Dictionary name: cif_core.dic

Dictionary version: 2.2
Dictionary last updated: 2001-01-11

_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, magnetic moments and directions, and so on.


loop_
_atom_site_label
_atom_site_fракt_x
_atom_site_fракt_y
_atom_site_fракt_z
_atom_site_U_iso_or_equiv
_atom_site_calc_attached_atom
_atom_site_calc_flag
_atom_site_adp_type
_atom_site_aniso_type_symbol
_atom_site_aniso_B_13
_atom_site_aniso_B_23
_atom_site_aniso_B_33
_atom_site_aniso_B_12
_atom_site_aniso_B_11


Example 4 - Hypothetical example to illustrate the description of a disordered methyl group. Assembly ‘M’ is a disordered methyl with configurations ‘A’ and ‘B’.

Example 5 - Illustration of the use of the _atom_site_adp_type standard code used to describe the type of atomic displacement parameters used for the site.

ATOM_SITE

Note: The provided text is a fragment of a larger document and does not include the full context or content. It is a snapshot of a part of the CIF dictionary, focusing on the ATOM_SITE category.
These are the standard anisotropic atomic displacement components in ångström squares which appear in the structure factor term:

\[ T = \exp \left( -2\pi^2 \sum_i \sum_j (U_i^{ij} h_i a_i^* a_j a^*_j) \right) \]

\( h \) is the Miller indices, \( a^* \) is the reciprocal-space cell lengths.

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

Appears in list containing `atom_site_aniso_label`. Related item(s): `atom_site_aniso_B` (conversion).

### `atom_site_attached_hydrogens`

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

Appears in list containing `atom_site_label` Where no value is given, the assumed value is 0.

Example(s): '2' (water oxygen), '1' (hydroxyl oxygen), '4' (ammonium nitrogen)

### `atom_site_B_equiv_geom_mean`

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

\[ B_{\text{equiv}} = (B_{11} B_{22} B_{33})^{1/3} \]

\( B_s \) is the principal components of the orthogonalised \( B^i \).

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

Appears in list containing `atom_site_label`. The permitted range is 0.0–\( \infty \). Related item(s): `atom_site_B_iso_or_equiv` (alternate), `atom_site_U_equiv_geom_mean` (conversion).

### `atom_site_B_iso_or_equiv`

Isotropic atomic displacement parameter, or equivalent isotropic atomic displacement parameter, \( B_{\text{equiv}} \), in ångström squared, calculated from anisotropic temperature factor parameters.

\[ B_{\text{equiv}} = \left( \frac{1}{3} \right) \sum_i \sum_j \left( B_{ij} a_i a_j a_k a_l \right) \]

\( a \) is the real-space cell lengths, \( a^* \) is the reciprocal-space cell lengths, \( B^i = 8\pi^2 U^i \).

Ref: Fischer, R. X. & Tillmanns, E. (1988). *Acta Cryst.* C44, 775–776. The IUCr Commission on Nomenclature recommends against the use of \( B \) for reporting atomic displacement parameters. \( U \), being directly proportional to \( B \), is preferred.

Appears in list containing `atom_site_label`. The permitted range is 0.0–\( \infty \). Related item(s): `atom_site_B_equiv_geom_mean` (alternate), `atom_site_U_iso_or_equiv` (conversion).

### `atom_site_calculated_attached_atom`

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 '1'.

### `atom_site_calc_flag`

A standard code to signal if 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'.

\( d \) determined from diffraction measurements

\( calc \) calculated from molecular geometry

\( dum \) dummy site with meaningless coordinates

Appears in list containing `atom_site_label`. Where no value is given, the assumed value is 'd'.

### `atom_site_Cartn_x`

### `atom_site_Cartn_y`

### `atom_site_Cartn_z`

The atom site coordinates in ångström specified according to a set of orthogonal Cartesian axes related to the cell axes as specified by the `atom_sites_Cartn_transform_axes` description.

Related item(s): `atom_site_fractions` (alternate). Appears in list containing `atom_site_label`.

### `atom_site_chemical_conn_number`

This number links an atom site to the chemical connectivity list. It must match a number specified by `chemical_conn_atom_number`.

Appears in list containing `atom_site_label`. Must match data name `chemical_conn_atom_number`. The permitted range is 1–\( \infty \).

### `atom_site_constraints`

A description of the constraints applied to parameters at this site during refinement. See also `atom_site_refinement_flags` and `refine_ls_number_constraints`.

Appears in list containing `atom_site_label`. Where no value is given, the assumed value is '1'.

Example(s): 'psp=1.0-psp(2n3)'
_atom_site_disorder_assembly (char)
A code which identifies a cluster of atoms that show long range positional disorder but are locally ordered. Within each such cluster of atoms, _atom_site_disorder_group is used to identify the sites that are simultaneously occupied. This field is only needed if there is more than one cluster of disordered atoms showing independent local order.

Appears in list containing _atom_site_label.

Example(s): 'A' (disordered methyl assembly with groups 1 and 2), 'Bi' (disordered sites related by a mirror), 'Si' (disordered sites independent of symmetry) [atom_site]

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

Appears in list containing _atom_site_label.

Example(s): '1' (unique disordered site in group 1), '2' (unique disordered site in group 2), '-1' (symmetry-independent disordered site) [atom_site]

_atom_site_fraction_x
_atom_site_fraction_y
_atom_site_fraction_z (numb)
Atom site coordinates as fractions of the _cell_length_values.

Related item(s): _atom_site_Cartn (alternate). Appears in list containing _atom_site_label. Where no value is given, the assumed value is '0.0'. [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 underline character. Underline separators are only used if higher-order components exist. If an intermediate component is not used it may be omitted provided the underline separators are inserted. For example the label 'C233_...SS' is acceptable and represents the components C, 233, ‘., and ggg. Each label may have a different number of components.

Appears in list as essential element of loop structure. May match subdirectory data 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_bond_atom_site_label_3, _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_tag (com)
Example(s): 'Cl2', 'Ca3P2B', 'Fe3+17+', 'H1281+', 'boro2Na', 'C_a_phe_63_a-0', 'Zn_Zn_301_A-0' [atom_site]

_atom_site_label_component_0
_atom_site_label_component_1
_atom_site_label_component_2
_atom_site_label_component_3
_atom_site_label_component_4
_atom_site_label_component_5
_atom_site_label_component_6 (char)
Component 0 is normally a code which matches identically with one of the _atom_type_symbol codes. If this is the case then the rules governing the _atom_type_symbol code apply. If, however, the data item _atom_site_type_symbol is also specified in the atom site list, component 0 need not match this symbol or adhere to any of the _atom_type_symbol rules. Component 1 is referred to as the "atom number". When component 0 is the atom type code, it is used to number the sites with the same atom type. This component code must start with at least one digit which is not followed by a + or − sign (to distinguish it from the component 0 rules). Components 2 to 6 contain the identifier, residue, sequence, asymmetry identifier and alternate codes, respectively. These codes may be composed of any characters except an underline.

Appears in list containing _atom_site_label. [atom_site]

_atom_site_occupancy (numb)
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. Where no value is given, the assumed value is '1.0'. The permitted range is 0.0 to 1.0. [atom_site]

_atom_site_refinement_flags (char)
A concatenated series of single-letter flags which indicate the refinement restraints or constraints applied to this site.

. no refinement constraints
S special position constraint on site
R rigid group refinement of site
T riding-atom site attached to non-riding atom
D distance or angle restraint on site
U thermal displacement constraints
Uiso or U^2 restraint (rigid bond)
P partial occupancy constraint

Appears in list containing _atom_site_label. [atom_site]
_atom_site_restraints

A description of restraints applied to specific parameters at this site during refinement. See also _atom_site_refinement_flags and _refine_is_number_restraints.

Appears in list containing _atom_site_label.

Example(s): 'restrained to planar ring' [atom_site]

_atom_site_symmetry_multiplicity (numb)

Appears in list containing _atom_site_label. The permitted range is 1→192.

_atom_site_type_symbol (char)
A code to identify the atom specie(s) 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. May match subsidiary data name(s) _atom_site_aniso_type_symbol. Must match data name _atom_type_symbol.

Example(s): 'Cu', 'Cu2+', 'dummy', 'Fe3+Ni2+', 'S-', 'H', 'H(2ES)' [atom_site]

_atom_site_U_equiv_geom_mean (numb)
Equivalent isotropic atomic displacement parameter, \( U_{eq} \), in nm\(^2\), calculated as the geometric mean of the anisotropic atomic displacement parameters.

\[
U_{eq} = (U_{11}U_{22}U_{33})^{1/3}
\]

\( U_{ij} \) are the principal components of the orthogonalised \( U_{ij} \).

Appears in list containing _atom_site_label. The permitted range is 0.0→∞. Related item(s): _atom_site_B_iso_or_equiv (alternate), _atom_site_B_equiv_geom_mean (conversion).

_atom_site_U_iso_or_equiv (numb)
Isotropic atomic displacement parameter, or equivalent isotropic atomic displacement parameter, \( U_{iso} \), in nm\(^2\), calculated from anisotropic atomic displacement parameters.

\[
U_{iso} = (1/3) \sum_{ij} (U_{ij}a_i^*a_j^*)
\]

\( a_i \) = the real-space cell lengths, \( a_i^* \) = the reciprocal-space cell lengths.

Elements of a 3 × 1 translation vector used in the transformation of Cartesian coordinates to fractional coordinates. The 3 × 1 translation is defined in _atom_sites_fractions_translation_vectors.

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

Matrix elements used to transform Cartesian coordinates to fractional coordinates. The axial alignments of this transformation are described in _atom_sites_fractions_translation_matrixes. The 3 × 1 translation is defined in _atom_sites_fractions_translation_vectors.

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

Elements of a 3 × 1 translation vector used in the transformation of Cartesian coordinates to fractional coordinates. The 3 × 1 translation is defined in _atom_sites_fractions_translation_vectors. The axial alignments of this transformation are described in _atom_sites_fractions_translation_matrixes.

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

The effective intra- and intermolecular bonding radii in Ångströms of this atom type.

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

The effective intra- and intermolecular bonding radii in Ångströms of this atom type.

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

The effective intra- and intermolecular bonding radii in Ångströms of this atom type.

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

The effective intra- and intermolecular bonding radii in Ångströms of this atom type.
The Cromer–Mann scattering-factor coefficients used to calculate the scattering factors for this atom type.


Appears in list containing _atom_type_symbol. [atom_type]

The imaginary and real components of the anomalous dispersion scattering factors, f" and f', in electrons, for this atom type and the radiation given in _dифф.radiation.wavelength. [atom_type]

Appears in list containing _atom_type_symbol. Where no value is given, the assumed value is '0.0'. [atom_type]

Reference to source of real and imaginary dispersion corrections for scattering factors used for this atom type. [atom_type]

Example(s): 'International Tables Vol. IV Table 2.3.1' [atom_type]

The bound coherent scattering length in femtometres for the atom type at the isotopic composition used for the diffraction experiment. [atom_type]

Appears in list containing _atom_type_symbol. Where no value is given, the assumed value is '0.0'. [atom_type]

Reference to source of scattering factors or scattering lengths used for this atom type. [atom_type]

Example(s): 'International Tables Vol. IV Table 2.4.6B' [atom_type]

A table of scattering factors as a function of (sinθ)/λ. This table should be well commented to indicate the items present. Regularly formatted lists are strongly recommended. [atom_type]

Appears in list containing _atom_type_symbol. [atom_type]

The code used to identify the atom specie(s) representing this atom type. Normally this code is the element symbol. The code may be composed of any character except an underline with the additional proviso that digits designate an oxidation state and must be followed by a + or - character. [atom_type]

Appears in list as essential element of loop structure. May match subsidiary data name(s): _atom_site_type_symbol. [atom_type]

Example(s): 'C', 'Cu2+', 'H(SEH)', 'dummy', 'FeNi' [atom_type]
_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(s):
: Department
Institute
Street
City and postcode
COUNTRY

<table>
<thead>
<tr>
<th>audit_author</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
</tr>
</tbody>
</table>

_aud_conform_dict_location

A file name or uniform resource locator (URL) where the conformant dictionary resides.

May appear in list containing _audit_conform_dict_name.

<table>
<thead>
<tr>
<th>audit_conform</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
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</tbody>
</table>

_aud_conform_dict_name

The string identifying the highest-level dictionary defining datanames used in this file.

May appear in list as essential element of loop structure.

<table>
<thead>
<tr>
<th>audit_conform</th>
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</table>

_aud_conform_dict_version

The version number of the conformant dictionary.

