(N_{\text{rest}}\) = the number of restraints (see _refine_ls_number_restraints) and \(N_{\text{param}}\) = 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 0.0 → ∞.
4. DATA DICTIONARIES

**_refine_ls_restrained_S_gt_**

The least-squares goodness-of-fit parameter $S'$ for significantly intense reflections (satisfying _refines threshold expression_ 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_.

\[
S' = \left( \frac{\sum |w_1| |y_{obs} - y_{calc}|^2 + \sum w_i |p_{calc} - p_{targ}|^2}{N_{ref} + N_{restr} - N_{param}} \right)^{1/2}
\]

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 [1/square of standard uncertainty (e.s.d.)], $p_{calc}$ = the calculated restraint values, $p_{targ}$ = the target restraint values, $w_i$ = the restraint weight, $N_{ref}$ = the number of reflections used in the refinement (see _refine_ls_number_reflns_obs_), $N_{restr}$ = the number of restraints (see _refine_ls_restrained_S_obs_), $N_{param}$ = 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_ls_restrained_S_obs_**

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_.

\[
S' = \left( \frac{\sum |w_1| |y_{obs} - y_{calc}|^2 + \sum w_i |p_{calc} - p_{targ}|^2}{N_{ref} + N_{restr} - N_{param}} \right)^{1/2}
\]

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 [1/square of standard uncertainty (e.s.d.)], $p_{calc}$ = the calculated restraint values, $p_{targ}$ = the target restraint values, $w_i$ = the restraint weight, $N_{ref}$ = the number of reflections used in the refinement (see _refine_ls_number_reflns_obs_), $N_{restr}$ = the number of restraints (see _refine_ls_restrained_S_obs_), $N_{param}$ = 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_ls_shift/su_max_lt_**

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 largest value of the shift divided by the final standard uncertainty is too small to measure.

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

**_refine_ls_shift/su_max_**

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

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

**_refine_ls_shift/su_mean_**

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

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

**_refine_ls_shift/su_max_lt_**

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 $0 \rightarrow \infty$.

**_refine_ls_structure_factor_coef_**

Structure-factor coefficient ($|F|/\sigma^2$ or $f\bar{f}$ used in the least-squares refinement process.

The data value must be one of the following:

- $F$ structure-factor magnitude
- $F$ structure-factor squared
- $I_{net}$ net intensity

Where no value is given, the assumed value is "$F$".

**_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*(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_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:

- `sigma` based on measured s.u.'s
- `unit` unit or no weights applied
- `calc` calculated weights applied

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

**_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 _refine_ls_R_factor_definitions_.

\[ wR = \left( \frac{\sum |w_1| |y_{obs} - y_{calc}|^2}{\sum w_i |y_{obs}|^2} \right)^{1/2} \]

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 $0 \rightarrow \infty$.
4.1. CORE DICTIONARY (CORECIF)

**REFINE_LS_CLASS**

Data items in the REFINE_LS_CLASS category record details (for each reflection class separately) about the reflections used for the structure refinement.


```plaintext
loop_
  _refine_ls_class_R_factor_gt
  _refine_ls_class_code
  0.057 'Main'
  0.074 'Com'
  0.044 'NbRefls'
  0.046 'LaRefls'
  0.112 'Sat1'
  0.177 'Sat2'
```

**_refine_ls_class_code** (char)

The code identifying a certain reflection class. This code must match a _reflns_class_code.

Examples: ‘1’, ‘m1’, ‘a2’.

Appears in list. Must match parent data name _reflns_class_code.

**_refine_ls_class_d_res_high** (num)

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 _refine_ls_class_code.

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

**_refine_ls_class_d_res_low** (num)

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 _refine_ls_class_code.

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

**_refine_ls_class_R_factor_all** (num)

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 _refine_ls_class_d_res_high and _refine_ls_class_d_res_low. This is the conventional $R$ factor.

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

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. See also _refine_ls_class_d_res_high and _refine_ls_class_d_res_low.

