**_atom_site_aniso_label** (*char*)

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

Appearance in list: yes.

**_atom_site_aniso_type_symbol** (*char*)

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

Appearance in list: yes. If looped, **`_atom_site_aniso_label`** must be present in the same list.

**_atom_site_aniso_U_11**
**_atom_site_aniso_U_12**
**_atom_site_aniso_U_13**
**_atom_site_aniso_U_22**
**_atom_site_aniso_U_23**
**_atom_site_aniso_U_33** (*numb*)

These are the standard anisotropic atomic displacement components which appear in the structure factor term: $\exp(-2\pi^2 \sum_i \sum_j U_{ij} h_i h_j a_i^* a_j^*)$. The components may be entered in any order.

Appearance in list: yes. If looped, **`_atom_site_aniso_label`** must be present in the same list. E.s.d. expected: yes. Default e.s.d. value: 0·0. The units extensions are: ‘ ’ (ångströms squared *1.0) ‘**`_pm`**’ (picometres squared /10000.) ‘**`_nm`**’ (nanometres squared *100.).

**_atom_site_attached_hydrogens** (*numb*)

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

Appearance in list: yes. If looped, **`_atom_site_label`** must be present in the same list. Where no value is given, the assumed value is ‘`0`’. The permitted range is 0→4.

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

**_atom_site_calc_attached_atom** (*char*)

The `_atom_site_label` of the atom site to which the ‘geometry-calculated’ atom site is attached.

Appearance in list: yes. If looped, **`_atom_site_label`** must be present in the same list. Where no value is given, the assumed value is ‘`.`’.

**_atom_site_calc_flag** (*char*)

A standard code to signal if the site data has been determined by diffraction data or calculated from the geometry of surrounding sites, or has been assigned dummy coordinates.

| | |
|---|---|
| **`d`** | determined from diffraction measurements |
| **`calc`** | calculated from molecular geometry |
| **`dum`** | dummy site with meaningless coordinates |

Appearance in list: yes. If looped, _atom_site_label must be present in the same list. Where no value is given, the assumed value is 'd'.

**_atom_site_Cartn_x**
**_atom_site_Cartn_y**
**_atom_site_Cartn_z** (*numb*)

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

Appearance in list: yes. If looped, _atom_site_label must be present in the same list. E.s.d. expected: yes. Default e.s.d. value: 0·0. The units extensions are: ' ' (ångströms *1.0) '_pm' (picometres /100.) '_nm' (nanometres *10.).

**_atom_site_chemical_conn_number** (*numb*)

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

Appearance in list: yes. If looped, _atom_site_label must be present in the same list. The permitted range is 1→ ∞.

**_atom_site_constraints** (*char*)

A description of the constraints applied to parameters at this site during refinement. See also _atom_site_refinement_flags and _refine_ls_number_constraints.

Appearance in list: yes. If looped, _atom_site_label must be present in the same list. Where no value is given, the assumed value is '.'.

Example(s): pop=1.0-pop(Zn3)

**_atom_site_description** (*char*)

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

Appearance in list: yes. If looped, _atom_site_label must be present in the same list. Where no value is given, the assumed value is '.'.

Example(s): 'Ag/Si disordered'

**_atom_site_disorder_group** (*char*)

A code to link disordered atom sites of a group that exist simultaneously in the crystal structure.

Appearance in list: yes. If looped, _atom_site_label must be present in the same list. Where no value is given, the assumed value is '.'.

Example(s): A

**_atom_site_fract_x**
**_atom_site_fract_y**
**_atom_site_fract_z** (*numb*)

Atom site coordinates as fractions of the _cell_length_ values.

Appearance in list: yes. If looped, _atom_site_label must be present in the same list. E.s.d. expected: yes. Default e.s.d. value: 0·0. Where no value is given, the assumed value is '0·0'.

**_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 *_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__ggg' is acceptable and represents the components C, 233, '', and ggg. Each label may have a different number of components.

Appearance in list: yes.

Example(s): C12, Ca3g28, Fe3+17, H*251, boron2a, C_a_phe_83_a_0, Zn_Zn_301_A_0

**_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, chain order and alternate codes, respectively. These codes may be composed of any characters except an underline.

Appearance in list: yes. If looped, _atom_site_label must be present in the same list.

**_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.

Appearance in list: yes. If looped, _atom_site_label must be present in the same list. E.s.d. expected: yes. Default e.s.d. value: 0·0. Where no value is given, the assumed value is '1·0'. The permitted range is 0·0→1·0.

**_atom_site_refinement_flags** (*char*)

A concatenated series of single-letter codes which indicate the refinement restraints or constraints applied to this site.

| | |
|---|---|
| . | no refinement constraints |
| S | special position constraint on site |
| G | rigid group refinement of site |
| R | riding atom site attached to non-riding atom |
| D | distance or angle restraint on site |
| T | thermal displacement constraints |
| U | $U_{iso}$ or $U_{ij}$ restraint (rigid bond) |
| P | partial occupancy constraint |

Appearance in list: yes. If looped, _atom_site_label must be present in the same list. Where no value is given, the assumed value is '.'.

**_atom_site_restraints** (*char*)

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

Appearance in list: yes. If looped, _atom_site_label must be present in the same list. Where no value is given, the assumed value is '.'.

Example(s): 'restrained to planar ring'

**_atom_site_symmetry_multiplicity** (*numb*)

The multiplicity of a site due to the space-group symmetry as is given in *International Tables for Crystallography*, Vol. A (1987).

Appearance in list: yes. If looped, _atom_site_label must be present in the same list. The permitted range is 1→192.

**_atom_site_thermal_displace_type** (*char*)

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

| | |
|---|---|
| Uani | anisotropic $U_{ij}$ |
| Uiso | isotropic $U$ |
| Uovl | overall $U$ |
| Umpe | multipole expansion $U$ |

Appearance in list: yes. If looped, _atom_site_label must be present in the same list.

**_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.

Appearance in list: yes. If looped, _atom_site_label must be present in the same list.

Example(s): Cu , Cu2+ , dummy , Fe3+Ni2+ , S- , H* , H(SDS)

**_atom_site_U_iso_or_equiv** (*numb*)

Isotropic atomic displacement parameter, or equivalent isotropic atomic displacement parameter calculated from anisotropic atomic displacement parameters. The latter must be calculated as $U_{(equiv)} = (1/3)\sum_i[\sum_j(U_{ij}a_i^* a_j^* A_i . A_j)]$ where $A$ are the real-cell and $a^*$ the reciprocal-cell lengths [see Fischer, R. X. & Tillmanns, E. (1988). *Acta Cryst.* C**44**, 775–776].

Appearance in list: yes. If looped, _atom_site_label must be present in the same list. E.s.d. expected: yes. Default e.s.d. value: 0·0. The permitted range is 0·0→10·0. The units extensions are: ' ' (ångströms squared *1.0) '_pm' (picometres squared /10000.) '_nm' (nanometres squared *100.).

**_atom_site_Wyckoff_symbol** (*char*)

The Wyckoff symbol (letter) as listed in the space-group section of *International Tables for Crystallography*, Vol. A (1987).

Appearance in list: yes. If looped, _atom_site_label must be present in the same list.

**_atom_sites_Cartn_tran_matrix_11**
**_atom_sites_Cartn_tran_matrix_12**
**_atom_sites_Cartn_tran_matrix_13**
**_atom_sites_Cartn_tran_matrix_21**
**_atom_sites_Cartn_tran_matrix_22**
**_atom_sites_Cartn_tran_matrix_23**
**_atom_sites_Cartn_tran_matrix_31**
**_atom_sites_Cartn_tran_matrix_32**
**_atom_sites_Cartn_tran_matrix_33** (*numb*)

Matrix elements used to transform fractional coordinates to orthogonal Cartesian coordinates. The axial alignments of this transformation are described in _atom_sites_Cartn_transform_axes.

$$\begin{pmatrix} 11 & 12 & 13 \\ 21 & 22 & 23 \\ 31 & 32 & 33 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}_{\text{fractional}} = \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}_{\text{Cartesian}}$$

**_atom_sites_Cartn_transform_axes** (*char*)

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

Example(s): 'a parallel to x; b in the plane of y & z'

**_atom_sites_solution_primary**
**_atom_sites_solution_secondary**
**_atom_sites_solution_hydrogens** (*char*)

Codes which identify the methods used to locate the initial atomic sites. The *_primary code identifies how the first atom sites were determined; the *_secondary code identifies how the remaining non-hydrogen sites were located; and the *_hydrogens code identifies how the hydrogens were located.

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

**_atom_type_analytical_mass_%** (*numb*)

Mass percentage of this atom type derived from chemical analysis.