May appear in list containing _audit_conform_dict_name.

<table>
<thead>
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<th>audit_conform</th>
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</table>

_aud_contact_author_address

The mailing address of the author of the data block to whom correspondence should be addressed.

Example(s):
: Department
Institute
Street
City and postcode
COUNTRY

<table>
<thead>
<tr>
<th>audit_contact_author</th>
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</table>

_aud_contact_author_email

The electronic mail address of the author of the data block to whom correspondence should be addressed.

Example(s):
: Department
Institute
Street
City and postcode
COUNTRY

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<th>audit_contact_author</th>
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_aud_contact_author_fax

The facsimile telephone number of the author of the data block to whom correspondence should be addressed.

Example(s):
: Department
Institute
Street
City and postcode
COUNTRY

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_aud_contact_author_phone

The telephone number of the author of the data block to whom correspondence should be addressed.

Example(s):
: Department
Institute
Street
City and postcode
COUNTRY

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_data_conform_dict_location[]

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 5HVP.

| loop_ |
|       |
|       |

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</table>
includes the international dialing prefix, the area code in parentheses, followed by the local number and any extension number prefixed by 'x', with no spaces.

Example(s): '12(34)9477330', '12(34)9477330x5543'

### audit_contact_author

Data items in the AUDIT_CONTACT_AUTHOR category detail about appears in list as essential element of loop structure. The value of /cell_angle_alpha, /cell_angle_beta, /cell_angle_gamma (numb)

Unit-cell angles in degrees of the reported structure. The values of _reflin_index_h, _k, _l must correspond to the cell defined by these values and _cell_length_a, _b and _c. The values of _diffrefl_refln_index_h, _k, _l may not correspond to these values if a cell transformation took place following the measurement of diffraction intensities. See also _diffrefl_reflns_transf_matrix._

Where no value is given, the assumed value is '90.0'. The permitted range is 0.0 to 180.0.

### cell_formula_units_Z

The number of the formula units in the unit cell as specified by /chemical_formula_structural, /chemical_formula_mol or /chemical_formula_sum. The permitted range is 1 to \(\infty\).

### cell_length_a

Unit-cell lengths in angstroms corresponding to the structure reported. 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 _diffrefl_refln_index_h, _k, _l may not correspond to these values if a cell transformation took place following the measurement of diffraction intensities. See also _diffrefl_reflns_transf_matrix._

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

### cell_measurement_pressure

The pressure in kilopascals at which the unit-cell parameters were measured (not the pressure used to synthesize the sample). The permitted range is 0.0 to \(\infty\).

### cell_measurement_radiation

Description of the radiation used to measure the unit-cell data. See also _cell_measurement_wavelength_. Example(s): 'neutron', 'Cu Kα', 'synchrotron'

### cell_measurement_reflns_used

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

### cell_measurement_theta_max

The maximum and minimum theta angles in degrees of reflections used to measure the unit cell. The permitted range is 0.0 to 90.0.
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 _diffn_radiation_wavelength_. The permitted range is 0.0–9.0 Å.

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

Example(s): 'pseudo-orthorhombic', 'standard setting from 45° deg rotation around c' [cell]

**_cell_special_details_**

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

\[a = _cell_length_a, b = _cell_length_b, c = _cell_length_c, \alpha = _cell_angle_alpha, \beta = _cell_angle_beta, \text{ and } \gamma = _cell_angle_gamma.\]

The permitted range is 0.0–9.0 Å³.

**_cell_measurement_refln_[]**

Data items in the CELL_MEASUREMENT_REFLN category record details about the reflections used in 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 of Rb_2S_2O_8 at room temperature (not yet published).

loop_
  _cell_measurement_refln_index_h
  _cell_measurement_refln_index_k
  _cell_measurement_refln_index_l
  _cell_measurement_refln_theta
  0  4  1  8.67
  0  3  2  9.45
  3  0  2  9.46
  4  1  8.93
  -2 -1 -2  7.53
  3  0  2  9.46
  4  1  8.93
  -2 -1 -2  7.53
# = = = = data truncated for brevity = = = =

_Miller indices of a reflection used for measurement of the unit cell._

Appears in list as essential element of loop structure.

_theta angle in degrees for the reflection used for measurement of the unit cell with the indices _cell_measurement_refln_index_.

Appears in list containing _cell_measurement_refln_index_. The permitted range is 0.0–90.0°.

**_chemical_[]**

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


\[
\text{trans-bis(tricyclohexylphosphine)tetracarbonylmolybdenum}(0)
\]

_Full names by which the compound is most commonly known._

**_chemical_absolute_configuration_**

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


_ad absolute configuration established by the structure determination of a compound containing a chiral reference molecule of known absolute configuration.

 thanking absolute configuration established by anomalous dispersion effects in diffraction measurements on the crystal.

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

_sym absolute configuration has not been established by anomalous dispersion effects in diffraction measurements on the crystal. An arbitrary choice of enantiomer has been made .

_absolute configuration is unknown, there being no firm chemical evidence for its assignment to hand and it having not been established by anomalous dispersion effects in diffraction measurements on the crystal._

_A description of the source of the compound under study, or of the parent molecule if a simple derivative is studied. This includes the place of discovery for minerals or the actual source of a natural product._

Example(s): 'From Norilsk (URSS)', 'Extracted from the bark of Cinchona Naturalis'.

**_chemical_melting_point_**

The temperature in kelvins at which a crystalline solid changes to a liquid.

The permitted range is 0.0–∞ K.

**_chemical_name_common_**

_Trivial name by which the compound is commonly known._

Example(s): '1-bromoenestradiol'.

**_chemical_name_mineral_**

_Mineral name accepted by the International Mineralogical Association. Use only for natural minerals. See also _chemical_compound_source._

Example(s): 'chalcopyrite'.

<table>
<thead>
<tr>
<th>_chemical_name_structure_type</th>
<th>(char)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Commonly used structure-type name. Usually only applied to minerals or inorganic compounds.</td>
<td></td>
</tr>
</tbody>
</table>

Example(s): 'perovskite', ' sphalerite', 'A15' [chemical]

<table>
<thead>
<tr>
<th>_chemical_name_systematic</th>
<th>(char)</th>
</tr>
</thead>
<tbody>
<tr>
<td>IUPAC or Chemical Abstracts full name of compound.</td>
<td></td>
</tr>
</tbody>
</table>

Example(s): '1-bromostra-1,3,5(10)-triene-3,17\'-b-diol' [chemical]

<table>
<thead>
<tr>
<th>_chemical_optical_rotation</th>
<th>(char)</th>
</tr>
</thead>
<tbody>
<tr>
<td>The optical rotation in solution of the compound is specified in the following format:</td>
<td></td>
</tr>
</tbody>
</table>

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

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 in 100 ml of solution, SORT is the signed value (preceded by a + or a – sign) of 100α/lc, where c is the signed optical rotation in degrees measured in a cell of length l in dm and c is the value of CONC in g, and SOLV is the chemical formula of the solvent. |        |

Example(s): ' [α]_{25}^\circ = +108 (c = 3.42, CHCl3) ' [chemical]

<table>
<thead>
<tr>
<th><em>chemical_conn_atom</em>[]</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Data items in the <em>chemical_conn_atom</em> and <em>chemical_conn_bond</em> categories record details about the 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 <em>chemical_conn_atom</em> 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 <em>chemical_conn_atom</em> and <em>chemical_conn_bond</em> data items will always describe a complete chemical entity.</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>_chemical_conn_atom_number</th>
<th>(numb)</th>
</tr>
</thead>
<tbody>
<tr>
<td>The net integer charge assigned to this atom. This is the formal charge assignment normally found in chemical diagrams.</td>
<td></td>
</tr>
</tbody>
</table>

Appears in list containing _chemical_conn_atom_type_symbol_. Where no value is given, the assumed value is '0'. The permitted range is -6 to 6. |        |

Example(s): '1' (for an ammonium nitrogen), '-1' (for a chloride ion) [chemical_conn_atom]

<table>
<thead>
<tr>
<th>_chemical_conn_atom_display_x</th>
<th>(numb)</th>
</tr>
</thead>
<tbody>
<tr>
<td>The 2D Cartesian coordinates ((x, y)) of the position of this atom in a recognisable 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. If absent, values will be assigned by the journal or database staff.</td>
<td></td>
</tr>
</tbody>
</table>

Appears in list containing _chemical_conn_atom_type_symbol_. The permitted range is 0.0 to 1.0. [chemical_conn_atom]

<table>
<thead>
<tr>
<th>_chemical_conn_atom_NCA</th>
<th>(numb)</th>
</tr>
</thead>
<tbody>
<tr>
<td>The number of connected atoms excluding terminal hydrogen atoms.</td>
<td></td>
</tr>
</tbody>
</table>

Appears in list containing _chemical_conn_atom_type_symbol_. The permitted range is 0–∞. [chemical_conn_atom]

<table>
<thead>
<tr>
<th>_chemical_conn_atom_NH</th>
<th>(numb)</th>
</tr>
</thead>
<tbody>
<tr>
<td>The total number of hydrogen atoms attached to this atom, regardless of whether they are included in the refinement or the <em>atom_site</em> list. This number will be the same as <em>atom_site_attached hydrogens</em> only if none of the hydrogen atoms appear in the <em>atom_site</em> list.</td>
<td></td>
</tr>
</tbody>
</table>

Appears in list containing _chemical_conn_atom_type_symbol_. The permitted range is 0–∞. [chemical_conn_atom]

<table>
<thead>
<tr>
<th>_chemical_conn_atom_number</th>
<th>(numb)</th>
</tr>
</thead>
<tbody>
<tr>
<td>The chemical sequence number to be associated with this atom.</td>
<td></td>
</tr>
</tbody>
</table>

Appears in list containing _chemical_conn_atom_type_symbol_. May match subsidiary data name(s): _atom_site_chemical_conn_number, _chemical_conn_bond_atom_1, _chemical_conn_bond_atom_2. The permitted range is 1–∞. [chemical_conn_atom]
The chemical bond type associated with the connection between the two sites _chemical_conn_atom_type_symbol_ and _chemical_conn_atom_.


Loop:

_chemical_conn_atom_ 1
_chemical_conn_atom_ 2

<table>
<thead>
<tr>
<th>bond_type</th>
<th>atom_1</th>
<th>atom_2</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 1 doub 4 3 sing 4 2 sing</td>
<td>4 3 sing 6 5 sing 7 6 sing</td>
<td>8 7 sing 8 3 sing 10 2 sing</td>
</tr>
<tr>
<td>12 9 doub 12 11 sing 12 10 sing</td>
<td>13 11 sing 14 13 sing 15 14 sing</td>
<td>16 15 sing 16 11 sing 17 5 sing</td>
</tr>
<tr>
<td>18 5 sing 19 6 sing 20 6 sing</td>
<td>21 7 sing 22 7 sing 23 8 sing</td>
<td>24 8 sing 25 13 sing 26 13 sing</td>
</tr>
</tbody>
</table>


Loop:

_chemical_conn_atom_ 1
_chemical_conn_atom_ 2

<table>
<thead>
<tr>
<th>bond_type</th>
<th>atom_1</th>
<th>atom_2</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 3 doub 4 2 sing</td>
<td>4 3 sing 6 5 sing 7 6 sing</td>
<td>8 7 sing 8 3 sing 10 2 sing</td>
</tr>
<tr>
<td>12 9 doub 12 11 sing 12 10 sing</td>
<td>13 11 sing 14 13 sing 15 14 sing</td>
<td>16 15 sing 16 11 sing 17 5 sing</td>
</tr>
<tr>
<td>18 5 sing 19 6 sing 20 6 sing</td>
<td>21 7 sing 22 7 sing 23 8 sing</td>
<td>24 8 sing 25 13 sing 26 13 sing</td>
</tr>
</tbody>
</table>

**_chemical_formula_**

**Example 1 - based on data set TOZ of Willis, Beckwith & Toczer ([1991]. Acta Cryst. C47, 2276–2277).**

\[
\text{_chemical_formula_moiety_} = \text{C18 H25 N O3} \\
\text{_chemical_formula_sum_} = \text{C18 H25 N O3} \\
\text{_chemical_formula_weight_} = 303.40
\]

**Example 2 - based on data set 9597gaus of Alyea, Ferguson & Kannan ([1996b]. Acta Cryst. C47, 2276–2277).**

\[
\text{_chemical_formula_moiety_} = \text{'C40 H66 Mo O4 P2'} \\
\text{_chemical_formula_sum_} = \text{'C40 H66 Mo O4 P2'} \\
\text{_chemical_formula_weight_} = 768.81
\]

**_chemical_formula_analysis_**

Formula determined by standard chemical analysis including trace elements. See _chemical_formula_ for rules for writing chemical formulas. Parentheses are used only for standard uncertainties (c.s.d.’s).