Appears in list containing _refine_ls_class_code.

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

**_refine_ls_class_R_Fsqd_factor** (num)

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 _reflns_threshold_expression) and 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.

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

Appears in list containing \_refine_ls_class_code
The permitted range is \( 0 \rightarrow \infty \). [refine_ls]

\_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 \_refins_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 specified reflections.

Appears in list containing \_refine_ls_class_code
The permitted range is \( 0 \rightarrow \infty \). [refine_ls]

\_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.

\[
wR = \left( \frac{\sum |Y_{\text{obs}} - Y_{\text{calc}}|^2 \sum |wY_{\text{obs}}|^2}{\sum |wY_{\text{obs}}|^2} \right)^{1/2},
\]
where \( Y_{\text{obs}} \) = the observed amplitudes specified by \_refine_ls_structure_factor_coef, \( Y_{\text{calc}} \) = 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_all_definitions.

Appears in list containing \_refine_ls_class_code
The permitted range is \( 0 \rightarrow \infty \). [refine_ls]

**REFLIN**

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


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

Appears in list containing \_refln_index_. [refln]

\_refln_B_calc \_refln_B_meas (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_index_. [refln]

\_refln_class_code (char)
The code identifying the class to which this reflection has been assigned. This code must match a value of \_refins_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_index._ Must match parent data name \_refln_class_code. [refln]

\_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_index._ Must match parent data name \_exptl_crystal_id. [refln]

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

Appears in list containing \_refln_index._
The permitted range is \( 0 \rightarrow \infty \). [refln]
The calculated, measured and standard uncertainty (derived from measurement) of the structure factors (in electrons for X-ray diffraction).

Appears in list containing _refln_index_.

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_.

Classification of a reflection indicating its status with respect to inclusion in the refinement and the calculation of R factors.

Appears in list containing _refln_index_.

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.

The calculated, measured and standard uncertainty (derived from measurement) of the intensity, all in the same arbitrary units as _refln_intensity_.

Appears in list containing _refln_index_.

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

Appears in list containing _refln_index_.

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

Classification of a reflection indicating its status with respect to inclusion in the refinement and the calculation of R factors.

Appears in list containing _refln_index_.

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.

Appears in list containing _refln_index_.

Code identifying the wavelength in the _diffrn_radiation_list. See _diffrn_radiation_wavelength_id.

Appears in list containing _refln_index_. Must match parent data name _diffrn_radiation_wavelength_id.
REFLN

4. DATA DICTIONARIES

**REFLNS**

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


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</tr>
<tr>
<td><em>reflns_d_resolution_high</em></td>
<td>0.8733</td>
</tr>
<tr>
<td><em>reflns_d_resolution_low</em></td>
<td>11.9202</td>
</tr>
</tbody>
</table>

**_reflns_d_resolution_high_**

The highest and lowest resolution in Ångström for the reflections. The permitted range is 0 → ∞.

**_reflns_d_resolution_low_**

The lowest and lowest resolution in Ångström for the reflections. These are the smallest and largest d values. The permitted range is 0 → ∞.

**_reflns_Friedel_coverage_**

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_(crystal class) is the number of reflections obtained on averaging under the symmetry of the crystal class and _N_(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_.

The permitted range is 0.0 → 1.0.

**_reflns_limit_h_max_**

Miller indices limits for the reported reflections. These need not be the same as the _diffrn_refln_limit_values._

**_reflns_limit_h_min_**

**_reflns_limit_k_max_**

**_reflns_limit_k_min_**

**_reflns_limit_l_max_**

**_reflns_limit_l_min_**

**_reflns_number_gt_**

The number of reflections in the _refln_ list (not the _diffrn_refln_list_) that are significantly intense, satisfying the criterion specified by _reflns_threshold_expression_. 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_.

The permitted range is 0 → ∞.

Related item: _reflns_number_observed_ (alternate)

**_reflns_number_observed_**

The number of ‘observed’ reflections in the _refln_ list (not the _diffrn_refln_list_). The observed reflections satisfy the threshold criterion specified by _reflns_threshold_expression_ (or the deprecated item _reflns_observed_criterion_). They may include Friedel-equivalent reflections 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_.