Appearance in list: yes. If looped, _atom_type_symbol must be present in the same list. The permitted range is 0·0→ ∞.

**_atom_type_description** (*char*)

A description of the atom(s) designated by this atom type. In most cases this will be the element name and oxidation state of a single atom species. For disordered or nonstoichiometric structures it will describe a combination of atom species.

Appearance in list: yes. If looped, _atom_type_symbol must be present in the same list.

Example(s): deuterium, 0·34Fe+0·66Ni

**_atom_type_number_in_cell** (*numb*)

Total number of atoms of this atom type in the unit cell.

Appearance in list: yes. If looped, _atom_type_symbol must be present in the same list. The permitted range is 0→ ∞.

**_atom_type_oxidation_number** (*numb*)

Formal oxidation state of this atom type in the structure.

Appearance in list: yes. If looped, _atom_type_symbol must be present in the same list. Where no value is given, the assumed value is '0'. The permitted range is −6→6.

**_atom_type_radius_bond**
**_atom_type_radius_contact** *(numb)*

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

Appearance in list: yes. If looped, **_atom_type_symbol** must be present in the same list. The permitted range is 0·0→4·0. The units extensions are: ' ' (ångströms *1.0) '_pm' (picometres /100.) '_nm' (nanometres *10.).

**_atom_type_scat_Cromer_Mann_a1**
**_atom_type_scat_Cromer_Mann_a2**
**_atom_type_scat_Cromer_Mann_a3**
**_atom_type_scat_Cromer_Mann_a4**
**_atom_type_scat_Cromer_Mann_b1**
**_atom_type_scat_Cromer_Mann_b2**
**_atom_type_scat_Cromer_Mann_b3**
**_atom_type_scat_Cromer_Mann_b4**
**_atom_type_scat_Cromer_Mann_c** *(numb)*

The Cromer–Mann scattering-factor coefficients used to calculate the scattering factors for this atom type. May be entered in any order. See *International Tables for X-ray Crystallography*, Vol. IV, Table 2.2B (1974); or *International Tables for Crystallography*, Vol. C, Tables 6.1.1.4 and 6.1.1.5 (1991).

Appearance in list: yes. If looped, **_atom_type_symbol** must be present in the same list.

**_atom_type_scat_dispersion_imag**
**_atom_type_scat_dispersion_real** *(numb)*

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 _diffrn_radiation_wavelength.

Appearance in list: yes. If looped, **_atom_type_symbol** must be present in the same list. Where no value is given, the assumed value is '0·0'.

**_atom_type_scat_source** *(char)*

Reference to source of scattering factors used for this atom type.

Appearance in list: yes. If looped, **_atom_type_symbol** must be present in the same list.

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

**_atom_type_scat_versus_stol_list** *(char)*

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

Appearance in list: yes. If looped, **_atom_type_symbol** must be present in the same list.

**_atom_type_symbol** *(char)*

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.

Appearance in list: yes.

Example(s): C, Cu2+, H(SDS), dummy, FeNi

**_audit_creation_date** *(char)*

A date that the CIF was created. The date format is yy-mm-dd.

Example(s): 90-07-12

**_audit_creation_method** *(char)*

A description of how data was entered into the CIF.

Example(s): 'spawned by the program QBEE'

**_audit_update_record** *(char)*

A record of any changes to the CIF. The update format is a date (yy-mm-dd) followed by a description of the changes. The latest update entry is added to the bottom of this record.

Example(s): '90-07-15 Updated by the Co-editor'

**_cell_angle_alpha**
**_cell_angle_beta**
**_cell_angle_gamma** *(numb)*

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

E.s.d. expected: yes. Default e.s.d. value: 0·0. Where no value is given, the assumed value is '90·0'. The permitted range is 0·0→180·0.

**_cell_formula_units_Z** *(numb)*

The number of the formula units in the unit cell as specified by _chemical_formula_structural, _chemical_formula_moiety or _chemical_formula_sum.

The permitted range is 1→ ∞.

**_cell_length_a**
**_cell_length_b**
**_cell_length_c** *(numb)*

Unit-cell lengths corresponding to the structure reported. The values of _refln_index_h, *_k, *_l must correspond to the cell defined by these values and _cell_angle_ values. The values of _diffrn_refln_index_h, *_k, *_l may not correspond to these values if a cell transformation took place following the measurement of diffraction intensities. See also _diffrn_reflns_transf_matrix_.

E.s.d. expected: yes. Default e.s.d. value: 0·0. The permitted range is 0·0→ ∞. The units extensions are: ' ' (ångströms *1.0) '_pm' (picometres /100.) '_nm' (nanometres *10.).

**_cell_measurement_pressure** *(numb)*

The pressure at which the unit-cell parameters were measured (not the pressure used to synthesize the sample).

E.s.d. expected: yes. Default e.s.d. value: 0·0. The units extensions are: ' ' (kilopascals *1.0) '_GPa' (gigapascals *1.0E+6).

**_cell_measurement_radiation** *(char)*

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

Example(s): neutron, 'Cu K\a', synchrotron

**_cell_measurement_refln_index_h**
**_cell_measurement_refln_index_k**
**_cell_measurement_refln_index_l** *(numb)*

Miller indices of a reflection used for unit-cell measurements.

Appearance in list: yes.

**_cell_measurement_refln_theta** (*numb*)

Theta angle in degrees for the reflection used for unit-cell measurement with the indices _cell_measurement_refln_index_.

Appearance in list: yes. If looped, _cell_measurement_refln_index_ must be present in the same list. The permitted range is 0·0→90·0.

**_cell_measurement_reflns_used** (*numb*)

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

**_cell_measurement_temperature** (*numb*)

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

E.s.d. expected: yes. Default e.s.d. value: 0·0. The permitted range is 0·0→ ∞. The units extensions are: ‘ ’ (Kelvin +0) ‘_C’ (Celsius +273.0).

**_cell_measurement_theta_max**
**_cell_measurement_theta_min** (*numb*)

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

The permitted range is 0·0→90·0.

**_cell_measurement_wavelength** (*numb*)

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

The permitted range is 0·0→ ∞. The units extensions are: ‘ ’ (ångströms *1.0) ‘_pm’ (picometres /100.) ‘_nm’ (nanometres *10.).

**_cell_special_details** (*char*)

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_volume** (*numb*)

Volume calculated from _cell_length_ and _cell_angle_ values.

E.s.d. expected: yes. Default e.s.d. value: 0·0. The permitted range is 0·0→ ∞. The units extensions are: ‘ ’ (cubic ångströms *1.0) ‘_pm’ (cubic picometres /1.0E+6) ‘_nm’ (cubic nanometres *1000.).

**_chemical_compound_source** (*char*)

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 (USSR)'`, `'Extracted from the bark of Cinchona Naturalis'`

**_chemical_conn_atom_charge** (*numb*)

The net integer charge assigned to this atom. This is the formal charge assignment normally found in chemical diagrams.

Appearance in list: yes. If looped, _chemical_conn_atom_type_symbol must be present in the same list. Where no value is given, the assumed value is ‘0’. The permitted range is −6→6.

Example(s): `1` (for an ammonium nitrogen), `−1` (for a chloride ion)

**_chemical_conn_atom_display_x**
**_chemical_conn_atom_display_y** (*numb*)

The 2D Cartesian coordinates ($x$, $y$) of the position of this atom in a recognizable chemical diagram. The coordinate origin is at the lower left corner, the $x$ axis is horizontal and the $y$ axis is vertical. The coordinates must lie in the range 0·0 to 1·0. These coordinates can be obtained from projections of a suitable uncluttered view of the molecular structure. If absent, values will be assigned by the journals' or database staff.

Appearance in list: yes. If looped, _chemical_conn_atom_type_symbol must be present in the same list. The permitted range is 0·0→1·0.

**_chemical_conn_atom_NCA** (*numb*)

The number of connected atoms excluding terminal hydrogen atoms.

Appearance in list: yes. If looped, _chemical_conn_atom_type_symbol must be present in the same list. The permitted range is 0→ ∞.

**_chemical_conn_atom_NH** (*numb*)

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

Appearance in list: yes. If looped, _chemical_conn_atom_type_symbol must be present in the same list. The permitted range is 0→ ∞.

**_chemical_conn_atom_number** (*numb*)

The chemical sequence number to be associated with this atom.

Appearance in list: yes. If looped, _chemical_conn_atom_type_symbol must be present in the same list. The permitted range is 1→ ∞.

**_chemical_conn_atom_type_symbol** (*char*)

A code identifying the atom type. This code must match an _atom_type_symbol code in the _atom_type_ list; or be a recognizable element symbol.