Example(s): Fe2.46(2) Ni1.60(3) S4' [chemical_formula]

**_chemical_formula_iupac_**

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.
The permitted range is 1.0–∞. 

Example(s):
- [Co Re (C12 H22 F)2 (C 8) 6]·0.5C H3 · H·+

Example(s):
- C7 H4 Cl Hg N 0.3 S·
- C’12 H17 N0 S 1+·
- C’12 H16 N2 06·
- (Cd 2+)3, (O6 N6 Cr 3–)2, 2(H2 0)·

Example(s):
- Ca ((Cl 0)3 0) 2 (H2 0)6·
- (Pt (N H3)2 (O5 H7 N3) 0)2 (Cl 0)42·

Example(s):
- C18 H19 N7 06 S·

Formula mass in daltons measured by a non-diffraction experiment. The permitted range is 1.0–∞.

Example 1: based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.
Appears in list containing _citation_id.  [citation]

_citation_book_publisher (char)
The name of the publisher of the citation; relevant for book chapters.
Appears in list containing _citation_id.  [citation]

_citation_book_publisher_city (char)
The location of the publisher of the citation; relevant for book chapters.
Appears in list containing _citation_id.  [citation]

_citation_book_title (char)
The title of the book in which the citation appeared; relevant for book chapters.
Appears in list containing _citation_id.  [citation]

_citation_coordinate_linkage (char)
_citation_coordinate_linkage states whether or not this citation is concerned with precisely the set of coordinates given in the data block. If, for instance, the publication described the same structure, but the coordinates had undergone further refinement prior to creation of the data block, the value of this data item would be 'no'.
no  citation unrelated to current coordinates
n  abbreviation for "no"
yes  citation related to current coordinates
y  abbreviation for "yes"
Appears in list containing _citation_id.  [citation]

_citation_country (char)
The country of publication; relevant for both journal articles and book chapters.
Appears in list containing _citation_id.  [citation]

_citation_database_id_Medline (num)
Accession number used by Medline to categorize a specific bibliographic entry.
Appears in list containing _citation_id.  The permitted range is 1-9999.
Example(s): '89064067'  [citation]

_citation_id (char)
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 subsidiary data name(s): _citation_author_citation_id, _citation_editor_citation_id.
Example(s): 'primary', '1', '2', '3'  [citation]

_citation_journal_abbrev (char)
Abbreviated name of the journal cited as given in the Chemical Abstracts Service Source Index.
Appears in list containing _citation_id.  [citation]

Example(s): 'J. Mol. Biol.'  [citation]

_citation_journal_id_ASTM (char)
The American Society for the Testing of Materials (ASTM) code assigned to the journal cited (also referred to as the CODEN designator of the Chemical Abstracts Service); relevant for journal articles.
Appears in list containing _citation_id.  [citation]

_citation_journal_id_CSD (char)
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.  [citation]

Example(s): '0070'  [citation]

_citation_journal_id_ISSN (char)
The International Standard Serial Number (ISSN) code assigned to the journal cited; relevant for journal articles.
Appears in list containing _citation_id.  [citation]

Example(s): 'Journal of Molecular Biology'  [citation]

_citation_journal_full (char)
Full name of the journal cited; relevant for journal articles.
Appears in list containing _citation_id.  [citation]

Example(s): 'Journal of Molecular Biology'  [citation]

_citation_journal_issue (char)
Issue number of the journal cited; relevant for journal articles.
Appears in list containing _citation_id.  [citation]

Example(s): '2'  [citation]

_citation_journal_volume (char)
Volume number of the journal cited; relevant for journal articles.
Appears in list containing _citation_id.  [citation]

Example(s): '174'  [citation]

_citation_language (char)
Language in which the citation appears.
Appears in list containing _citation_id.  [citation]

Example(s): 'german'  [citation]

_citation_page_first (char)
The first and last pages of the citation; relevant for both journal articles and book chapters.
Appears in list containing _citation_id.  [citation]
_citation_special_details (char)
A description of special aspects that describe the relationship of the contents of the data block to the literature item cited. Appears in list containing _citation_id.
Example(s):
'citation relates to this precise coordinate set',
'relates to earlier low-resolution structure',
[citation]

_citation_title (char)
The title of the citation; relevant for both journal articles and book chapters. Appears in list containing _citation_id.
Example(s):
'Structure of Diferric Dukovtransferrin at 2.30 Å Resolution'.
[citation]

_citation_year (num)
The year of the citation; relevant for both journal articles and book chapters. Appears in list containing _citation_id.
Example(s): 1994
[citation]

_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:
loop_
   _citation_author_citation_id _citation_author_name _citation_author_citation_id
   _citation_author_name
   primary 'Fitzgerald, P. M. D.'
   primary 'McKeever, B. M.'
   primary 'Springer, J. P.'
   primary 'Heimbach, J. C.'
   primary 'Herber, W. K.'
   primary 'Dixon, R. A. F.'
   primary 'Darke, P. L.'
   'Navia, M. A.' 2 'Fitzgerald, P. M. D.'
   'McKeever, B. M.' 2 'Lee, C.-T.'
   'Heimbach, J. C.' 2 'Herber, W. K.'
   'Springer, J. P.' 2 'Darke, P. L.'
   'Navia, M. A.' 3 'Fitzgerald, P. M. D.'
   'Springer, J. P.' 3 'Lee, C.-T.'
   'Heimbach, J. C.' 3 'Herber, W. K.'
   'Sigal, I. S.' 3 'Darke, P. L.'

_citation_author_citation_id (char)
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 data name _citation_id.
[citation_author]

_citation_author_name (char)
Name of an author of the citation; relevant for both journal articles 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_author]

_citation_author_ordinal (char)
This data name defines the order of the author’s name in the list of authors of a citation. Appears in list.
[citation_author]

_loop_citation_editor ()
Data items in the CITATION_EDITOR category record details about the editor associated with the book or book chapter citations in the _citation_list.
Example 1 - hypothetical example:
loop_
   _citation_editor_citation_id _citation_editor_name
   _citation_editor_citation_id
   5 'McKeever, B. M.'
   5 'Navia, M. A.'
   5 'Fitzgerald, P. M. D.'
   5 'Springer, J. P.'

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

_citation_editor_name (char)
Name of an editor of the citation; relevant for 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]

_citation_editor_ordinal (char)
This data name defines the order of the editor’s name in the list of editors of a citation. Appears in list.
[citation_editor]
Data items in the COMPUTING category record details about the computational programs used in the crystal structure analysis.


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.


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


Remarks about how the crystal was treated prior to intensity measurement. Particularly relevant when intensities were measured at low temperature.

Example(s): 'equilibrated in hutch for 24 hours', 'flash frozen in liquid nitrogen', 'slow cooled with direct air stream'

Fraction of unique (symmetry-independent) reflections measured out to \_diffrn\_refns\_theta\_full.

Appears in list. The permitted range is 0→1.0.

Fraction of unique (symmetry-independent) reflections measured out to \_diffrn\_refns\_theta\_max.

Appears in list. The permitted range is 0→1.0.

Special details of the diffraction measurement process. Should include information about source instability, crystal motion, degradation and so on.

Example(s): The results may not be entirely reliable as the measurement was made during a heat wave when the air-conditioning had failed.
The resolution of an area detector, in pixels/mm.

Related item(s):

- _diffrn_attenuator_attenuator_code
- _diffrn_attenuator_attenuator_material
- _diffrn_attenuator_attenuator_scale
- _diffrn_detector_type
- _diffrn_detector_dtime
- _diffrn_detector_material
- _diffrn_measurement_method
- _diffrn_measurement_details
- _diffrn_measurement_device

The permitted range is 0.0→∞.

A description of special aspects of the radiation detector.

The permitted range is

The deadtime in microseconds of the detector used to measure the diffraction intensities.

The detector used to measure the diffraction intensities.

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

The general class of the radiation detector.

The resolution of an area detector, in pixels/mm.
The elements of the diffractometer orientation matrix. These define the dimensions of the reciprocal cell and its orientation to the local diffractometer axes. See _diffn_orient_matrix_type.

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

<table>
<thead>
<tr>
<th>loop_</th>
<th>_diffn_orient_refln_angle_kappa</th>
<th>_diffn_orient_refln_angle_phi</th>
<th>_diffn_orient_refln_angle_theta</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-0.1429</td>
<td>1.87</td>
<td>-0.0226</td>
</tr>
<tr>
<td>2</td>
<td>-0.0558</td>
<td>-0.0230</td>
<td>0.05048</td>
</tr>
<tr>
<td>3</td>
<td>0.0587</td>
<td>0.0038</td>
<td>0.05048</td>
</tr>
<tr>
<td>4</td>
<td>-0.1766</td>
<td>0.0038</td>
<td>0.05048</td>
</tr>
<tr>
<td>5</td>
<td>0.0277</td>
<td>0.0038</td>
<td>0.05048</td>
</tr>
</tbody>
</table>

The indices of a reflection used to define the orientation matrix. See _diffn_orient_refln_index_h, _diffn_orient_refln_index_k and _diffn_orient_refln_index_l.


- _diffn_orient_matrix_UB_11: -0.04170
- _diffn_orient_matrix_UB_12: -0.0226
- _diffn_orient_matrix_UB_21: -0.00380
- _diffn_orient_matrix_UB_22: -0.0558
- _diffn_orient_matrix_UB_31: 0.0587
- _diffn_orient_matrix_UB_32: 0.1766
- _diffn_orient_matrix_UB_33: 0.0277

_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._

Data items in the DIFFRN category detail the measurement device used to support the crystal during data collection.

**Example:** 'profile data from \(q/2q\) scans'
_diffn_radiation_collimation  (char)
The collimation or focusing applied to the radiation.
Example(s): '0.3 nm double-pinhole', 'focusing mirrors' [diffn_radiation]

_diffn_radiation_filter_edge  (numb)
Absorption edge in Ångströms of the radiation filter used.
The permitted range is 0.0→∞. [diffn_radiation]

_diffn_radiation_inhomogeneity  (numb)
Half-width in millimetres of the incident beam in the direction perpendicular to the diffraction plane.
The permitted range is 0.0→∞. [diffn_radiation]

_diffn_radiation_monochromator  (char)
The method used to obtain monochromatic radiation. If a monochromator crystal is used the material and the indices of the Bragg reflection are specified.
Example(s): 'Zr filter', 'Ge 220', 'none', 'equatorial mounted graphite' [diffn_radiation]

_diffn_radiation_polarisation_norm  (numb)
The angle in degrees, as viewed from the specimen, between the perpendicular component of the polarisation and the diffraction plane. See _diffn_radiation_polarisation_ratio.
The permitted range is −180.0→180.0. [diffn_radiation]

_diffn_radiation_polarisation_ratio  (numb)
Polarisation ratio of the diffraction beam incident on the crystal. It is the ratio of the perpendicularly polarised to the parallel polarised component of the radiation. The perpendicular component forms an angle of _diffn_radiation_polarisation_norm to the normal to the diffraction plane of the sample (i.e. the plane containing the incident and reflected beams).
The permitted range is 0.0→∞. [diffn_radiation]

_diffn_radiation_probe  (char)
The nature of the radiation used (i.e. name of subatomic particle or region of the electromagnetic spectrum). It is strongly encouraged that this field be specified so that the probe radiation can be simply determined.
_x-ray  
_neutron  
_electron  
_gamma  [diffn_radiation]

_diffn_radiation_type  (char)
The type of the radiation. This represents a finer-grained level of description than _diffn_radiation_probe and is typically a description of the X-ray wavelength in Siegbahn notation.
Example(s): 'Cu Kα', 'Cu Kα1', 'Cu K-L2,3', 'white-beam' [diffn_radiation]

_diffn_radiation_xray_symbol  (char)
The IUPAC symbol for the X-ray wavelength for probe radiation.
K-L "S"  K_{01} in older Siegbahn notation
K-L "2"  K_{02} in older Siegbahn notation
K-M "S"  K_{β1} in older Siegbahn notation
K-L "2,3" use where K-L_{3} and K-L_{2} are not resolved [diffn_radiation]

_diffn_radiation_wavelength  (numb)
The radiation wavelength in Ångströms.
May appear in list containing _diffn_radiation_wavelength_id. The permitted range is 0.0→∞. [diffn_radiation]

_diffn_radiation_wavelength_id  (char)
An arbitrary code identifying each value of _diffn_radiation_wavelength. Items in the DIFFRN_RADIATION category are looped when multiple wavelengths are used. This code is used to link with the _diffn_refln_list. It must match with one of the _diffn_refln_wavelength_id codes.
Appears in list as essential element of loop structure. May match subsidiary data name(s): _diffn_refln_wavelength_id.
Example(s): 'x1', 'x2', 'neut' [diffn_radiation]

_diffn_radiation_wavelength_xr  (numb)
The relative weight of a wavelength identified by the code _diffn_radiation_wavelength_id in the list of wavelengths.
Appears in list containing _diffn_radiation_wavelength_id.
Where no value is given, the assumed value is '1.0'. The permitted range is 0.0→1.0. [diffn_radiation]
_diffrn_refln_[]

Data items in the DIFFRN_REFLN category record details about the intensities measured in the diffraction experiment. The DIFFRN_REFLN data items refer to individual intensity measurements, and must be included in looped lists. (The DIFFRN_REFLNS data items specify the parameters that apply to all intensity measurements. The DIFFRN_REFLNS data items are not looped.)