The permitted range is 0 → ∞.

**_reflns_number_total_**

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_.

The permitted range is 0 → ∞.

**_reflns_observed_criterion_**

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

**_reflns_threshold_expression_**

The 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.

Example: ‘\(I > 2\sigma(I)\)’.

**_reflns_special_details_**

The criteria used to classify a reflection as ‘observed’. This criterion is usually expressed in terms of a \(\sigma(F)\) or \(\sigma(F^2)\) threshold.

Example: ‘\([I > 2\sigma(I)]\)’.

**_reflns_class_code_**

The code identifying a certain reflection class.

Appears in list. May match child data name(s): _refln_class_code_.

Exampes: ‘\(1\)’, ‘\(m1\)’, ‘\(a2\)’.

**REFLNS_CLASS**

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

Example 2 – corresponding to the one-dimensional incommensurately modulated structure of K2SeO₄.

<table>
<thead>
<tr>
<th>REFNLS_CLASS</th>
<th>(char)</th>
</tr>
</thead>
<tbody>
<tr>
<td><em>reflns_class_number_gt</em></td>
<td>594</td>
</tr>
<tr>
<td><em>reflns_class_code</em></td>
<td>'Main'</td>
</tr>
<tr>
<td><em>reflns_class_code</em></td>
<td>'Sat1'</td>
</tr>
<tr>
<td><em>reflns_class_code</em></td>
<td>'Sat2'</td>
</tr>
</tbody>
</table>

**_reflns_class_code_**

The code identifying a certain reflection class.

Appears in list. May match child data name(s): _refln_class_code_.

Exampes: ‘\(1\)’, ‘\(m1\)’, ‘\(a2\)’.
For each reflection class, the resolution in Ångströms for the reflections used in the refinement. This is the smallest $d$ value.

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

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

Example 1 – based on standard test data set p622 of the Xtal distribution


loop
   _reflns_scale_group_code
   _reflns_scale_meas_F
   1 .895447
   2 .912743

The permitted range is $0.0 \rightarrow \infty$.
Data items in the REFLNS_Shell category record details about the reflections used to determine the ATOM_SITE data items, as broken down by shells of resolution.

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

<table>
<thead>
<tr>
<th>reflns_shell_d_res_high</th>
<th>reflns_shell_d_res_low</th>
<th>reflns_shell_meanI_over_uI_gt</th>
<th>reflns_shell_meanI_over_uI_gt</th>
<th>reflns_shell_meanI_over_uI_gt</th>
<th>reflns_shell_meanI_over_uI_gt</th>
</tr>
</thead>
<tbody>
<tr>
<td>31.38 3.82 69.8 5024 2560 96.8 1.98</td>
<td>3.82 3.03 26.1 7413 2364 95.1 3.85</td>
<td>3.03 2.65 10.5 5640 2123 86.2 6.37</td>
<td>2.65 2.41 6.4 4322 1882 76.8 8.01</td>
<td>2.41 2.23 4.3 3247 1714 70.4 9.86</td>
<td>2.23 2.10 3.1 1140 812 33.3 13.99</td>
</tr>
</tbody>
</table>

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 this resolution shell.

Appears in list.

The permitted range is 0 → ∞.

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

Appears in list.

The total number of measurements made for this resolution shell.

Appears in list.

The total number of reflections classified as 'observed' (see _reflns_observed_criterion) measured for this resolution shell.

Appears in list.

The total number of reflections measured for this resolution shell.

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

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

The permitted range is 0 → 100.0.