Appearance in list: yes.

**_chemical_conn_bond_atom_1**
**_chemical_conn_bond_atom_2** (*numb*)

Atom numbers which must match with chemical sequence numbers specified as _chemical_conn_atom_number values. These link the bond connection to the chemical numbering and atom sites.

Appearance in list: yes. The permitted range is 1→ ∞.

**_chemical_conn_bond_type** (*char*)

The chemical bond type associated with the connection between the two sites `_chemical_conn_bond_atom_1` and `*_2`.

| | |
|---|---|
| `sing` | single bond |
| `doub` | double bond |
| `trip` | triple bond |
| `quad` | quadruple bond |
| `arom` | aromatic bond |
| `poly` | polymeric bond |
| `delo` | delocalized double bond |
| `pi` | pi bond |

Appearance in list: yes. If looped, `_chemical_conn_bond_atom_1` must be present in the same list. Where no value is given, the assumed value is '`sing`'.

**_chemical_formula_appendix** (*These are notes only*)

`_chemical_formula_` items specify the composition and chemical properties of the compound. The formula data items must agree with those that specify the density, unit-cell and $Z$ values.

The following rules apply to the construction of the data items `_chemical_formula_analytical`, `*_structural` and `*_sum`. For the data item `*_moiety` the formula construction is broken up into residues or moieties, *i.e.* groups of atoms that form a molecular unit or molecular ion. The rules given below apply within each moiety but different requirements apply to the way that moieties are connected (see `_chemical_formula_moiety`).

1. Only recognized element symbols may be used.
2. Each element symbol is followed by a 'count' number. A count of '1' may be omitted.
3. A space or parenthesis must separate each element symbol and its count.
4. Where a group of elements is enclosed in parentheses, the multiplier for the group must follow the closing parentheses. That is, all element and group multipliers are assumed to be printed as subscripted numbers. [An exception to this rule exists for `*_moiety` formulae where pre- and post-multipliers are permitted for molecular units].
5. Unless the elements are ordered in a manner that corresponds to their chemical structure, as in `_chemical_formula_structural`, the order of the elements within any group or moiety should be: C, H followed by the other elements in alphabetical order of their symbol. This is the 'Hill' system used by *Chemical Abstracts*. This ordering is used in `_chemical_formula_moiety` and `_chemical_formula_sum`.

**_chemical_formula_analytical** (*char*)

Formula determined by standard chemical analysis including trace elements. See `_chemical_formula_appendix` for rules for writing chemical formulae. Parentheses are used only for e.s.d.'s.

Example(s): `'Fe2.45(2) Ni1.60(3) S4'`

**_chemical_formula_moiety** (*char*)

Formula with each discrete bonded residue or ion shown as a separate moiety. See above `_chemical_formula_appendix` for rules for writing chemical formulae. In addition to the general formulae requirements, the following rules apply:

1. Moieties are separated by commas ', '.
2. The order of elements within a moiety follows general rule 5 in `_chemical_formula_appendix`.
3. Parentheses are not used within moieties but may surround a moiety. Parentheses may not be nested.
4. Charges should be placed at the end of the moiety. The charge '+' or '−' may be preceded by a numerical multiplier and should be separated from the last (element symbol + count) by a space. Pre- or post-multipliers may be used for individual moieties.

Example(s): `'C7 H4 Cl Hg N O3 S'`
`'C12 H17 N4 O S 1+, C6 H2 N3 O7 1-'`
`'C12 H16 N2 O6, 5(H2 O1)'`
`'(Cd 2+)3, (C6 N6 Cr 3-)2, 2(H2 O)'`

**_chemical_formula_structural** (*char*)

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

Example(s): `'Ca ((Cl O3)2 O)2 (H2 O)6'`
`'(Pt (N H3)2 (C5 H7 N3 O)2) (Cl O4)2'`

**_chemical_formula_sum** (*char*)

See above `_chemical_formula_appendix` for the rules for writing chemical formulae in which all discrete bonded residues and ions are summed over the constituent elements, following the ordering given in general rule 5 in `_chemical_formula_appendix`. Parentheses are not normally used.

Example(s): `'C18 H19 N7 O8 S'`

**_chemical_formula_weight** (*numb*)

Formula mass in daltons. This mass should correspond to the formulae given under `_chemical_formula_structural`, `*_moiety` or `*_sum` and, together with the $Z$ value and cell parameters, should yield the density given as `_exptl_crystal_density_diffrn`.

The permitted range is $1{\cdot}0 \rightarrow \infty$.

**_chemical_formula_weight_meas** (*numb*)

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

The permitted range is $1{\cdot}0 \rightarrow \infty$.

**_chemical_melting_point** (*numb*)

The melting point of the crystal.

The permitted range is $0{\cdot}0 \rightarrow \infty$. The units extensions are: '` `' (Kelvin +0) '`_C`' (Celsius +273·0).

**_chemical_name_common** (*char*)

Trivial name by which compound is commonly known.

Example(s): `1-bromoestradiol`

**_chemical_name_mineral** (*char*)

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

Example(s): `chalcopyrite`

**_chemical_name_structure_type** (*char*)

Commonly used structure-type name. Usually only applied to minerals or inorganic compounds.

Example(s): `perovskite`, `sphalerite`, `A15`

**_chemical_name_systematic** (*char*)

IUPAC or *Chemical Abstracts* full name of compound.

Example(s): `1-bromoestra-1,3,5(10)-triene-3,17\b-diol`

**_computing_cell_refinement**
**_computing_data_collection**
**_computing_data_reduction**
**_computing_molecular_graphics**
**_computing_publication_material**
**_computing_structure_refinement**
**_computing_structure_solution** (*char*)

Software used in the processing of this data. Give the program or package name and a brief reference.

Example(s): `'CAD4 (Enraf-Nonius)'`
`'DIFDAT, SORTRF, ADDREF (XTAL3.0, 1990)'`
`'FRODO (Jones, 1986) & ORTEP (Johnson, 1965)'`
`'CRYSTALS (Watkin, 1988)'`
`'SHELX85 (Sheldrick, 1985)'`

**_database_code_CAS**
**_database_code_CSD**
**_database_code_ICSD**
**_database_code_MDF**
**_database_code_NBS**
**_database_code_PDF** (*char*)

The codes are assigned by databases: *Chemical Abstracts*; Cambridge Structural (organic and metal-organic compounds); Inorganic Crystal Structure; Metals Data File (metal structures); NBS (NIST) Crystal Data Database (lattice parameters) and the Powder Diffraction File (JCPDS/ICDD).

**_database_journal_ASTM**
**_database_journal_CSD** (*char*)

The ASTM coden for a journal as given in the Chemical Source List and the journal code used in the Cambridge Structural Database.

**_diffrn_ambient_pressure** (*numb*)

The pressure at which the diffraction data were measured.

E.s.d. expected: yes. Default e.s.d. value: 0·0. The permitted range is $0{\cdot}0 \rightarrow \infty$. The units extensions are: `' '` (kilopascals *1.0) `'_GPa'` (gigapascals *1.0E+6).

**_diffrn_ambient_temperature** (*numb*)

The mean temperature at which the diffraction data were measured.

E.s.d. expected: yes. Default e.s.d. value: 0·0. The permitted range is $0{\cdot}0 \rightarrow \infty$. The units extensions are: `' '` (Kelvin +0) `'_C'` (Celsius +273·0).

**_diffrn_attenuator_code** (*char*)

A code associated with a particular attenuator setting. This code is referenced by the `_diffrn_refln_attenuator_code` which is stored with the diffraction data. See `_diffrn_attenuator_scale`.

Appearance in list: yes.

**_diffrn_attenuator_scale** (*numb*)

The intensity scale associated with a particular attenuator setting identified by `_diffrn_attenuator_code`.

Appearance in list: yes. If looped, `_diffrn_attenuator_code` must be present in the same list. The permitted range is $1{\cdot}0 \rightarrow \infty$.

**_diffrn_measurement_device** (*char*)

Description of the diffractometer or camera used to measure the diffraction intensities.

Example(s): `'Gandolfi 114mm powder camera'`

**_diffrn_measurement_method** (*char*)

Method used to measure diffraction data.

Example(s): `'profile data from theta/2theta scans'`

**_diffrn_orient_matrix_type** (*char*)

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

**_diffrn_orient_matrix_UB_11**
**_diffrn_orient_matrix_UB_12**
**_diffrn_orient_matrix_UB_13**
**_diffrn_orient_matrix_UB_21**
**_diffrn_orient_matrix_UB_22**
**_diffrn_orient_matrix_UB_23**
**_diffrn_orient_matrix_UB_31**
**_diffrn_orient_matrix_UB_32**
**_diffrn_orient_matrix_UB_33** (*numb*)

The elements of the diffractometer orientation matrix. These define the dimensions of the reciprocal cell and its orientation to the local diffractometer axes. See `_diffrn_orient_matrix_type`.