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

Loop:

_diffrn_refln_index_h_
_diffrn_refln_index_k_
_diffrn_refln_index_l_
_diffrn_refln_angle_omega_
_diffrn_refln_index_h_2_
_diffrn_refln_index_k_2_
_diffrn_refln_index_l_2_
_diffrn_refln_angle_omega_2_
_diffrn_refln_index_h_3_
_diffrn_refln_index_k_3_
_diffrn_refln_index_l_3_
_diffrn_refln_angle_omega_3_

Appears in list containing _diffrn_refln_index_. Must match data name _diffrn_attenuator_code_.

_diffrn_refln_class_code_ (char)
The code identifying the class to which this reflection has been assigned. This code must match a value of _diffrn_reflns_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 mm = \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 cell.

Appears in list containing _diffrn_refln_index_. Must match data name _diffrn_reflns_class_code_.

_diffrn_refln_counts_bg_1_ (numb)
_diffrn_refln_counts_bg_2_ (numb)
_diffrn_refln_counts_net_ (numb)
_diffrn_refln_counts_peaks_ (numb)
_diffrn_refln_counts_total_ (numb)

The diffractometer counts for the measurements: background before any subsequent cell transformations.

Appears in list containing _diffrn_refln_index_.

_diffrn_refln_cryystal_id_ (char)

Code identifying each crystal if multiple crystals are used. Is used to link with _exptlystal_id_ in the _exptl_crystal_ list.

Appears in list containing _diffrn_refln_index_. Must match data name _exptl_crystal_id_.

_diffrn_refln_detect_slit_horiz_ (numb)
_diffrn_refln_detect_slit_vert_ (numb)

Total slit apertures in degrees in the diffraction plane (*/horiz) and perpendicular to the diffraction plane (*/vert).

Appears in list containing _diffrn_refln_index_. The permitted range is 0.0–90.0.

_diffrn_refln_elapsed_time_ (numb)

Elapsed time in minutes from the start of diffraction measurement to the measurement of this intensity.

Appears in list containing _diffrn_refln_index_. The permitted range is 0.0–\infty.

_diffrn_refln_index_h_ **_**
_diffrn_refln_index_k_ **_**
_diffrn_refln_index_l_ **_**

Miller indices of a measured reflection. These need not match the _refln_index_. **_** _**_ _**_ values if a transformation of the original measured cell has taken place. Details of the cell transformation are described in _diffrn_reflns_reduction_process_. See also _diffrn_reflns_transf_matrix_.

Appears in list as essential element of loop structure.

_diffrn_refln_angle_omega_ (numb)

The diffractometer angles in degrees of a reflection. These correspond to the specified orientation matrix and the original measured cell before any subsequent cell transformations.

Appears in list containing _diffrn_refln_index_.

_diffrn_refln_attenuator_code_ (char)
The code identifying the attenuator setting for this reflection. This code must match one of the _diffrn_attenuator_code_ values.
**DIFFRN_REFLN**

- **_diffrn_refln_intensity_net** (numb)
  
  Net intensity calculated from the diffraction counts after the attenuator and standard scales have been applied.

  Appears in list containing **_diffrn_refln_index**. The permitted range is 0–∞.

- **_diffrn_refln_intensity_sigma** (numb)
  
  This definition has been superseded and is retained here only for archival purposes. Use instead **_diffrn_refln_intensity_u** Standard uncertainty (c.o.d.) of the net intensity calculated from the diffraction counts after the attenuator and standard scales have been applied.

  Appears in list containing **_diffrn_refln_index**. The permitted range is 0–∞.

- **_diffrn_refln_intensity_u** (numb)
  
  Standard uncertainty of the net intensity calculated from the diffraction counts after the attenuator and standard scales have been applied.

  Related item(s): **_diffrn_refln_intensity_sigma** (alternate).

  Appears in list containing **_diffrn_refln_index**. The permitted range is 0–∞.

- **_diffrn_refln_scale_group_code** (char)
  
  The code identifying the scale applying to this reflection. This code must match with a specified **_diffrn_scale_group_code** value.

  Appears in list containing **_diffrn_refln_index**. Must match data name **_diffrn_scale_group_code**.

- **_diffrn_refln_scan_mode** (char)
  
  The code identifying the mode of scanning with a diffractometer. See **_diffrn_refln_scan_width** and **_diffrn_refln_scan_mode_backgd**.

  Appears in list containing **_diffrn_refln_index**.

- **_diffrn_refln_scan_mode_backgd** (char)
  
  The code identifying the mode of scanning a reflection to measure the background intensity.

  Appears in list containing **_diffrn_refln_index**.

- **_diffrn_refln_scan_rate** (numb)
  
  The rate of scanning a reflection to measure the intensity in degrees per minute.

  Appears in list containing **_diffrn_refln_index**. The permitted range is 0–∞.

- **_diffrn_refln_scan_time_backgd** (numb)
  
  The time spent measuring each background in seconds.

  Appears in list containing **_diffrn_refln_index**. The permitted range is 0–∞.

- **_diffrn_refln_scan_width** (numb)
  
  The scan width in degrees of the scan mode defined by the code **_diffrn_refln_scan_mode**.

  Appears in list containing **_diffrn_refln_index**. The permitted range is 0.0–90.0.

- **_diffrn_refln_sint/lambda** (numb)
  
  The (sinθ)/λ value in reciprocal angstroms for this reflection.

  Appears in list containing **_diffrn_refln_index**. The permitted range is 0.0–∞.

- **_diffrn_refln_standard_code** (char)
  
  A code identifying that this reflection was measured as a standard intensity. The value must be ‘.’ or match one of the **_diffrn_standard_refln_code** values.

  Appears in list containing **_diffrn_refln_index**. Must match data name **_diffrn_standard_refln_code**.


- **_diffrn_refln_wavelength** (numb)
  
  The mean wavelength in ångströms of 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_refln_index**. The permitted range is 0.0–∞.

- **_diffrn_refln_wavelength_id** (char)
  
  Code identifying the wavelength in the **_diffrn_radiation_list**.

  Appears in list containing **_diffrn_refln_index**. Must match data name **_diffrn_radiation_wavelength_id**.

  Example(s): ’x1’, ’x2’, ’neut’.

---

**_diffrn_refln_[]**

Data items in the DIFFRN_REFLNS category record details about the set of intensities measured in the diffraction experiment. The DIFFRN_REFLNS data items specify the parameters that apply to all intensity measurements. The DIFFRN_REFLNS data items are not looped. (The DIFFRN_REFLNS data items refer to individual intensity measurements, and must be included in looped lists.)


<table>
<thead>
<tr>
<th>Data Item</th>
<th>Value</th>
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<tr>
<td>_diffrn_reflns_number</td>
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<td>_diffrn_reflns_av_equivalents</td>
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<tr>
<td>_diffrn_reflns_theta_max</td>
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</tr>
</tbody>
</table>
The permitted range is 0.0.

Elements of the matrix used to transform the diffraction reflection indices into the reflection indices. 

\[
\begin{pmatrix}
11 & 12 & 13 \\
21 & 22 & 23 \\
31 & 32 & 33
\end{pmatrix}
\]

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 K$_2$SeO$_4$. 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.

Loop details about the classes of reflections measured in the diffraction experiment.

**Example 1** - example corresponding to the one-dimensional incommensurately modulated structure of K$_2$SeO$_4$. 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.

Loop details about the classes of reflections measured in the diffraction experiment.
DIFFRN_REFLNS_CLASS

_diffrrn_reflns_class_code (char)
The code identifying a certain reflection class.
Appears in list as essential element of loop structure. May match sub-
sidiary data name(s): _diffrrn_reflns_class_code.
Example(s): '1', 'm1', 's2' [diffrrn_reflns_class]

_diffrrn_reflns_class_description (char)
Description of each reflection class.
Appears in list containing _diffrrn_reflns_class_code.
Example(s): 'm=1 first order satellites',
'BHOLO common projection reflections' [diffrrn_reflns_class]

_diffrrn_reflns_class_d_res_high (numb)
The highest resolution in ångströms for the interplanar spacing
in the reflections of each measured reflection class. This is the
smallest d value for this reflection class.
Appears in list containing _diffrrn_reflns_class_code. The per-
mitted range is 0.0→∞.
Example(s): [diffrrn_reflns_class]

_diffrrn_reflns_class_d_res_low (numb)
The lowest resolution in ångströms for the interplanar spacing
in the reflections of each measured reflection class. This is the
largest d value for this reflection class.
Appears in list containing _diffrrn_reflns_class_code. The per-
mitted range is 0.0→∞.
Example(s): [diffrrn_reflns_class]

_diffrrn_reflns_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 _diffrrn_reflns_class_code. The per-
mitted range is 0→∞.
Example(s): [diffrrn_reflns_class]

_diffrrn_scale_group_code (char)
The code identifying a specific measurement group (e.g. for
multi-film or multi-crystal data). The code must match a
_diffrrn_scale_group_code in the reflection list.
Appears in list as essential element of loop structure. May match sub-
sidiary data name(s): _diffrrn_scale_group_code.
Example(s): '1', '2', '3', 's1', 'A', 'B', 'c1', 'c2',
'c3' [diffrrn_scale_group]

_diffrrn_scale_group_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
_diffrrn_refln_ or _reln_ list on a common scale.
Appears in list containing _diffrrn_scale_group_code. The per-
mitted range is 0.0→∞.
Example(s): [diffrrn_scale_group]

_diffrrn_source[]
Data items in the DIFFRN_SOURCE category record details of the source of radiation used in the diffraction experiment.
Example 1 - based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP

_diffrrn_source 'rotating anode X-ray tube'
_diffrrn_source_type 'Rigaku RU-200'
_diffrrn_source_current 100
_diffrrn_source_power 50
_diffrrn_source_size '8 mm x 0.4 mm broad focus'

_diffrrn_radiation_source (char)
This definition has been superseded and is retained here only for
archival purposes. Use instead _diffrrn_source.
The source of radiation.
Example(s): [diffrrn_source]

_diffrrn_source (char)
The general class of the source of radiation.
Related item(s): _diffrrn_radiation_source (alternate).
Example(s): 'sealed X-ray tube', 'nuclear reactor',
'spallation source', 'electron microscope',
'rotating-anode X-ray tube', 'synchrotron'

_diffrrn_source_current (char)
The current in milliamperes at which the radiation source was
operated.
The permitted range is 0.0→∞.
Example(s): [diffrrn_source]

_diffrrn_source_details (char)
A description of special aspects of the source used.
Example(s): [diffrrn_source]

_diffrrn_source_power (numb)
The power in kilowatts at which the radiation source was
operated.
The permitted range is 0.0→∞.
Example(s): [diffrrn_source]

_diffrrn_source_size (char)
The dimensions of the source as viewed from the sample.
Example(s): '8mm x 0.4 mm fine-focus', 'broad focus'
Example(s): [diffrrn_source]
The chemical element symbol for the X-ray target (usually the anode) used for generation of X-rays. This can be used also for spallation sources.

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</table>

The voltage in kilovolts at which the radiation source was operated.

The permitted range is 0→∞.

_**diffrn_source_type**_ (char)

The make, model or name of the source of radiation.

Example(s): 'NSLS beamline X8C', 'Rigaku RU2000'

_**diffrn_source_voltage**_ (numb)

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

The permitted range is 0→∞.

_**diffrn_standards_number**_ (numb)

The number of unique standard reflections used in the diffraction measurements.

The permitted range is 0→∞.