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

Appears in list.
4.1. CORE DICTIONARY (CORECIF)

**SPACE_GROUP**

Contains all the data items that refer to the space group as a whole, such as its name or crystal system. They may be looped, for example, in a list of space groups and their properties. Only a subset of the SPACE_GROUP category items appear in the core dictionary. The remainder are found in the symmetry CIF dictionary. Space-group types are identified by their number as given in International Tables for Crystallography Vol. A. Specific settings of the space groups can be identified either by their Hall symbol or by specifying their symmetry operations. The commonly used Hermann–Mauguin symbol determines the space-group type uniquely but several different Hermann–Mauguin symbols may refer to the same space-group type. A Hermann–Mauguin symbol contains information on the choice of the basis, but not on the choice of origin. Different formats for the Hermann–Mauguin symbol are found in the symmetry CIF dictionary.

Example 1 – the monoclinic space group No. 15 with unique axis b.

```
  .space_group_id          1
  .space_group_name M-M   'C 2/c'
  .space_group_IT_number  15
  .space_group_name_Hall  '-C 2yc'
  .space_group_crystal_system monoclinic
```

**reflns_shell**

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 reflections classified as ‘observed’ (see _reflns_observed_criterion_) measured for this resolution shell.

Appears in list.

The permitted range is 0.0 → 100.0.

**reflns_shell_Rmerge_I_all**

The value of _Rmerge(I)_ for all reflections in a given shell.

\[
_{\text{Rmerge}}(I) = \frac{\sum (|I_j - \langle I \rangle|)}{\sum |I_j|},
\]

where \(I_j\) = the intensity of the \(j\)th observation of reflection \(i\), \(\langle I \rangle\) = 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 0.0 → \(\infty\).

**reflns_shell_Rmerge_F_all**

The value of _Rmerge(F) _for all reflections in a given shell.

\[
_{\text{Rmerge}}(F) = \frac{\sum (|F_j - \langle F \rangle|)}{\sum |F_j|},
\]

where \(F_j\) = the amplitude of the \(j\)th observation of reflection \(i\), \(\langle F \rangle\) = 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 0.0 → \(\infty\).

**reflns_shell_Rmerge_F_gt**

The value of _Rmerge(F) _for significantly intense reflections (see _reflns_threshold_expression_) in a given shell.

\[
_{\text{Rmerge}}(F) = \frac{\sum (|F_j - \langle F \rangle|)}{\sum |F_j|},
\]

where \(F_j\) = the amplitude of the \(j\)th observation of reflection \(i\), \(\langle F \rangle\) = 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 0.0 → \(\infty\).

**reflns_shell_Rmerge_F_obs**

The value of _Rmerge(F) _for all reflections classified as ‘observed’ (see _reflns_observed_criterion_) in a given shell.

\[
_{\text{Rmerge}}(F) = \frac{\sum (|F_j - \langle F \rangle|)}{\sum |F_j|},
\]

where \(F_j\) = the amplitude of the \(j\)th observation of reflection \(i\), \(\langle F \rangle\) = 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 0.0 → \(\infty\).

**reflns_shell_Rmerge_I_obs**

The value of _Rmerge(I) _for all reflections classified as ‘observed’ (see _reflns_observed_criterion_) in a given shell.

\[
_{\text{Rmerge}}(I) = \frac{\sum (|I_j - \langle I \rangle|)}{\sum |I_j|},
\]

where \(I_j\) = the intensity of the \(j\)th observation of reflection \(i\), \(\langle I \rangle\) = 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 0.0 → \(\infty\).

**reflns_shell_Rmerge_I_all**

The value of _Rmerge(I) _for all reflections in a given shell.

\[
_{\text{Rmerge}}(I) = \frac{\sum (|I_j - \langle I \rangle|)}{\sum |I_j|},
\]

where \(I_j\) = the intensity of the \(j\)th observation of reflection \(i\), \(\langle I \rangle\) = 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 0.0 → \(\infty\).
SPACE_GROUP