**_diffrn_orient_refln_angle_chi**
**_diffrn_orient_refln_angle_kappa**
**_diffrn_orient_refln_angle_phi**
**_diffrn_orient_refln_angle_psi** (*numb*)

Diffractometer angles in degrees of a reflection used to define the orientation matrix. See `_diffrn_orient_matrix_UB_` and `_diffrn_orient_refln_index_h`, `*_k` and `*_l`.

Appearance in list: yes. If looped, `_diffrn_orient_refln_index_` must be present in the same list.

**_diffrn_orient_refln_index_h**
**_diffrn_orient_refln_index_k**
**_diffrn_orient_refln_index_l** (*numb*)

The indices of a reflection used to define the orientation matrix. See `_diffrn_orient_matrix_type` and `_diffrn_orient_matrix_`

Appearance in list: yes.

**_diffrn_radiation_detector** *(char)*

The detector used to measure the diffraction intensities.

Appearance in list: both.

Example(s): `scintillation`, `LiI`, `'video tube'`, `'Kodak II film'`

**_diffrn_radiation_detector_dtime** *(numb)*

The deadtime in microseconds of `_diffrn_radiation_detector`.

Appearance in list: both. The permitted range is 0·0→ ∞.

**_diffrn_radiation_filter_edge** *(numb)*

Absorption edge of the radiation filter used.

Appearance in list: both. The permitted range is 0·0→ ∞. The units extensions are: ' ' (ångströms *1.0) **'_pm'** (picometres /100.) **'_nm'** (nanometres *10.).

**_diffrn_radiation_inhomogeneity** *(numb)*

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

Appearance in list: both. The permitted range is 0·0→ ∞.

**_diffrn_radiation_monochromator** *(char)*

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

Appearance in list: both.

Example(s): `'Zr filter'`, `'Ge 220'`, `none`, `'equatorial mounted graphite'`

**_diffrn_radiation_polarisn_norm** *(numb)*

The angle in degrees of the perpendicular polarisation component to the diffraction plane. See `_diffrn_radiation_polarisn_ratio`.

Appearance in list: both. The permitted range is 0·0→ ∞.

**_diffrn_radiation_polarisn_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 `_diffrn_radiation_polarisn_norm` to the normal to the diffraction plane of the sample (*i.e.* the plane containing the incident and reflected beams).

Appearance in list: both. The permitted range is 0·0→ ∞.

**_diffrn_radiation_source** *(char)*

The source of radiation.

Appearance in list: both.

Example(s): `'RU2 Rigaku Denki rotating Cu anode'`, `'fine focus Philips Mo tube'`, `'5MeV synchrotron'`, `'HIFAR reactor'`

**_diffrn_radiation_type** *(char)*

The nature of the radiation.

Appearance in list: both.

Example(s): `'Cu K\a'`, `neutron`, `electron`

**_diffrn_radiation_wavelength** *(numb)*

The radiation wavelength.

Appearance in list: both. The permitted range is 0·0→ ∞. The units extensions are: ' ' (ångströms *1.0) **'_pm'** (picometres /100.) **'_nm'** (nanometres *10.).

**_diffrn_radiation_wavelength_id** *(char)*

The code identifying each value of `_diffrn_radiation_wavelength`. The `_diffrn_radiation_` data is looped when multiple wavelengths are used. This code is used to link with the `_diffrn_refln_` list. It must match with one of the `_diffrn_refln_wavelength_id` codes.

Appearance in list: yes. If looped, **`_diffrn_radiation_ wavelength`** must be present in the same list.

Example(s): `x1,` `x2,` `neut`

**_diffrn_radiation_wavelength_wt** *(numb)*

The relative weight of a wavelength identified by the code `_diffrn_radiation_wavelength_id` in the list of wavelengths.

Appearance in list: yes. If looped, **`_diffrn_radiation_wavelength_id`** must be present in the same list. The permitted range is 0·0→1·0. Where no value is given, the assumed value is '1·0'.

**_diffrn_refln_angle_chi**
**_diffrn_refln_angle_kappa**
**_diffrn_refln_angle_omega**
**_diffrn_refln_angle_phi**
**_diffrn_refln_angle_psi**
**_diffrn_refln_angle_theta** *(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.

Appearance in list: yes. If looped, **`_diffrn_refln_index_`** must be present in the same list.

**_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.

Appearance in list: yes. If looped, **`_diffrn_refln_index_`** must be present in the same list.

**_diffrn_refln_counts_bg_1**
**_diffrn_refln_counts_bg_2**
**_diffrn_refln_counts_net**
**_diffrn_refln_counts_peak**
**_diffrn_refln_counts_total** *(numb)*

The diffractometer counts for the measurements: background before the peak, background after the peak, net counts after background removed, counts for peak scan or position, and the total counts (background plus peak).

Appearance in list: yes. If looped, **`_diffrn_refln_index_`** must be present in the same list. The permitted range is 0→ ∞.

**_diffrn_refln_crystal_id** (*char*)

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

Appearance in list: yes. If looped, `_diffrn_refln_index_` must be present in the same list.

**_diffrn_refln_detect_slit_horiz**
**_diffrn_refln_detect_slit_vert** (*numb*)

Total horizontal and vertical slit apertures in degrees.

Appearance in list: yes. If looped, `_diffrn_refln_index_` must be present in the same list. The permitted range is 0·0→90·0.

**_diffrn_refln_elapsed_time** (*numb*)

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

Appearance in list: yes. If looped, `_diffrn_refln_index_` must be present in the same list. The permitted range is 0·0→ $\infty$. The units extensions are: ‘ ’ (minutes *1.0) ‘`_sec`’ (seconds /60.) ‘`_hr`’ (hours *60.).

**_diffrn_refln_index_h**
**_diffrn_refln_index_k**
**_diffrn_refln_index_l** (*numb*)

Miller indices of a diffraction reflection. These need not match the `_refln_index_h`, `*_k`, `*_l` 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_`.

Appearance in list: yes.

**_diffrn_refln_intensity_net**
**_diffrn_refln_intensity_sigma** (*numb*)

Net intensity and e.s.d. calculated from the diffraction counts after the attenuator and standard scales have been applied.

Appearance in list: yes. If looped, `_diffrn_refln_index_` must be present in the same list. The permitted range is 0→ $\infty$.

**_diffrn_refln_scale_group_code** (*char*)

The code identifying the scale appling to this reflection. This code must match with a specified `_diffrn_scale_group_code` value.

Appearance in list: yes. If looped, `_diffrn_refln_index_` must be present in the same list.

**_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`.

| | |
|---|---|
| `om` | $\omega$ scan |
| `ot` | $\omega/2\theta$ scan |

Appearance in list: yes. If looped, `_diffrn_refln_index_` must be present in the same list.

**_diffrn_refln_scan_mode_backgd** (*char*)

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

| | |
|---|---|
| `st` | stationary counter background |
| `mo` | moving counter background |

Appearance in list: yes. If looped, `_diffrn_refln_index_` must be present in the same list.

**_diffrn_refln_scan_width** (*numb*)

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

Appearance in list: yes. If looped, `_diffrn_refln_index_` must be present in the same list. The permitted range is 0·0→90·0.

**_diffrn_refln_sint/lambda** (*numb*)

The sin $\theta$ over wavelength value for this reflection.

Appearance in list: yes. If looped, `_diffrn_refln_index_` must be present in the same list. The permitted range is 0·0→ $\infty$. The units extensions are: ‘ ’ (reciprocal ångströms *1.0) ‘`_pm`’ (reciprocal picometres *100.) ‘`_nm`’ (reciprocal nanometres /10.).

**_diffrn_refln_standard_code** (*char*)

The code identifying that this reflection was measured as a standard intensity. This is the case if the code matched one of the `_diffrn_standard_refln_code` values.

Appearance in list: yes. If looped, `_diffrn_refln_index_` must be present in the same list.

Example(s): `1`, `2`, `3`, `s1`, `s2`, `s3`, `A`, `B`, `C`

**_diffrn_refln_wavelength** (*numb*)

The mean wavelength of radiation used to measure diffraction for this reflection. This is an important parameter for data collected using energy dispersive detectors or the Laue method.