_**diffrn_standards_scale_sigma**_ (numb)

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

_**diffrn_standards_scale_u**_ (numb)

The standard uncertainty of the individual mean standard scales applied to the intensity data.

_**diffrn_standards_decay_%**_ (numb)

The percentage decrease in the mean of the intensities for the set of standard reflections 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.

_**diffrn_standards_interval_time**_ (numb)

The volume of the intensity data set.

_**diffrn_standards_interval_count**_ (numb)

The permitted range is 0→∞.

_**diffrn_standards_decay_%**_ (numb)

The permitted range is 0→∞.

_**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→∞.

_**diffrn_standards_number**_ (numb)

The number of unique standard reflections used in the diffraction measurements.

The permitted range is 0→∞.

_**diffrn_standards_scale_sigma**_ (numb)

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

_**diffrn_standards_scale_u**_ (numb)

The standard uncertainty of the individual mean standard scales applied to the intensity data.

_**diffrn_standards_decay_%**_ (numb)

The percentage decrease in the mean of the intensities for the set of standard reflections 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.

_**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→∞.

_**diffrn_standards_number**_ (numb)

The number of unique standard reflections used in the diffraction measurements.

The permitted range is 0→∞.

_**diffrn_standards_scale_sigma**_ (numb)

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

_**diffrn_standards_scale_u**_ (numb)

The standard uncertainty of the individual mean standard scales applied to the intensity data.

_**diffrn_standards_decay_%**_ (numb)

The percentage decrease in the mean of the intensities for the set of standard reflections 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.

_**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→∞.

_**diffrn_standards_number**_ (numb)

The number of unique standard reflections used in the diffraction measurements.

The permitted range is 0→∞.

_**diffrn_standards_scale_sigma**_ (numb)

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

_**diffrn_standards_scale_u**_ (numb)

The standard uncertainty of the individual mean standard scales applied to the intensity data.

_**diffrn_standards_decay_%**_ (numb)

The percentage decrease in the mean of the intensities for the set of standard reflections 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.

_**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→∞.

_**diffrn_standards_number**_ (numb)

The number of unique standard reflections used in the diffraction measurements.

The permitted range is 0→∞.
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 $0.0 \rightarrow \infty$. [exptl]

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

The permitted range is $0.0 \rightarrow 1.0$. [exptl]

The absorption correction type and method. The value ‘empirical’ should not be used unless no more detailed information is available.

Example(s): ‘Templ analytical’, ‘Templ analytical (measured)’, ‘Templ cylindrical’.

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

The permitted range is $1 \rightarrow \infty$. [exptl]

Any special information about the experimental work prior to the intensity measurement. See also _exptl(crystal prep)utation._

May appear in list containing _exptl(crystal id). The permitted range is $0.0 \rightarrow \infty$. [exptl]

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

$$F(000) = \left[ \sum_{i} f_{i}^{2} + \left( \sum_{i} f_{i} \right)^{2} \right]^{1/2}$$

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

May appear in list containing _exptl(crystal id). The permitted range is $0.0 \rightarrow \infty$. [exptl]
_exptl_crystal_id (char)
Code identifying each crystal if multiple crystals are used. It
is used to link with _diffn_refln_crystal_id in intensity
measurement and with _refln_crystal_id in the _refln_list.
Appears in list as essential element of loop structure. May
match subsidiary data name(s): _diffn_refln_crystal_id, _re-
fln_crystal_id.

_exptl_crystal_preparation (char)
Details of crystal growth and preparation of the crystal (e.g.
mounting) prior to the intensity measurements.
May appear in list containing _exptl_crystal_id.
Example(s):
`mounted in an argon-filled quartz capillary`

_exptl_crystal_pressure_history (char)
Relevant details concerning the pressure history of the sample.
May appear in list containing _exptl_crystal_id.

_exptl_crystal_length
_exptl_crystal_max
_exptl_crystal_id
_exptl_crystal_min
_exptl_crystal_rad
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 *rad item is its
radius and the *length item is its length. These may appear in
a list with _exptl_crystal_id if multiple crystals are used in the
experiment.
May appear in list containing _exptl_crystal_id. The permitted
range is 0.0→∞.

_exptl_crystal_thermal_history (char)
Relevant details concerning the thermal history of the sample.
May appear in list containing _exptl_crystal_id.

_exptl_crystal_face[]
Data items in the EXPTL.CRYSTAL FACE category record
details of the crystal faces.

Example 1 - based on structure PAWD2 of Vittal & Dean [(1996). Acta
Cryst. C52, 1180–1182].

_loop_
_exptl_crystal_face_index_h
_exptl_crystal_face_index_k
_exptl_crystal_face_index_l
_exptl_crystal_face_perp_dist
0 1 -2 1.8274
1 0 -2 .17571
-1 1 -2 .17845
-2 1 0 0.21010
-1 0 2 .18849
1 -1 2 .20605
2 -1 0 .24680
-1 2 0 .19688
0 1 2 .15206

_chem_
**_geom_angle_**

Data items in the GEOM_ANGLE category record details about the bond angles, as calculated from the contents of 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>
</tr>
</thead>
<tbody>
<tr>
<td>C2</td>
<td>C1 C5 111.6(2) 1.555 1.555 1.555 yes</td>
<td></td>
<td></td>
</tr>
<tr>
<td>O1</td>
<td>C2 C3 110.9(2) 1.555 1.555 1.555 yes</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C2</td>
<td>C2 O21 127.0(3) 1.555 1.555 1.555 yes</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C2</td>
<td>C3 N4 101.3(2) 1.555 1.555 1.555 yes</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C2</td>
<td>C3 N3 107(1) 1.555 1.555 1.555 no</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C2</td>
<td>C3 O21 122.2(3) 1.555 1.555 1.555 yes</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C2</td>
<td>C3 116.7(2) 1.555 1.555 1.555 yes</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**_geom_bond_**

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


<table>
<thead>
<tr>
<th>Loop</th>
<th>geom_bond_atom_site_label_1</th>
<th>geom_bond_atom_site_label_2</th>
</tr>
</thead>
<tbody>
<tr>
<td>C2</td>
<td>C1 1.342(4) 1.555 1.555 1.555 yes</td>
<td></td>
</tr>
<tr>
<td>C5</td>
<td>C1 1.439(3) 1.555 1.555 1.555 yes</td>
<td></td>
</tr>
<tr>
<td>C2</td>
<td>C3 1.512(4) 1.555 1.555 1.555 yes</td>
<td></td>
</tr>
<tr>
<td>C2</td>
<td>C2 O21 1.199(4) 1.555 1.555 yes</td>
<td></td>
</tr>
<tr>
<td>C3</td>
<td>N4 1.465(3) 1.555 1.555 yes</td>
<td></td>
</tr>
<tr>
<td>C3</td>
<td>C3 1.537(4) 1.555 1.555 1.555 yes</td>
<td></td>
</tr>
<tr>
<td>C3</td>
<td>N3 1.20(3) 1.555 1.555 yes</td>
<td></td>
</tr>
<tr>
<td>C5</td>
<td>C5 1.472(3) 1.555 1.555 yes</td>
<td></td>
</tr>
</tbody>
</table>

**_geom_angle_** (numb)

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

**_geom_angle_publ_flag_** (char)

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

**_geom_bond_** (numb)

The intramolecular bond distance in Angstroms. Appears in list containing _geom_bond_atom_site_label_. The permitted range is 0.0–∞. **_geom_bond_publ_flag_** (char)

This code signals if the bond distance is referred to in a publication or should be placed in a list of significant bond distances.
The bond valence calculated from the bond valence model.

Appears in list containing _geom_bond_valence_ (numb)

The bond valence calculated from the bond valence model.

Appears in list containing _geom_bond_valence_ (numb)

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


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_.

The torsion angle is the angle of twist required to superimpose the projection of the vector site2-site1 onto the projection of the vector site3-site4. Clockwise torsions are positive, anticlockwise torsions are negative.


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

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_frac_x_, _atom_site_frac_y_ and _atom_site_frac_z_. It must match a number given in _symmetry_equiv_pos_site_id_. k, l and m refer to the translations that are subsequently applied to the symmetry transformed coordinates to generate the atom used in calculating the hydrogen bond. These translations (x, y, z) are related to (k, l, m) by the relations k = 5 + x, l = 5 + y, m = 5 + z. By adding 5 to the translations, the use of negative numbers is avoided.

Appears in list containing _geom_hbond_atom_site_label_.

Example(s): 1. {no symmetry or translation to site}, '4' (4th symmetry operation applied), '7_645Y' (7th symm. posn. on x; -b on y)

GEOM_TORSION

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

Example 1 - based on data set CLPHO6 of Ferguson, Ruhl, McKervey 

loop_

_geom_torsion_atom_site_label_1
_geom_torsion_atom_site_label_2
_geom_torsion_atom_site_label_3
_geom_torsion_atom_site_label_4
_geom_torsion_site symmetry_1
_geom_torsion_site symmetry_2
_geom_torsion_site symmetry_3
_geom_torsion_site symmetry_4
_geom_torsion_publ_flag

<table>
<thead>
<tr>
<th>C(9)</th>
<th>O(2)</th>
<th>C(7)</th>
<th>C(2)</th>
<th>71.82(2)</th>
<th>...</th>
<th>yes</th>
</tr>
</thead>
<tbody>
<tr>
<td>C(7)</td>
<td>O(2)</td>
<td>C(9)</td>
<td>C(10)</td>
<td>-168.01(3)</td>
<td>...</td>
<td>2.666 yes</td>
</tr>
<tr>
<td>C(10)</td>
<td>O(3)</td>
<td>C(8)</td>
<td>C(6)</td>
<td>-167.73(3)</td>
<td>...</td>
<td>yes</td>
</tr>
<tr>
<td>C(8)</td>
<td>O(3)</td>
<td>C(10)</td>
<td>C(9)</td>
<td>-69.72(2)</td>
<td>...</td>
<td>2.666 yes</td>
</tr>
<tr>
<td>O(1)</td>
<td>C(1)</td>
<td>C(2)</td>
<td>C(3)</td>
<td>-179.5(4)</td>
<td>...</td>
<td>no</td>
</tr>
<tr>
<td>O(1)</td>
<td>C(11)</td>
<td>C(2)</td>
<td>C(7)</td>
<td>-0.6(1)</td>
<td>...</td>
<td>no</td>
</tr>
</tbody>
</table>
Data items in the JOURNAL_INDEX category are used to list terms employed in generating the journal indexes. Normally the creator of a CIF will not specify these data items. The data names are not defined in the Dictionary because they are for journal use only.


Example 2 - based on a paper by Coleman, Patrick, Andersen & Retting ([1996], Acta Cryst. C52, 1525–1527.}

The name and address of the author submitting the manuscript for publication. 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(s):
; Professor George Ferguson
Department of Chemistry and Biochemistry
University of Guelph
Ontario
Canada
N1G 2W1
;
_publ_contact_author_address
The address of the author submitting the manuscript and data block. This is the person contacted by the journal editorial staff.

Example(s):
; Department of Chemistry and Biochemistry
University of Guelph
Ontario
Canada
N1G 2W1
;
_publ_contact_author_email (char)
Email address in a format recognisable to international networks.

Example(s): 'name@host.domain.country', 'bn@ucr.org'

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

Example(s): '12(34)9477334', '12(34)349477334'

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

Example(s): 'Professor George Ferguson'

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

Example(s): '12(34)9477330', '12(34)349477330x5643'

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

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

Example(s): 'Tex file created by FrameMaker on a Sun 3/260'

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

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

_publ_requested_category (char)
The category of paper submitted. For submission to Acta Crystallographica Section C or Acta Crystallographica Section E, only those codes indicated for use with those journals should be used.

FA Full article
FI Full submission - inorganic (Acta C)
FU Full submission - organic (Acta C)
PM Full submission - metal-organic (Acta C)
CI CIF-access paper - inorganic (Acta C)
CO CIF-access paper - organic (Acta C)
CM CIF-access paper - metal-organic (Acta C)
EI Electronic submission - inorganic (Acta E)
EO Electronic submission - organic (Acta E)
EM Electronic submission - metal-organic (Acta E)
AD Addenda & Errata (Acta C, Acta E)
SC Short Communication

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

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

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

_publ_section_title
_publ_section_title_footnote
_publ_section_synopsis
_publ_section_abstract
_publ_section_comment
_publ_section_introduction
_publ_section_exptl_prep
_publ_section_exptl_refinement
_publ_section_exptl_solution
_publ_section_discussion
_publ_section_acknowledgements
_publ_section_references
_publ_section_figure_captions
_publ_section_table_legends

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.