4. DATA DICTIONARIES

<table>
<thead>
<tr>
<th><strong>SPACE_GROUP</strong></th>
<th><strong>cif_core.dic</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>space_group_id</td>
<td>(char)</td>
</tr>
<tr>
<td>This is an identifier needed if space_group_items are looped. Appears in list as essential element of loop structure. May match child data name(s):</td>
<td></td>
</tr>
<tr>
<td>[space_group]</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>space_group_IT_number</th>
<th>(num)</th>
</tr>
</thead>
<tbody>
<tr>
<td>The number as assigned in International Tables for Crystallography Vol. A, specifying the proper affine class (i.e. the orientation-preserving affine class) of space groups (crystallographic space-group type) to which the space group belongs. This number defines the space-group type but not the coordinate system in which it is expressed. May appear in list containing space_group_id. The permitted range is 1 → 230. Related item: space_group_name_Hall or list the symmetry operations.</td>
<td></td>
</tr>
<tr>
<td>[space_group]</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>space_group_name_H-M_alt</th>
<th>(char)</th>
</tr>
</thead>
<tbody>
<tr>
<td>_space_group_name_H-M_alt allows any Hermann–Mauguin symbol to be given. The way in which this item is used is determined by the user and in general is not intended to be interpreted by computer. It may, for example, be used to give one of the extended Hermann–Mauguin symbols given in Table 4.3.2.1 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. 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. In order for the defaults to work correctly, the identity operation should have space_group_symop_id or symmetry_equiv_pos_site_id set to 1, and space_group_symop_operation_xyz or symmetry_equiv_pos_as_xyz set to x, y, z; i.e. the operation labelled 1 should be the identity operation. May appear in list containing space_group_id. Related item: symmetry_equiv_pos_site_id (alternate). Where no value is given, the assumed value is '1'.</td>
<td></td>
</tr>
<tr>
<td>[space_group]</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>space_group_symop_operation_xyz</th>
<th>(char)</th>
</tr>
</thead>
<tbody>
<tr>
<td>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. In order for the defaults to work correctly, the identity operation should have space_group_symop_id or symmetry_equiv_pos_site_id set to 1, and space_group_symop_operation_xyz or symmetry_equiv_pos_as_xyz set to x, y, z; i.e. the operation labelled 1 should be the identity operation. May appear in list containing space_group_id. Related item: symmetry_equiv_pos_site_id (alternate). Where no value is given, the assumed value is '1'.</td>
<td></td>
</tr>
<tr>
<td>[space_group]</td>
<td></td>
</tr>
</tbody>
</table>

SYMMETRY

Data items in the SYMMETRY category record details about the space-group symmetry.


- symmetry_cell_setting  orthorhombic
- symmetry_space_group_name_H-M  ‘P 21 21 21’
- symmetry_space_group_name_Hall  ‘P 2ac 2ab’

_symmetry_equiv_pos_as_xyz

_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

_SYMMETRY_EQUIV

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


_loop_

_symmetry_equiv_pos_as_xys


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

1 1 1
2 2 1
3 3 1
4 4 1

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
4. DATA DICTIONARIES

VALENCE_PARAM

_valence_param_atom_1
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_atom_1_valence
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_atom_2
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_atom_2_valence
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_B
The bond-valence parameter $B$ used in the expression

$$s = \exp\left(\frac{(R_o - R)}{B}\right),$$

where $s$ is the valence of a bond of length $R$.

Appears in list containing _valence_param_id

_valence_param_details
Details of or comments on the bond-valence parameters.
Appears in list containing _valence_param_id

_valence_param_id
An identifier for the valence parameters of a bond between the given atoms.
Appears in list.

_valence_ref_id
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

_valence_param_Ro
The bond-valence parameter $R_o$ used in the expression

$$s = \exp\left(\frac{(R_o - R)}{B}\right),$$

where $s$ is the valence of a bond of length $R$.

Appears in list containing _valence_param_id

VALENCE_REF

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

_valence_ref_id
An identifier for items in this category. Parent of _valence_ref_id, which must have the same value.
Appears in list containing _valence_param_id. May match child data name(s): _valence_ref_id

_valence_ref_reference
Literature reference from which the valence parameters identified by _valence_param_id were taken.
Appears in list containing _valence_ref_id

cif_core.dic