Appearance in list: yes. If looped, `_diffrn_refln_index_` must be present in the same list. The permitted range is 0·0→ $\infty$. The units extensions are: ‘ ’ (ångströms *1.0) ‘`_pm`’ (picometres /100.) ‘`_nm`’ (nanometres *10.).

**_diffrn_refln_wavelength_id** (*char*)

Code identifying the wavelength in the `_diffrn_radiation_` list.

Appearance in list: yes. If looped, `_diffrn_refln_index_` must be present in the same list.

Example(s): `x1, x2, neut`

**_diffrn_reflns_av_R_equivalents** (*numb*)

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

The permitted range is 0·0→ $\infty$.

**_diffrn_reflns_av_sigmaI/netI** (*numb*)

Measure $[\sum |\sigma(I)| / \sum |net(I)|]$ for all measured reflections.

The permitted range is 0·0→ $\infty$.

**_diffrn_reflns_limit_h_max**
**_diffrn_reflns_limit_h_min**
**_diffrn_reflns_limit_k_max**
**_diffrn_reflns_limit_k_min**
**_diffrn_reflns_limit_l_max**
**_diffrn_reflns_limit_l_min** (*numb*)

The index limits of the diffraction reflection data specified by `_diffrn_refln_index_h`, `*_k`, `*_l`.

**_diffrn_reflns_number** (*numb*)

The total number of measured diffraction data.

The permitted range is 0→ $\infty$.

**_diffrn_reflns_reduction_process** *(char)*

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

Example(s): 'data averaged using Fisher test'

**_diffrn_reflns_theta_max**
**_diffrn_reflns_theta_min** *(numb)*

Theta angle limits in degrees for the measured diffraction data.

The permitted range is 0·0→90·0.

**_diffrn_reflns_transf_matrix_11**
**_diffrn_reflns_transf_matrix_12**
**_diffrn_reflns_transf_matrix_13**
**_diffrn_reflns_transf_matrix_21**
**_diffrn_reflns_transf_matrix_22**
**_diffrn_reflns_transf_matrix_23**
**_diffrn_reflns_transf_matrix_31**
**_diffrn_reflns_transf_matrix_32**
**_diffrn_reflns_transf_matrix_33** *(numb)*

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

$$(h \quad k \quad l)_{\rm diffraction} \begin{pmatrix} 11 & 12 & 13 \\ 21 & 22 & 23 \\ 31 & 32 & 33 \end{pmatrix} = (h' \quad k' \quad l')$$

**_diffrn_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 _diffrn_refln_scale_group_code in the reflection list.

Appearance in list: yes.

Example(s): 1, 2, 3 , s1, A, B, c1, c2, c3

**_diffrn_scale_group_I_net** *(numb)*

The intensity scale for a specific measurement group identified by _diffrn_scale_group_code.

Appearance in list: yes. The permitted range is 0·0→ ∞.

**_diffrn_special_details** *(char)*

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

**_diffrn_standard_refln_code** *(char)*

The code identifying a reflection measured as a standard reflection with the indices _diffrn_standard_refln_index_. This is the same code as the _diffrn_refln_standard_code in the _diffrn_refln_ list.

Appearance in list: yes. If looped, _diffrn_standard_refln_index_ must be present in the same list.

Example(s): 1, 2, 3, s1, A, B

**_diffrn_standard_refln_index_h**
**_diffrn_standard_refln_index_k**
**_diffrn_standard_refln_index_l** *(numb)*

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

Appearance in list: yes.

**_diffrn_standards_decay_%** *(numb)*

The percentage variation of the mean intensity for all standard reflections.

The permitted range is 0·0→ ∞.

**_diffrn_standards_interval_count**
**_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 e.s.d. of the individual mean standard scales applied to the intensity data.

The permitted range is 0·0→ ∞.

**_exptl_absorpt_coefficient_mu** *(numb)*

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

The permitted range is 0·0→ ∞. The units extensions are: ' ' (reciprocal millimetres *1.0) '_cm' (reciprocal centimetres /10.).

**_exptl_absorpt_correction_T_max**
**_exptl_absorpt_correction_T_min** *(numb)*

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

The permitted range is 0·0→1·0.

**_exptl_absorpt_correction_type** *(char)*

The absorption correction type and method.

| | |
|---|---|
| analytical | analytical from crystal shape |
| integration | integration from crystal shape |
| empirical | empirical from diffraction data |
| refdelf | refined from $\Delta F$ |
| sphere | spherical |
| cylinder | cylindrical |
| none | no absorption correction applied |

**_exptl_absorpt_process_details** *(char)*

Description of the absorption process applied to the data.

Example(s): 'Tompa analytical'

**_exptl_crystal_colour** *(char)*

The colour of the crystal.

Example(s): 'Dark green'

**_exptl_crystal_density_diffrn** *(numb)*

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

The permitted range is 0·0→ ∞.

**_exptl_crystal_density_meas** (*numb*)

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

The permitted range is 0·0→ ∞.

**_exptl_crystal_density_meas_temp** (*numb*)

Temperature in Kelvin that `_exptl_crystal_density_meas` was determined at.

The permitted range is 0·0→ ∞.

**_exptl_crystal_density_method** (*char*)

The method used to measure `_exptl_crystal_density_meas`.

**_exptl_crystal_description** (*char*)

A description of the crystal quality and habit. Dimensional data is better placed in the `_exptl_crystal_face_` data items.

**_exptl_crystal_F_000** (*numb*)

The number of electrons in the crystal unit cell $F(000)$.

The permitted range is 1→ ∞.

**_exptl_crystal_face_diffr_chi**
**_exptl_crystal_face_diffr_kappa**
**_exptl_crystal_face_diffr_phi**
**_exptl_crystal_face_diffr_psi** (*numb*)

The diffractometer angle settings in degrees for a specific crystal face associated with `_exptl_crystal_face_perp_dist`.

Appearance in list: yes. If looped, `_exptl_crystal_face_perp_dist` must be present in the same list.

**_exptl_crystal_face_index_h**
**_exptl_crystal_face_index_k**
**_exptl_crystal_face_index_l** (*numb*)

Miller indices of the crystal face associated with the value `_exptl_crystal_face_perp_dist`.

Appearance in list: yes. If looped, `_exptl_crystal_face_perp_dist` must be present in the same list.

**_exptl_crystal_face_perp_dist** (*numb*)

The perpendicular distance of the face to centre of rotation of the crystal.

Appearance in list: yes. The permitted range is 0·0→ ∞. The units extensions are: ' ' (millimetres *1.0) '_cm' (centimetres *10.0).

**_exptl_crystal_id** (*char*)

Code identifying each crystal if multiple crystals are used. Is used to link with `_diffrn_refln_crystal_id` in diffraction data and with `_refln_crystal_id` in the `_refln_` list.

Appearance in list: yes.

**_exptl_crystal_preparation** (*char*)

Details of crystal growth and preparation of the crystal (*e.g.* mounting) prior to the diffraction measurements.

Example(s): `'mounted in an argon-filled quartz capillary'`

**_exptl_crystal_size_max**
**_exptl_crystal_size_mid**
**_exptl_crystal_size_min**
**_exptl_crystal_size_rad** (*numb*)

The maximum, medial and minimum dimensions of the crystal. If the crystal is a sphere or a cylinder then the `*_rad` item is the radius. These may appear in a list with `_exptl_crystal_id` if multiple crystals used in the experiment.

Appearance in list: both. If looped, `_exptl_crystal_id` must be present in the same list. The permitted range is 0·0→ ∞. The units extensions are: ' ' (millimetres *1.0) '_cm' (centimetres *10.0).

**_exptl_crystals_number** (*numb*)

The total number of crystals used in the data measurement.

The permitted range is 1→ ∞.

**_exptl_special_details** (*char*)

Any special information about the experimental work prior to the diffraction measurement. See also `_exptl_crystal_preparation`.

**_geom_angle** (*numb*)

Angle in degrees bounded by the `_geom_angle_atom_site_label_1`, `*_2` and `*_3`. Site at `*_2` is at the apex of the angle.

Appearance in list: yes. If looped, `_geom_angle_atom_site_label_` must be present in the same list. E.s.d. expected: yes. Default e.s.d. value: 0·0.

**_geom_angle_atom_site_label_1**
**_geom_angle_atom_site_label_2**
**_geom_angle_atom_site_label_3** (*char*)

The labels of the three atom sites which define the angle specified by `_geom_angle`. These must match labels specified as `_atom_site_label` in the atom list. Label 2 identifies the site at the apex of the angle.

Appearance in list: yes.

**_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.

| | |
|---|---|
| `no` | do not include angle in special list |
| `yes` | do include angle in special list |

Appearance in list: yes. If looped, `_geom_angle_atom_site_label_` must be present in the same list.