_loop_ _publ_author_[]

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

Example(s):
- Willis, Anthony C., Research School of Chemistry, Australian National University, GPO Box 4, Canberra, ACT, Australia 2601.

_publ_author_address  (char)
The address of a publication author. If there is more than one author this will be looped with _publ_author_name.

Example(s):
- Department Institute Street City and postcode COUNTRY ; [publ_author]

_publ_author_footnote  (char)
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.

Example(s): 'On leave from U. Western Australia', 'Also at Department of Biophysics' [publ_author]

_publ_author_name  (char)
The name of a publication author. If there are multiple authors they 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.


_loop_ _publ_body_[]

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


_publ_body_title  (char)

A text section of a submitted paper. Appears in list containing _publ_body_element.

Example(s):
- 'Introduction', 'Theory', 'In...', 'As the wide...', 'The two-channel...'
- subsection 3.1 'The two-channel entropy S\[\D\rr(r)\]'...
- subsection 3.2 'Uniform vs informative prior model densities'...
- subsection 3.2.1 'Use of uniform models'...
- Straightforward algebra leads to expressions analogous to...

_publ_body_format  (char)

The functional role of the associated text section.

Example(s):
- section 1 Introduction
- section 2 Theory
- As the wide dynamic range involved in the total electron density...
- The two-channel method for retrieval of the deformation electron density...
- Straightforward algebra leads to expressions analogous to...

_publ_body_element  (char)

Appendix

Example(s):
- subsection 3.1 'The two-channel entropy S\[\D\rr(r)\]
- subsection 3.2 'Uniform vs informative prior model densities'
- subsection 3.2.1 'Use of uniform models'
- Straightforward algebra leads to expressions analogous to...
_publ_body_format (char)
Code indicating the appropriate typesetting conventions for accented characters and special symbols in the text section.
- ascii: no coding for special symbols
- cif: CIF convention
- latex: \LaTeX\
- rtf: Rich Text Format
- sgml: SGML (ISO 8879)
- tex: \TeX\
- troff: troff or nroff

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

_publ_body_label (char)
Code identifying the section of text. The combination of this with _publ_body_element must be unique.
Appears in list as essential element of loop structure. Uniqueness of loop packet tested on _publ_body_element.

Example(s): '1', '1.1', '2.1.3'

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

_publ_manuscript_incl_extra_defn (char)
Flags whether the corresponding data item marked for inclusion in a journal request list is a standard CIF definition or not.
- no: not a standard CIF data name
- y: abbreviation for "yes"

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

_publ_manuscript_incl_extra_info (char)
A short note indicating the reason why the author wishes the corresponding data item marked for inclusion in the journal request list to be published.
Appears in list containing _publ_manuscript_incl_extra_item.

_publ_manuscript_incl_extra_item (char)
Specifies the inclusion of specific data into a manuscript which is not normally requested by the journal. The values of this item are the extra data names (which must be enclosed in single quotes) that will be added to the journal request list.
Appears in list as essential element of loop structure.

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


**Example 2** - hypothetical example including both standard CIF data items and a non-CIF quantity which the author wishes to list.
The nature of the absolute structure and how it was determined.

The measure of absolute structure as defined by Rogers. The

The highest resolution in Ångström for the interplanar spacing

The permitted range is 0.0 → 1.0.

The measure of absolute structure defined as by Flack. For
centrosymmetric structures the only permitted value, if the data
name is present, is ‘inapplicable’ represented by ‘.’. For non-
centrosymmetric structures the value must lie in the 99.97%
Gaussian confidence interval $-3u < \eta < 1 + 3u$ and a stan-
dard uncertainty (e.s.d.) $u$ must be supplied. The _enumer-
atation_range of $0.0:1.0$ is correctly interpreted as meaning
$(0.0 - 3u) < \eta < (1.0 + 3u)$.


The permitted range is $-1.0$ → $1.0$.

The measure of absolute structure as defined by Rogers. The
value must lie in the 99.97% Gaussian confidence interval $-1 - 3u < \eta < 1 + 3u$ and a standard uncertainty (e.s.d.) $u$ must be supplied. The _enumeration_range of $-1.0:1.0$ is correctly interpreted as meaning $(-1.0 - 3u) < \eta < (1.0 + 3u)$.


The permitted range is $-1.0$ → $1.0$.

The highest resolution in Ångström for the interplanar spacing
in the reflections used in refinement. This is the smallest d value.

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

The lowest resolution in Ångström for the interplanar spacing
in the reflections used in refinement. This is the highest d value.

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

The extinction coefficient used to calculate the correction
factor applied to the structure-factor data. The nature of the
extinction coefficient is given in the definitions of _refine ls_extinction_expression and _refine ls_extinction_method. For the ‘Zachariasen’ method it is the $r^*$ 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 ‘p’ value. Note that the magnitude of these values is usually of the order of 1000.

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


Example(s): ‘3472(ES)’ (Zachariasen coefficient $r^* = 0.3475 \times 10^3$)

A description or reference of 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.


Copenhagen: Munksgaard.

A description of the extinction correction method applied with
the data item _refine ls_extinction_coef. This description
should include information about the correction method, either
‘Becker–Coppens’ or ‘Zachariasen’. The latter is sometimes re-
ferred to as the ‘Larson’ method even though it employs Zachari-
asen’s formula. The Becker–Coppens procedure is referred to as
‘type 1’ when correcting secondary extinction dominated by the
mosaic spread; as ‘type 2’ when secondary extinction is domi-
nated by particle size and includes a primary extinction compo-
nent; and as ‘mixed’ when there is a mixture of types 1 and 2. For
the Becker–Coppens method it is also necessary to set the mosaic
distribution as either ‘Gaussian’ or ‘Lorentzian’; and the nature
of the extinction as ‘isotropic’ or ‘anisotropic’. Note that if either
the ‘mixed’ or ‘anisotropic’ corrections are applied the multi-
ple coefficients cannot be contained in _extinction_coef and
must be listed in _refine_special_details.


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

Example(s): ‘B-C type 2 Gaussian isotropic’, ‘none’.

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

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

$Y_{obs}$ = 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/σ²), $u$ = standard uncertainty, $N_{ref}$ = the number of reflections used in the refinement, $N_{param}$ = the number of refined parameters, and the sum $\sum$ is taken over the specified reflections.

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

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

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

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

Related item(s): _refine ls_goodness_of_fit_obs_ (alternate). The permitted range is 0.0 → \( \infty \).

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

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

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

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

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

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

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

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

Treatment of hydrogen atoms in the least-squares refinement.

- reflall: refined all H parameters
- refxyz: refined H coordinates only
- refU: refined H U only
- noref: no refinement of H parameters

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

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_.

Where no value is given, the assumed value is 1.0. The permitted range is 0 → \( \infty \).

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 → \( \infty \).

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

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

The number of restrained parameters. These are parameters which are not directly dependent on another refined parameter. Often restrained parameters 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 → \( \infty \).
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_vh_factor_definitions.

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

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

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

Residual factor R(I) for significantly intense reflections (satisfying _refine_ls_threshold_expression) and included in the refinement. This is most often calculated in Rietveld refinements of powder data, where it is referred to as R$_{\text{I}}$ or R$_{\text{I(ris)}}$.

\[ I = \sum \frac{|I_{\text{obs}}| - |I_{\text{calc}}|}{\sum |I_{\text{obs}}|} \]

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

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

Residual factor for the reflections classified as 'observed' (see _refine_ls_structure_factor_coef). \( Y_{\text{calc}} \) = the observed coefficients (see _refine_ls_structure_factor_coef), \( w \) = the least-squares reflection weight \([1/\text{square of standard uncertainty (e.s.d.)}])\), \( P_{\text{calc}} \) = the calculated restraint values, \( P_{\text{target}} \) = 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), \( N_{\text{param}} \) = 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 → \( \infty \).

Residual factor (alternate). The permitted range is 0.0 → \( \infty \).
\_\texttt{refine\_ls\_restrained\_S\_obs} (numb)

This definition has been superseded and is retained here only for archival purposes. Use instead \_\texttt{refine\_ls\_restrained\_S\_gt}

The least-squares goodness-of-fit parameter \( S \) for observed reflections, after the final cycle of least squares. This parameter explicitly includes the restraints applied in the least-squares process. See also \_\texttt{refine\_ls\_summary\_of\_fit\_definitions}.

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

where \( Y_{\text{obs}} \) is the observed coefficients (see \_\texttt{refine\_ls\_structure\_factor\_coef}), \( Y_{\text{calc}} \) is the calculated coefficients (see \_\texttt{refine\_ls\_structure\_factor\_coef}), \( w \) is the least-squares reflection weight [\( 1/\text{square of standard uncertainty (e.s.d.)} \)], \( P_{\text{calc}} \) is the calculated restraint values, \( P_{\text{target}} \) is the target restraint values, \( N_{\text{ref}} \) is the number of reflections used in the refinement (see \_\texttt{refine\_ls\_number\_refines}), \( N_{\text{restr}} \) is the number of restraints (see \_\texttt{refine\_ls\_number\_restraints}), \( N_{\text{sum}} \) is the number of refined parameters (see \_\texttt{refine\_ls\_number\_parameters})). The sum \( \sum \) is taken over the specified reflections, and the sum \( \sum \) is taken over the restraints.

\_\texttt{refine\_ls\_shift/\text{ed}_\text{max}} (numb)

This definition has been superseded and is retained here only for archival purposes. Use instead \_\texttt{refine\_ls\_shift/\text{su}_\text{max}}

The largest ratio of the final least-squares parameter shift divided by the final standard uncertainty (\( \text{s.u.} \), formerly described as estimated standard deviation, \( \text{e.s.d.} \)).

\_\texttt{refine\_ls\_shift/\text{ed}_\text{mean}} (numb)

This definition has been superseded and is retained here only for archival purposes. Use instead \_\texttt{refine\_ls\_shift/\text{su}_\text{mean}}

The average ratio of the final least-squares parameter shift divided by the final standard uncertainty (\( \text{s.u.} \), formerly described as estimated standard deviation, \( \text{e.s.d.} \)).

\_\texttt{refine\_ls\_shift/\text{su}_\text{max}} (numb)

The largest ratio of the final least-squares parameter shift divided by the final standard uncertainty.

\text{Related item(s)}: \_\texttt{refine\_ls\_shift/\text{ed}_\text{max}} (alternate). The permitted range is \( 0.0 \rightarrow \infty \).

\_\texttt{refine\_ls\_shift/\text{su}_\text{mean}} (numb)

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

\text{Related item(s)}: \_\texttt{refine\_ls\_shift/\text{ed}_\text{mean}} (alternate). The permitted range is \( 0.0 \rightarrow \infty \).

\_\texttt{refine\_ls\_structure\_factor\_coef} (char)

Structure-factor coefficient \( [F, F^2 \text{ or } I] \), used in the least-squares refinement process.

\( F \) structure factor magnitude

\( F_{\text{sqd}} \) structure factor squared

\( I_{\text{net}} \) net intensity

Where no value is given, the assumed value is \( F' \).

\_\texttt{refine\_ls\_weighting\_details} (char)

A description of special aspects of the weighting scheme used in least-squares refinement. Used to describe the weighting when the value of \_\texttt{refine\_ls\_weighting\_scheme} is specified as 'calc'.

\text{Example(s)}:

\text{Sigdel model of Koenig-Hendricks on:}

\text{Sigdel = A sig + B sig*(sin(\varpi)/1 - 1/6)}

\text{A sig = 22.0, B sig = 150.0 at the beginning of refinement.}

\text{A sig = 16.0, B sig = 60.0 at the end of refinement.}

\_\texttt{refine\_ls\_weighting\_scheme} (char)

The weighting scheme applied in the least-squares process. The standard code may be followed by a description of the weight (but \textit{see} \_\texttt{refine\_ls\_weighting\_details} for a preferred approach).

\text{sigma} based on measured s.u.'s

\text{unit} unit or no weights applied

\text{calc} calculated weights applied

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

\_\texttt{refine\_ls\_wR\_factor\_all} (numb)

Weighted residual factors for all reflections. The reflections also satisfy the resolution limits established by \_\texttt{refine\_ls\_d\_res\_high} and \_\texttt{refine\_ls\_d\_res\_low}. See also the \_\texttt{refine\_ls\_R\_factor\_definitions}.

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

where \( Y_{\text{obs}} \) is the observed amplitude specified by \_\texttt{refine\_ls\_structure\_factor\_coef}, \( Y_{\text{calc}} \) is the calculated amplitude specified by \_\texttt{refine\_ls\_structure\_factor\_coef}, \( w \) is the least-squares weight, and the sum \( \sum \) is taken over the specified reflections.