**_geom_angle_site_symmetry_1**
**_geom_angle_site_symmetry_2**
**_geom_angle_site_symmetry_3** (*char*)

The symmetry code of each atom site as the symmetry equivalent position number 'n' and the cell translation number 'mmm'. These numbers are combined to form the code 'n mmm' or n_mmm. 'n' is the sequence number of the symmetry elements as listed in `_symmetry_equiv_pos_as_xyz`. 'mmm' are the concatenated cell translations along $x$, $y$, $z$ with respect to the base number 555. The symmetry transformation is applied to the coordinates given by `_atom_site_fract_x`, `*_y`, `*_z` identified by `_atom_site_label`. If there are no cell translations the translation number may be omitted. If no symmetry operations or translations are applicable then a single period '.' may be used.

Appearance in list: yes. If looped, _geom_angle_atom_site_label_ must be present in the same list.

Example(s): . (no symmetry or translation to site), 4 (4th symmetry operation applied), 7_645 (7th symm. posn; +*a* on *x*; −*b* on *y*)

**_geom_bond_atom_site_label_1**
**_geom_bond_atom_site_label_2** (*char*)

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

Appearance in list: yes.

**_geom_bond_distance** (*numb*)

The intramolecular bond distance.

Appearance in list: yes. If looped, _geom_bond_atom_site_label_ must be present in the same list. E.s.d. expected: yes. Default e.s.d. value: 0·0. The permitted range is 0·0→ ∞. The units extensions are: ' ' (ångströms *1.0) The units extensions are: '_pm' (picometres /100.) '_nm' (nanometres *10.).

**_geom_bond_publ_flag** (*char*)

Signals if the bond distance is referred to in a publication or should be placed in a list of special bond distances.

| | |
|---|---|
| no | do not include bond in special list |
| yes | do include bond in special list |

Appearance in list: yes. If looped, _geom_bond_atom_site_label_ must be present in the same list.

**_geom_bond_site_symmetry_1**
**_geom_bond_site_symmetry_2** (*char*)

The symmetry code of each atom site as the symmetry-equivalent position number 'n' and the cell translation number 'mmm'. These numbers are combined to form the code 'n mmm' or n_mmm. 'n' is the sequence number of the symmetry elements as listed in _symmetry_equiv_pos_as_xyz. 'mmm' are the concatenated cell translations along *x*, *y*, *z* with respect to the base number 555. The symmetry transformation is applied to the coordinates given by _atom_site_fract_x,*_y, *_z identified by _atom_site_label. If there are no cell translations the translation number may be omitted. If no symmetry operations or translations are applicable then a single period '.' may be used.

Appearance in list: yes. If looped, _geom_bond_atom_site_label_ must be present in the same list.

Example(s): . (no symmetry or translation to site), 4 (4th symmetry operation applied), 7_645 (7th symm. posn; +*a* on *x*; −*b* on *y*)

**_geom_contact_atom_site_label_1**
**_geom_contact_atom_site_label_2** (*char*)

The labels of two atom sites that are within contact distance. The labels must match _atom_site_label codes in the atom list.

Appearance in list: yes.

**_geom_contact_distance** (*numb*)

The interatomic contact distance.

Appearance in list: yes. If looped, _geom_contact_atom_site_label_ must be present in the same list. E.s.d. expected: yes. Default e.s.d. value: 0·0. The permitted range is 0·0→ ∞. The units extensions are: ' ' (ångströms *1.0) The units extensions are: '_pm' (picometres /100.) '_nm' (nanometres *10.).

**_geom_contact_publ_flag** (*char*)

Signals if the contact distance is referred to in a publication or should be placed in a list of special contact distances.

| | |
|---|---|
| no | do not include distance in special list |
| yes | do include distance in special list |

Appearance in list: yes. If looped, _geom_contact_atom_site_label_ must be present in the same list.

**_geom_contact_site_symmetry_1**
**_geom_contact_site_symmetry_2** (*char*)

The symmetry code of each atom site as the symmetry equivalent position number 'n' and the cell translation number 'mmm'. These numbers are combined to form the code 'n mmm' or n_mmm. 'n' is the sequence number of the symmetry elements as listed in _symmetry_equiv_pos_as_xyz. 'mmm' are the concatenated cell translations along *x*, *y*, *z* with respect to the base number 555. The symmetry transformation is applied to the coordinates given by _atom_site_fract_x,*_y, *_z identified by _atom_site_label. If there are no cell translations the translation number may be omitted. If no symmetry operations or translations are applicable then a single period '.' may be used.

Appearance in list: yes. If looped, _geom_contact_atom_site_label_ must be present in the same list.

Example(s): . (no symmetry or translation to site), 4 (4th symmetry operation applied), 7_645 (7th symm. posn; +*a* on *x*; −*b* on *y*)

**_geom_special_details** (*char*)

The description of geometrical information not covered by the existing _geom_ data names, such as least-squares planes.

**_geom_torsion** (*numb*)

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, W. & Prelog, V. (1960). *Endeavour*, **16**, 521–528.

Appearance in list: yes. If looped, _geom_torsion_atom_site_label_ must be present in the same list. E.s.d. expected: yes. Default e.s.d. value: 0·0.

**_geom_torsion_atom_site_label_1**
**_geom_torsion_atom_site_label_2**
**_geom_torsion_atom_site_label_3**
**_geom_torsion_atom_site_label_4** (*char*)

The labels of the four atom sites which define the torsion angle specified by _geom_torsion. These must match codes specified as _atom_site_label in the atom list. The torsion angle definition should be that of Klyne, W. & Prelog, V. (1960). *Endeavour*, **16**, 521–528. The vector direction *_label_2 to *_label_3 is the viewing direction, and the torsion angle is the angle of twist required to superimpose the projection of the vector site 2–site 1 onto the projection of the vector site 3–site 4. Clockwise torsions are positive, anticlockwise torsions are negative.

Appearance in list: yes.

**_geom_torsion_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.

| | |
|---|---|
| no | do not include distance in special list |
| yes | do include distance in special list |

Appearance in list: yes. If looped, _geom_torsion_atom_site_label_ must be present in the same list.

**_geom_torsion_site_symmetry_1**
**_geom_torsion_site_symmetry_2**
**_geom_torsion_site_symmetry_3**
**_geom_torsion_site_symmetry_4** (*char*)

The symmetry code of each atom site as the symmetry-equivalent position number 'n' and the cell translation number 'mmm'. These numbers are combined to form the code 'n mmm' or n_mmm. 'n' is the sequence number of the symmetry elements as listed in `_symmetry_equiv_pos_as_xyz`. 'mmm' are the concatenated cell translations along $x$, $y$, $z$ with respect to the base number 555. The symmetry transformation is applied to the coordinates given by `_atom_site_fract_x`, `*_y`, `*_z` identified by `_atom_site_label`. If there are no cell translations the translation number may be omitted. If no symmetry operations or translations are applicable then a single period '.' may be used.

Appearance in list: yes. If looped, `_geom_torsion_atom_site_label_` must be present in the same list.

Example(s): `.` (no symmetry or translation to site), `4` (4th symmetry operation applied), `7_645` (7th symm. posn; $+a$ on $x$; $-b$ on $y$)

**_journal_coden_ASTM**
**_journal_coden_Cambridge**
**_journal_coeditor_address**
**_journal_coeditor_code**
**_journal_coeditor_email**
**_journal_coeditor_fax**
**_journal_coeditor_name**
**_journal_coeditor_notes**
**_journal_coeditor_phone**
**_journal_date_accepted**
**_journal_date_from_coeditor**
**_journal_date_to_coeditor**
**_journal_date_printers_final**
**_journal_date_printers_first**
**_journal_date_proofs_in**
**_journal_date_proofs_out**
**_journal_date_recd_copyright**
**_journal_date_recd_electronic**
**_journal_date_recd_hard_copy**
**_journal_issue**
**_journal_name_full**
**_journal_page_first**
**_journal_page_last**
**_journal_suppl_publ_number**
**_journal_suppl_publ_pages**
**_journal_techeditor_address**
**_journal_techeditor_code**
**_journal_techeditor_email**
**_journal_techeditor_fax**
**_journal_techeditor_name**
**_journal_techeditor_notes**
**_journal_techeditor_phone**
**_journal_volume**
**_journal_year** (*char*)

Data items specified by the journal staff.

**_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`.

Appearance in list: both.

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

**_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, precedes the first names or initials.

Appearance in list: both.

Example(s): `'Bleary, Percival R.'`
```
"O'Neil, F.K."
'Van den Bossche, G.'
'Yang, D.-L.'
'Simonov, Yu.A'
```

**_publ_contact_author** (*char*)

The name and address of the author submitting the manuscript and CIF. This is the person contacted by the journal editorial staff.

Example(s):
```
; Professor Dr. J.U. Blogs
  Department of Structural Chemistry
  RRDD Institute of Technology
  Building #6-M57
  Highho Street
  Citytown 64664
  COUNTRYHERE
;
```

**_publ_contact_author_email** (*char*)

Email address in a form recognizable to international networks.

Example(s): `name@host.domain.country`, `uur5@banjo.bitnet`

**_publ_contact_author_fax** (*char*)

Facsimile telephone number with international code in parentheses.

Example(s): `'(12) 34 947 7334'`

**_publ_contact_author_phone** (*char*)

Telephone number with international code in parentheses and any extension number preceded by 'ext'.

Example(s): `'(12) 34 947 7330 ext 5543'`

**_publ_contact_letter** (*char*)

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

**_publ_manuscript_creation** (*char*)

A description of the wordprocessor 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 3/280'`

**_publ_manuscript_incl_extra_item**
**_publ_manuscript_incl_extra_info**
**_publ_manuscript_incl_extra_defn** (*char*)

These data items are used to specify the need to include specific data into a manuscript which is not normally requested by the journal. `*_item` specifies the data name; `*_info` provides the reasons for the inclusion; and `*_defn` flags whether this is a standard definition or not (flags are 'yes' or 'no'). The example shows how these three items are looped. Note that *_item names *must* be enclosed in single quotes.

Appearance in list: yes.

Example(s):

```
'_atom_site_symmetry_multiplicity'   'special sites' yes
'_chemical_compound_source'          'rare material' yes
'_reflns_d_resolution_high' 'limited data a problem' yes
'_crystal_magnetic_permeability'      'new quantity'  no
```

**_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_coeditor_name** (*char*)

The Co-editor's name requested to process the submitted manuscript.

**_publ_requested_journal** (*char*)

The journal's name requested for publication.

**_publ_section_title**
**_publ_section_abstract**
**_publ_section_comment**
**_publ_section_introduction**
**_publ_section_experimental**
**_publ_section_discussion**
**_publ_section_acknowledgements**
**_publ_section_references**
**_publ_section_figure_captions**
**_publ_section_table_legends** (*char*)

The sections of a manuscript if submitted in parts. As an alternative see _publ_manuscript_text and _publ_manuscript_processed.

**_refine_diff_density_max**
**_refine_diff_density_min** (*numb*)

The largest and smallest density in the final difference Fourier map.

E.s.d. expected: yes. Default e.s.d. value: 0·0. The units extensions are: ' ' (electrons per cubic ångström *1.0) '_pm' (electrons per cubic picometre *1.0E+6) '_nm' (electrons per cubic nanometre /1000.).

**_refine_ls_abs_structure_details** (*char*)

The nature of the absolute structure and how it was determined. For example, to describe the nature of the Friedel data used.

**_refine_ls_abs_structure_Flack** (*numb*)

This measure of absolute structure (enantiomorph or polarity) is defined in the paper by Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.

E.s.d. expected: yes. Default e.s.d. value: 0·0. The permitted range is 0·0→1·0.

**_refine_ls_abs_structure_Rogers** (*numb*)

This measure of absolute structure (enantiomorph or polarity) is defined in the paper by Rogers, D. (1981). *Acta Cryst.* A**37**, 734–741.

E.s.d. expected: yes. Default e.s.d. value: 0·0.

**_refine_ls_extinction_coef** (*numb*)

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 will be the $r^*$ value; for the 'B–C type 1 isotropic' method it is the '$g$' value, and for 'B–C type 2 isotropic' corrections it is the '$\rho$' value. Note that the magnitude of these values is usually of the order of 10000.

E.s.d. expected: yes. Default e.s.d. value: 0·0.

Example(s): 3472(52) (Zachariasen coefficient $r^* = 0{\cdot}347(5) \times 10^4$)

**_refine_ls_extinction_expression** (*char*)

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.

Example(s): 'Equ (22) p292 "Crystallographic Computing" Munksgaard 1970'

**_refine_ls_extinction_method** (*char*)

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 'Becker–Coppens' [Becker, P. J. & Coppens, P. (1974). *Acta Cryst.* A**30**, 129–153] or 'Zachariasen' [Zachariasen, W.H. (1967). *Acta Cryst.* **23**, 558–564]. The latter is sometimes referred to as the 'Larson' method [Larson, A. C. (1967). *Acta Cryst.* **23**, 664–665] even though it employs Zachariasen'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 dominated by particle size and includes a primary extinction component; and as 'mixed' when there is a mixture of types 1 and 2. For the B–C 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 multiple 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'

**_refine_ls_goodness_of_fit_all**
**_refine_ls_goodness_of_fit_obs** (*numb*)

The least-squares goodness-of-fit parameter $S$ for all data, and for observed data, after the final cycle of refinement. Ideally account should be taken of parameters restrained in the least squares. The goodness-of-fit parameter $S$ is defined as $S = [\sum(w|Y_m - Y_c|^2)/(N_{ref} - N_{param})]^{1/2}$ where the sum is over the specified reflection data; $N_{ref}$ is the number of reflections used in the refinement; $N_{param}$ is the number of refined parameters; $Y_m$ and $Y_c$ are the measured and calculated coefficients specified in `_refine_ls_structure_factor_coef`; and $w$ is the least-squares weight [1/(e.s.d. squared)]. See also `_refine_ls_restrained_S_` definitions.

E.s.d. expected: yes. Default e.s.d. value: 0·0. The permitted range is 0·0→ ∞.

**`_refine_ls_hydrogen_treatment`** (*char*)

Treatment of hydrogen atoms in the least-squares refinement.

| | |
|---|---|
| `refall` | refined all H parameters |
| `refxyz` | refined H coordinates only |
| `refU` | refined H $U$ only |
| `noref` | no refinement of H parameters |

Where no value is given, the assumed value is `'refxyz'`.

**`_refine_ls_matrix_type`** (*char*)

Type of matrix used to accumulate the least-squares derivatives.

| | |
|---|---|
| `full` | full |
| `fullcycle` | full with fixed elements per cycle |
| `atomblock` | block diagonal per atom |
| `userblock` | user-defined blocks |
| `diagonal` | diagonal elements only |
| `sparse` | selected elements only |

Where no value is given, the assumed value is `'full'`.

**`_refine_ls_number_constraints`** (*numb*)

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

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

**`_refine_ls_number_parameters`** (*numb*)

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

The permitted range is 0→ ∞.

**`_refine_ls_number_reflns`** (*numb*)

Number of reflections contributing to least-squares derivatives.

The permitted range is 0→ ∞.

**`_refine_ls_number_restraints`** (*numb*)

The number of restrained parameters. These are parameters which are not directly dependent on another refined parameter. 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→ ∞.

**`_refine_ls_R_factor_all`**
**`_refine_ls_R_factor_obs`** (*numb*)

Residual factors for all reflection data, and for reflection data classified as 'observed' (see `_reflns_observed_criterion`). $R = (\sum ||F_m| - |F_c|| / \sum |F_m|)$; $F_m$ and $F_c$ are measured and calculated structure factors. This is the conventional $R$ factor. See also `_refine_ls_wR_factor_` definitions.

The permitted range is 0·0→ ∞.

**`_refine_ls_restrained_S_all`**
**`_refine_ls_restrained_S_obs`** (*numb*)

The least-squares goodness-of-fit parameter $S'$ for all data, and for observed data, after the final cycle of least squares. This parameter explicitly includes the restraints applied in the least-squares process. $S' = \{[\sum(w|Y_m - Y_c|^2) + \sum_r(w_r|P_c - P_t|^2)]/(N_{ref} + N_{restr} - N_{param})\}^{1/2}$ where the sum $\sum$ is over the specified reflection data; $\sum_r$ is over the restraint data; $N_{ref}$ is the number of reflections used in the refinement (see `_refine_ls_number_reflns`); $N_{param}$ is the number of refined parameters (see `_refine_ls_number_parameters`); $N_{restr}$ is the number of restraints (see `_refine_ls_number_restraints`); $Y_m$ and $Y_c$ are the measured and calculated coefficients specified in `_refine_ls_structure_factor_coef`; $P_c$ and $P_t$ are the calculated and target restraint values; $w$ is the least-squares reflection weight [1/(e.s.d. squared)] and $w_r$ is the restraint weight. See also `_refine_ls_goodness_of_fit_` definitions.

The permitted range is 0·0→ ∞.