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

\_\texttt{refine\_ls\_wR\_factor\_gt} (numb)

Weighted residual factors for significantly intense reflections (satisfying \_\texttt{refine\_ls\_threshold\_expression}) included in the refinement. The reflections also satisfy the resolution limits established by \_\texttt{refine\_ls\_d\_res\_high} and \_\texttt{refine\_ls\_d\_res\_low}. See also the \_\texttt{refine\_ls\_R\_factor\_definitions}.

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

where \( Y_{\text{obs}} \) is the observed amplitude specified by \_\texttt{refine\_ls\_structure\_factor\_coef}, \( Y_{\text{calc}} \) is the calculated amplitude specified by \_\texttt{refine\_ls\_structure\_factor\_coef}, \( w \) is the least-squares weight, and the sum \( \sum \) is taken over the specified reflections.

\text{Related item(s)}: \_\texttt{refine\_ls\_wR\_factor\_obs} (alternate). The permitted range is \( 0.0 \rightarrow \infty \).
This definition has been superseded and is retained here only for archival purposes. Use instead _refine_ls_wR_factor_gt_

Weighted residual factors for the reflections classified as ‘observed’ (see _refins_observed_criterion_ and included in the refinement. The reflections also satisfy the resolution limits established by _refine_ls_d_res_high_ and _refine_ls_d_res_low_. See also the _refine_ls_R_factor_ref_ definitions.

$$wR = \sqrt{\frac{\sum w(Y_{\text{obs}} - Y_{\text{calc}})^2}{\sum wY_{\text{obs}}^2}}$$

$Y_{\text{obs}}$ is the observed amplitude specified by _refine_ls_structure_factor_coeff_, $Y_{\text{calc}}$ is the calculated amplitude specified by _refine_ls_structure_factor_coeff_, $w$ is the least-squares weight, and the sum $\sum$ is taken over the specified reflections.

The permitted range is 0.0 → ∞.

**_refine_special_details_**

Description of special aspects of the refinement process.

**Example 1 - example for a modulated structure extracted from van Smaalen ([1991]. J. Phys.: Condens. Matter, 3, 1247–1263.)**

loop _refine_ls_class_R_factor_all_
  _refine_ls_class_code_
  0.659 'main'
  0.678 'com'
  0.664 'NbdRef1'
  0.664 'LaRef1'
  0.112 'Sat1'
  0.177 'Sat2'

For each reflection class, the highest resolution in ångström for the reflections used in 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 → ∞.

**_refine_ls_class_d_res_high_**

For each reflection class, the lowest resolution in ångström for the reflections used in 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 → ∞.

**_refine_ls_class_d_res_low_**

For each reflection class, the residual factor for all reflections, and for significantly intense reflections (see _refins_threshold_expression_) and included in the refinement. This is the conventional $R$ factor.

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

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

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

**_refine_ls_class_R_Fsqd_factor_**

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 _refins_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_.

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

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

Appears in list containing _refine_ls_class_code_. The permitted range is 0.0 → ∞.
the refinement. This is most often calculated in Rietveld refinement of powder data, where it is referred to as $R_\text{wp}$ or $R_\text{merge}$.

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

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

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

`refine_is_class`<br>`wR or all`<br>`(num)`

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_is_class_d_res_high` and `refine_is_class_d_res_low`.

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

$Y(\text{obs})$ = the observed amplitude specified by `refine_isstructure_factor_coef`. $Y(\text{calc})$ = the calculated amplitude specified by `refine_isstructure_factor_coef`, $w$ = the least-squares weight, and the sum $\sum$ is taken over the reflections of this class. See also `refine_is_class_B_factor` definitions.

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

---


```bash
loop_  
  _refln_index_h  _refln_index_k  _refln_index_l  
  _refln_F_squared_calc  
  _refln_F_squared_meas  
  _refln_F_squared_sigma  
  _refln_include_status  
2 0 0 85.57 58.90 1.45 o 
3 0 0 15718.18 15631.06 30.40 o 
4 0 0 55613.11 49840.09 61.86 o 
5 0 0 246.85 241.86 10.02 o 
6 0 0 82.16 69.97 1.93 o 
# = - - - data truncated for brevity = - - -
```

---


```bash
loop_  
  _refln_index_h  _refln_index_k  _refln_index_l  
  _refln_F_meas  
  _refln_F_calc  
  _refln_F_sigma  
  _refln_include_status  
  _refln_scale_group_code  
0 0 6 34.935 36.034 3.143 o 1 
0 0 12 42.599 40.855 2.131 o 1 
0 1 1 59.172 57.976 4.719 o 1 
0 1 2 89.694 94.741 4.325 o 1 
0 1 6 6.755 7.102 0.895 < 1 
# = - - - data truncated for brevity = - - -
```

---

**_refln_A_calc**<br>`(num)`

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

$$A = |F| \cos(\text{phase})$$

Appears in list containing `refln_index`. [ref ln]

`refln_B_calc`<br>`(num)`

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`. [ref ln]

`refln_class_code`<br>`(char)`

The code identifying the class to which this reflection has been assigned. This code must match a value of `refine_is_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 data name `refln_class_code`. [ref ln]

`refln_d_spacing`<br>`(num)`

The $d$ spacing in ångströms for this reflection. It is related to the $(\sin\theta)/\lambda$ value by the expression $\text{refln_d_spacing} = 2/(\text{refln_sin/lambda})$.

Appears in list containing `refln_index`. The permitted range is 0.0→∞. [gsb band]

`refln_crystal_id`<br>`(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 data name `exptl_crystal_id`. [ref ln]

`refln_F_calc`<br>`(num)`

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`. [ref ln]

`refln_F_scaled_calc`<br>`refln_F_scaled_meas`<br>`refln_F_scaled_sigma`<br>`(num)`
Appears in list containing _refln_index_.  

_class_  

Classification of a reflection so as to indicate its status with respect to inclusion in refinement and calculation of $R$ factors.

- o (lower-case letter o for 'observed')
  - satisfies $\text{refln\_ls\_d\_res\_low}$
  - satisfies $\text{refln\_ls\_d\_res\_high}$
  - exceeds $\text{refln\_threshold\_expression}$
- <
  - satisfies $\text{refln\_ls\_d\_res\_high}$
  - satisfies $\text{refln\_ls\_d\_res\_low}$
  - does not exceed $\text{refln\_threshold\_expression}$
- x unreliable measurement – not used
- h does not satisfy $\text{refln\_ls\_d\_res\_high}$
- l does not satisfy $\text{refln\_ls\_d\_res\_low}$

Related item(s): _refln\_observed\_status (alternate). Appears in list containing _refln_index_. Where no value is given, the assumed value is 'o'.

## _refln_index_h_  

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

Appears in list as essential element of loop structure.

## _refln_intensity_calc_  

## _refln_intensity_meas_  

## _refln_intensity_sigma_  

The calculated, measured and standard uncertainty (derived from measurement) of the intensity, in the measured units.

Appears in list containing _refln_index_.

## _refln_mean_path_length_tbar_  

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

Appears in list containing _refln_index_.

## _refln_observed_status_  

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

Classification of a reflection so as to indicate its status with respect to inclusion in refinement and calculation of $R$ factors.

## _refln_phase_calc_  

The calculated structure-factor phase in degrees.

Appears in list containing _refln_index_.

## _refln_phase_meas_  

The measured structure-factor phase in degrees.

Appears in list containing _refln_index_.

## _refln_refinement_status_  

Status of reflection in the structure refinement process.

- incl included in ls process
- excl excluded from ls process
- extn excluded due to extinction

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

## _refln_scale_group_code_  

Code identifying the structure-factor scale. This code must correspond to one of the _refln\_scale\_group\_code values.

Appears in list containing _refln_index_. Must match data name _refln\_scale\_group\_code_.

Example(s): '1', '2', '3', 's1', 'A', 'B', 'c1', 'c2', 'c3' [refln]

## _refln_sint_/lambda_  

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

Appears in list containing _refln_index_. The permitted range is $0.0 \rightarrow \infty$.

## _refln_symmetry_epsilon_  

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

Appears in list containing _refln_index_. The permitted range is $1 \rightarrow 48$.

## _refln_symmetry_multiplicity_  

The number of reflections symmetry-equivalent under the Laue symmetry to the present reflection. In the Laue symmetry, Friedel opposites ($hkl$ and $-h-k-l$) are equivalent. Tables of symmetry-equivalent reflections are available in International Tables for Crystallography, Volume A (1987), section 10.2.

Appears in list containing _refln_index_. The permitted range is $1 \rightarrow 48$.

## _refln_wavelength_  

The mean wavelength in ångströms of 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_. The permitted range is $0.0 \rightarrow \infty$.

## _refln_wavelength_id_  

Code identifying the wavelength in the _diffrn\_radiation\_list. See _diffrn\_radiation\_wave\_length\_id_.

Appears in list containing _refln_index_. Must match data name _diffrn\_radiation\_wave\_length\_id_.

Example(s): '1' [refln]
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.


<table>
<thead>
<tr>
<th>Related item(s):</th>
<th>reflns_number_observed (alternate).</th>
<th>REFLNS_number_gt</th>
<th>reflns_number_observed</th>
<th>reflns_number_total</th>
<th>reflns_observedCriterion</th>
<th>reflns_special_details</th>
<th>reflns_threshold_expression</th>
</tr>
</thead>
<tbody>
<tr>
<td>reflns_limit_h_min</td>
<td>0</td>
<td>reflns_limit_h_max</td>
<td>6</td>
<td>reflns_limit_k_min</td>
<td>0</td>
<td>reflns_limit_k_max</td>
<td>17</td>
</tr>
<tr>
<td>reflns_d_resolution_high</td>
<td>0.8733</td>
<td>reflns_d_resolution_low</td>
<td>11.9202</td>
<td>reflns_d_resolution_high</td>
<td>0.8733</td>
<td>reflns_d_resolution_low</td>
<td>11.9202</td>
</tr>
</tbody>
</table>

The permitted range is 0→∞.

**reflns_d_resolution_high**

The highest and lowest resolution in ångströms for the interplanar spacings in the reflections. These are the smallest and largest d values.

The permitted range is 0.0→∞.

**reflns_d_resolution_low**

**reflns_Friedel_coverage**

The proportion of Friedel related reflections present in the number of the ‘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_reflns_list, N(\text{Crystal class}) is the number of reflections obtained on averaging under the symmetry of the crystal class, N(\text{Laue symmetry}) is the number of reflections obtained on averaging under the Laue symmetry.

Examples: (a) For centrosymmetric structures its value 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 \(hk\) is equivalent to \(-h-k-l\) in the crystal class and all Friedel pairs \{hk; \(-h-k-l\}\} have been measured. (c) For whole-sphere data in space group \(Pmm2\), the value will be <1.0 because although reflections \(hk\) and \(-h-k-l\) are not equivalent when \(hk\) indices are non-zero, they are when \(l = 0\). (d) For a crystal in the group \(Pnm2\) measurements of the two inequivalent octants \(h \geq 0, k \geq 0, l \leq 0\) 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 zero value for _reflns_Friedel_coverage_.

The permitted range is 0.0→1.0.

**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_. It 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. The special characteristics of the reflections included in the _refln_ list should be given in the item _reflns_special_details_.

**reflns_number_observed**

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

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 _reflns_observedCriterion_). They may include Friedel equivalent reflections according to the nature of the structure and the procedures used. The special characteristics of the reflections included in the _refln_ list should be given in the item _reflns_special_details_.

**reflns_number_total**

The total number of reflections in the _refln_ list (not the _diffrn_refln_ list). It 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. The 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_observedCriterion**

**reflns_special_details**

**reflns_threshold_expression**

The threshold, usually based on multiples of \(u(I)\), \(u(F^2)\) or \(u(F)\), that serves to identify significantly intense reflections, the number of which is given by _reflns_number_gt_. These reflections are used in the calculation of _reflns_is_h_factor_gt_.

Related item(s): _reflns_observedCriterion_ (alternate).

Example(s): ‘\(I > 2u(I)\)’

**reflns**

**reflns_limit_h_min**

**reflns_limit_h_max**

**reflns_limit_k_min**

**reflns_limit_k_max**

**reflns_limit_l_min**

**reflns_limit_l_max**

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

Related item(s): _reflns_observedCriterion_ (alternate).
**Example 1**: example corresponding to the one-dimensional incommensurate modulated structure of K$_2$SeO$_4$.

```
loop_
  _reflns_class_number_gt
  _reflns_class_code
  584 'Main'
  226 'Set1'
  50 'Set2'
```

**_reflns_class_code** (char)

The code identifying a certain reflection class.

Appears in list. May match subsidiary data name(s): _reflns_class_code.

Example(s): 't', 'm1', 's2'

**_reflns_class_description** (char)

Description of each reflection class.

Appears in list containing _reflns_class_code.

Example(s): 'w1 first order satellites', 'HOLo common projection reflections'

**_reflns_class_d_res_high** (numb)

For each reflection class the highest resolution in ångströms for the interplanar spacing in the reflections used in refinement. This is the smallest d value.

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

**_reflns_class_d_res_low** (numb)

For each reflection class the lowest resolution in ångströms for the interplanar spacing in the reflections used in refinement. This is the largest d value.

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

**_reflns_class_number_gt** (numb)

For each reflection class, the number of significantly intense reflections (see _reflns_threshold_expression) in the _reflns_list (not the _diffn_reflns_list). It 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. The special characteristics of the reflections included in the _reflns_list should be given in the item _reflns_special_details.

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

**_reflns_class_number_total** (numb)

For each reflection class, the total number of reflections in the _reflns_list (not the _diffn_reflns_list). It 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. The special characteristics of the reflections included in the _reflns_list should be given in the item _reflns_special_details.

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

---

**_reflns_class_R_factor_all**

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

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

F_{\text{obs}} = \text{observed structure-factor amplitudes}, F_{\text{calc}} = \text{calculated structure-factor amplitudes}, and the sum \( \sum \) is taken over the reflections of this class. See also _reflns_class_wfact or all definitions.

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

---

**_reflns_class_R_Fsqd_factor**

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 _reflns_class_d_res_high and _reflns_class_d_res_low.

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

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

Appears in list containing _reflns_class_code. The permitted range is 0.0→∞.
**REFLNS_CLASS**

`reflns_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 `reflns_class_d_res_high` and `reflns_class_d_res_low`.

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

\[ Y_{obs} = \text{the observed amplitude specified by} \, \text{refine_ls_structure_factor_coeff}, \quad Y_{calc} = \text{the calculated amplitude specified by} \, \text{refine_ls_structure_factor_coeff}, \]

\[ w = \text{the least-squares weight, and the sum} \sum \text{is taken over the reflections of this class. See also} \, \text{reflns_class_R_factor definitions.} \]

Appears in list containing `reflns_class_code`. The permitted range is 0.0–∞.

**_reflns_scale_[]**

Data items in the REFLNS_SCALE category record details about the structure factor scales. They are referenced from within the REFLN list through `reflns_scale_group_code`.  

```plaintext
loop_
  _reflns_scale_group_code
  _reflns_scale_meas_F
  1.05647
```

`reflns_scale_group_code` (char)

The code identifying a scale `reflns_scale_meas_.` These are linked to the `refln_` list by the `reflns_scale_group_code`. These codes need not correspond to those in the `differ` list.

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

`reflns_scale_meas_F`

`reflns_scale_meas_F_squared`

`reflns_scale_meas_intensity` (numb)

Scales associated with `reflns_scale_group_code`.  
Appears in list containing `reflns_scale_group_code`. The permitted range is 0.0–∞.

`reflns_shell_d_res_high` (numb)

The highest resolution in ångströms for the interplanar spacing in the reflections in this shell. This is the smallest `d` value.

Appears in list. The permitted range is 0.0–∞.  

`reflns_shell_d_res_low` (numb)

The lowest resolution in ångströms for the interplanar spacing in the reflections in this shell. This is the largest `d` value.

Appears in list. The permitted range is 0.0–∞.  

`reflns_shell_meanI_over_uI_gt` (numb)

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

Appears in list.  

`reflns_shell_meanI_over_uI_all` (numb)

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

Appears in list.  

`reflns_shell_meanI_over_uI_gt` (numb)

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

The ratio of the mean of the intensities of the significantly intense reflections (see `reflns_threshold_expression`) in this shell to the mean of the standard uncertainties of the intensities of the significantly intense reflections in the resolution shell.

Appears in list.  

`reflns_shell_meanI_over_uI_all` (numb)

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

The ratio of the mean of the intensities of the reflections classified as 'observed' (see `reflns_observed_criterion`) in this shell to the mean of the standard uncertainties of the intensities of the 'observed' reflections in the resolution shell.

Appears in list.
_reflns_shell_mean1_over_u1_gt  (numb)
The ratio of the mean of the intensities of the significantly intense reflections (see _reflns_threshold_expression) in this shell to the mean of the standard uncertainties of the intensities of the significantly intense reflections in the resolution shell.
Related item(s): _reflns_shell_mean1_over_sig1_gt (alternate). Appears in list. [reflns_shell]

_reflns_shell_number_measured_all  (numb)
The total number of reflections measured for this resolution shell.
Appears in list. The permitted range is 0.0→∞. [reflns_shell]

_reflns_shell_number_measured_gt  (numb)
The number of significantly intense reflections (see _reflns_threshold_expression) measured for this resolution shell.
Related item(s): _reflns_shell_number_measured_obs (alternate). Appears in list. The permitted range is 0.0→∞. [reflns_shell]

_reflns_shell_number_measured_obs  (numb)
This definition has been superseded and is retained here only for archival purposes. Use instead _reflns_shell_number_measured_gt.
The number of reflections classified as 'observed' (see _reflns_observed_criterion) measured for this resolution shell.
[reflns_shell]

_reflns_shell_number_possible  (numb)
The number of unique reflections it is possible to measure in this reflection shell.
Appears in list. The permitted range is 0→∞. [reflns_shell]

_reflns_shell_number_unique_all  (numb)
The total number of measured reflections resulting from merging measured symmetry-equivalent reflections for this resolution shell.
Appears in list. The permitted range is 0→∞. [reflns_shell]

_reflns_shell_number_unique_gt  (numb)
The total number of significantly intense reflections (see _reflns_threshold_expression) resulting from merging measured symmetry-equivalent reflections for this resolution shell.
Related item(s): _reflns_shell_number_unique_obs (alternate). Appears in list. The permitted range is 0→∞. [reflns_shell]

_reflns_shell_number_unique_obs  (numb)
This definition has been superseded and is retained here only for archival purposes. Use instead _reflns_shell_number_unique_gt.
The total number of reflections classified as 'observed' (see _reflns_observed_criterion) resulting from merging measured symmetry-equivalent reflections for this resolution shell.
[reflns_shell]

_reflns_shell_percent_possible_all  (numb)
The percentage of geometrically possible reflections represented by all reflections measured for this resolution shell.
Appears in list. The permitted range is 0.0→100.0. [reflns_shell]

_reflns_shell_percent_possible_gt  (numb)
The percentage of geometrically possible reflections represented by significantly intense reflections (see _reflns_threshold_expression) measured for this resolution shell.
Related item(s): _reflns_shell_percent_possible_obs (alternate). Appears in list. The permitted range is 0.0→100.0. [reflns_shell]

_reflns_shell_percent_possible_obs  (numb)
This definition has been superseded and is retained here only for archival purposes. Use instead _reflns_shell_percent_possible_gt.
The percentage of geometrically possible reflections represented by reflections classified as 'observed' (see _reflns_observed_criterion) measured for this resolution shell.
[reflns_shell]

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

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

$F_i$ = the amplitude of the $i$th observation of reflection $i$, $\langle F \rangle$ = the mean of the amplitudes of all observations of reflection $i$, the sum $\sum_i$ is taken over all reflections, and the sum $\sum_j$ is taken over all observations of each reflection.
Appears in list. The permitted range is 0.0→∞. [reflns_shell]

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

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

$F_i$ = the amplitude of the $i$th observation of reflection $i$, $\langle F \rangle$ = the mean of the amplitudes of all observations of reflection $i$, the sum $\sum_i$ is taken over all reflections, and the sum $\sum_j$ is taken over all observations of each reflection.
Related item(s): _reflns_shell_Rmerge_F_obs (alternate). Appears in list. The permitted range is 0.0→∞. [reflns_shell]

_reflns_shell_Rmerge_F_obs  (numb)
This definition has been superseded and is retained here only for archival purposes. Use instead _reflns_shell_Rmerge_F_gt.
The value of $R_{merge}(F)$ for reflections classified as 'observed' (see _reflns_observed_criterion) in a given shell.

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

$F_i$ = the amplitude of the $i$th observation of reflection $i$, $\langle F \rangle$ = the mean of the amplitudes of all observations of reflection $i$, the sum $\sum_i$ is taken over all reflections, and the sum $\sum_j$ is taken over all observations of each reflection.
[reflns_shell]
The value of \( R_{\text{merge}}(I) \) for all reflections in a given shell.
\[
R_{\text{merge}}(I) = \frac{\sum_i (\sum_j |I_{ij} - \langle I_i \rangle|)}{\sum_i (\sum_j |I_{ij}|)}
\]

\( I_i \) is the intensity of the jth observation of reflection i, \( \langle I_i \rangle \) is the mean of the intensities of all observations of reflection i, the sum \( \sum_j \) is taken over all observations, and the sum \( \sum_i \) is taken over all observations of each reflection.

Appears in list. The permitted range is 0.0–\( \infty \).

The value of \( R_{\text{merge}}(I) \) for significantly intense reflections (see _reflns_threshold_expression_) in a given shell.
\[
R_{\text{merge}}(I) = \frac{\sum_i (\sum_j |I_{ij} - \langle I_i \rangle|)}{\sum_i (\sum_j |I_{ij}|)}
\]

\( I_i \) is the intensity of the jth observation of reflection i, \( \langle I_i \rangle \) is the mean of the intensities of all observations of reflection i, the sum \( \sum_j \) is taken over all observations, and the sum \( \sum_i \) is taken over all observations of each reflection.

Related item(s): _reflns_shell_Rmerge_I_obs_ (alternate). Appears in list. The permitted range is 0.0–\( \infty \).

The value of \( R_{\text{merge}}(I) \) for reflections classified as ‘observed’ (see _reflns_observed_criterion_) in a given shell.
\[
R_{\text{merge}}(I) = \frac{\sum_i (\sum_j |I_{ij} - \langle I_i \rangle|)}{\sum_i (\sum_j |I_{ij}|)}
\]

\( I_i \) is the intensity of the jth observation of reflection i, \( \langle I_i \rangle \) is the mean of the intensities of all observations of reflection i, the sum \( \sum_j \) is taken over all observations, and the sum \( \sum_i \) is taken over all observations of each reflection.

Example(s): 'P 2ac 2ab', 'P 61 2 2 (0 0 -1)'.

Hermann–Mauguin space-group symbol. Note that the H–M symbol does not necessarily contain complete information about the symmetry and the space-group origin. If used always supply the full symbol from International Tables for Crystallography, Vol. A (1987) and indicate the origin and the setting if it is not implicit. If there is any doubt that the equivalent positions can be uniquely deduced from this symbol specify the _symmetry_equiv_pos_as_xyz_ or _symmetry_equiv_pos_as_xyz_ data items as well. Leave spaces between symbols referring to different axes.

Example(s): 'P 1 21/m 1', 'P 2/n 2/n 2/n (origin at -1)'.

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


Example 2 - based on data set TOZ of Willis, Beckwith & Tozer ([1991]. Acta Cryst. C47, 2276–2277). 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.
The element symbol of the second atom forming the bond whose valence parameters are given in this category. Appears in list.

_valence_param_atom_2_valence (numb)
The valence (formal charge) of the second atom whose bond valence parameters are given in this category. Appears in list.

_valence_param_B (numb)
The bond valence parameter $B$ used in the expression

$$s = \exp\left(\frac{R_0 - R}{B}\right)$$

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

_valence_param_details (char)
Details or comments on the bond valence parameters. Appears in list.

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

_valence_param_ref_id (char)
An identifier which links to the reference from which the bond valence parameters are taken. A child of_valence_ref_id which it must match. Appears in list. Must match data name_valence_ref_id.

_valence_param_Ro (numb)
The bond valence parameter $R_0$ used in the expression

$$s = \exp\left(\frac{R_0 - R}{B}\right)$$

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

_valence_ref_id (char)
An identifier for items in this category. Parent of_valence_ref_id which has the same value. Appears in list containing_valence_ref_id. May match subsidiary data name(s):_valence_ref_id. [valence_ref]

_valence_ref_reference (char)
Literature reference from which the valence parameters identified by_valence_param_ref_id were taken. Appears in list containing_valence_ref_id. [valence_ref]