**`_refine_ls_shift/esd_max`**
**`_refine_ls_shift/esd_mean`** (*numb*)

The largest and the average ratios of the final least-squares parameter shift divided by the final estimated standard deviation.

The permitted range is 0·0→ ∞.

**`_refine_ls_structure_factor_coef`** (*char*)

Structure-factor coefficient $|F|$, $F^2$ or $I$, used in the least-squares refinement process.

| | |
|---|---|
| `Inet` | net intensity |
| `Fsqd` | structure factor squared |
| `F` | structure-factor magnitude |

Where no value is given, the assumed value is `'F'`.

**`_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.

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

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

**`_refine_ls_wR_factor_all`**
**`_refine_ls_wR_factor_obs`** (*numb*)

Residual factors for all reflection data, and for reflection data classified as 'observed' (see `_reflns_observed_criterion`). $wR = [\sum(w|Y_m - Y_c|^2)/\sum(wY_m^2)]^{1/2}$ where $Y_m$ and $Y_c$ are the measured and calculated coefficients specified by the `_refine_ls_structure_factor_coef`; $w$ is the least-squares weight. See also the `_refine_ls_R_factor_` definitions.

The permitted range is 0·0→ ∞.

**_refine_special_details** (*char*)

Description of special aspects of the refinement process.

**_refln_A_calc**
**_refln_A_meas** (*numb*)

Calculated, measured structure-factor component $A = |F| \cos(\text{phase})$ in electrons.

Appearance in list: yes. If looped, `_refln_index_` must be present in the same list.

**_refln_B_calc**
**_refln_B_meas** (*numb*)

Calculated, measured structure-factor component $B = |F| \sin(\text{phase})$ in electrons.

Appearance in list: yes. If looped, `_refln_index_` must be present in the same list.

**_refln_crystal_id** (*char*)

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

Appearance in list: yes. If looped, `_refln_index_` must be present in the same list.

**_refln_F_calc**
**_refln_F_meas**
**_refln_F_sigma** (*numb*)

The calculated, measured and standard deviation (derived from measured data) of the structure factors, in electrons.

Appearance in list: yes. If looped, `_refln_index_` must be present in the same list.

**_refln_F_squared_calc**
**_refln_F_squared_meas**
**_refln_F_squared_sigma** (*numb*)

Calculated, measured and estimated standard deviations of the squared structure factors, in electrons squared.

Appearance in list: yes. If looped, `_refln_index_` must be present in the same list.

**_refln_index_h**
**_refln_index_k**
**_refln_index_l** (*numb*)

Miller indices of the reflection.

Appearance in list: yes.

**_refln_intensity_calc**
**_refln_intensity_meas**
**_refln_intensity_sigma** (*numb*)

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

Appearance in list: yes. If looped, `_refln_index_` must be present in the same list.

**_refln_mean_path_length_tbar** (*numb*)

Mean path length through the crystal for this reflection.

Appearance in list: yes. If looped, `_refln_index_` must be present in the same list. The units extensions are: ‘ ’ (millimetres *1.0) ‘`_cm`’ (centimetres *10.0).

**_refln_observed_status** (*char*)

Classification of a reflection. *E.g.* ‘observed’ or ‘unobserved’ according to a criterion specified in `_reflns_observed_criterion`.

| | |
|---|---|
| `o` | observed by `_reflns_observed_criterion` |
| `<` | unobserved by `_reflns_observed_criterion` |
| `-` | systematically absent reflection |
| `x` | unreliable measurement – not used |

Appearance in list: yes. If looped, `_refln_index_` must be present in the same list. Where no value is given, the assumed value is ‘`o`’.

**_refln_phase_calc**
**_refln_phase_meas** (*numb*)

The calculated and measured structure-factor phase in degrees.

Appearance in list: yes. If looped, `_refln_index_` must be present in the same list.

**_refln_refinement_status** (*char*)

Status of reflection in the structure refinement process.

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

Appearance in list: yes. If looped, `_refln_index_` must be present in the same list. Where no value is given, the assumed value is ‘`incl`’.

**_refln_scale_group_code** (*char*)

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

Appearance in list: yes. If looped, `_refln_index_` must be present in the same list.

Example(s): `1`, `2`, `3`, `s1`, `A`, `B`, `c1`, `c2`, `c3`

**_refln_sint/lambda** (*numb*)

The $(\sin\theta)/\lambda$ for this reflection.

Appearance in list: yes. If looped, `_refln_index_` must be present in the same list. The permitted range is $0{\cdot}0 \rightarrow \infty$. The units extensions are: ‘ ’ (reciprocal ångströms *1.0) ‘`_pm`’ (reciprocal picometres *100.) ‘`_nm`’ (reciprocal nanometres /10.).

**_refln_symmetry_epsilon** (*numb*)

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

Appearance in list: yes. If looped, `_refln_index_` must be present in the same list. The permitted range is $1 \rightarrow 32$.

**_refln_symmetry_multiplicity** (*numb*)

The number of symmetry-equivalent reflections. The equivalent reflections have the same structure-factor value because of the space-group symmetry and the Friedel relationship.

Appearance in list: yes. If looped, `_refln_index_` must be present in the same list. The permitted range is $1 \rightarrow 24$.

**_refln_wavelength** (*numb*)

The mean wavelength of radiation used to measure this reflection. This is an important parameter for data collected using energy-dispersive detectors or the Laue method.

Appearance in list: yes. If looped, `_refln_index_` must be present in the same list. The permitted range is 0·0→ ∞. The units extensions are: `' '` (ångströms *1.0) `'_pm'` (picometres /100.) `'_nm'` (nanometres *10.).

**_refln_wavelength_id** (*char*)

Code identifying the wavelength in the `_diffrn_radiation_list`. See `_diffrn_radiation_wavelength_id`.

Appearance in list: yes. If looped, `_refln_index_` must be present in the same list.

**_reflns_d_resolution_high**
**_reflns_d_resolution_low** (*numb*)

The highest and lowest resolution for the interplanar spacings in the reflection data. These are the smallest and largest $d$ values.

The permitted range is 0·0→ ∞. The units extensions are: `' '` (ångströms *1.0) `'_pm'` (picometres /100.) `'_nm'` (nanometres *10.).

**_reflns_limit_h_max**
**_reflns_limit_h_min**
**_reflns_limit_k_max**
**_reflns_limit_k_min**
**_reflns_limit_l_max**
**_reflns_limit_l_min** (*numb*)

Miller indices limits for the reflection data. These need not be the same as the `_diffrn_reflns_limit_` values.

**_reflns_number_total**
**_reflns_number_observed** (*numb*)

The total number of reflections, and the number of 'observed' reflections, in the `_refln_` list (not the `_diffrn_refln_` list). The observed reflections satisfy the `_reflns_observed_criterion`. This may contain Friedel equivalent reflections according to the nature of the structure and the procedures used. The item `_reflns_special_details` describes the reflection data.

The permitted range is 0→ ∞.

**_reflns_observed_criterion** (*char*)

The criterion used to classify a reflection as 'observed'. This criterion is usually expressed in terms of an e.s.d. threshold.

Example(s): `>2sigma(I)`

**_reflns_scale_group_code** (*char*)

The code identifying a scale `_reflns_scale_meas_`. These are linked to the `_refln_` list by the `_refln_scale_group_code`.

Appearance in list: yes. If looped, `_reflns_scale_meas_` must be present in the same list.

**_reflns_scale_meas_F**
**_reflns_scale_meas_F_squared**
**_reflns_scale_meas_intensity** (*numb*)

Scales associated with `_reflns_scale_group_code`. These codes may not correspond to those in the `_diffrn_scale_` list.

Appearance in list: yes. If looped, `_reflns_scale_group_code` must be present in the same list. The permitted range is 0·0→ ∞.

**_reflns_special_details** (*char*)

A description of reflection data not covered by the other data names. It should include details of the Friedel reflection data.

**_symmetry_cell_setting** (*char*)

The cell settings for this space-group symmetry.

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

**_symmetry_equiv_pos_as_xyz** (*char*)

Symmetry equivalent position in the '*xyz*' representation. Except for the space group $P1$, this data will be repeated in a loop. The format of the data item is as per *International Tables for Crystallography*, Vol. A (1987). All equivalent positions should be entered, including those for lattice centring and a centre of symmetry, if present.

Appearance in list: yes.

Example(s): `'-y+x,-y,1/3+z'`

**_symmetry_Int_Tables_number** (*numb*)

Space-group number from *International Tables for Crystallography*, Vol. A (1987).

**_symmetry_space_group_name_Hall** (*char*)

Hall space-group symbol [Hall, S. R. (1981). *Acta Cryst.* A**37**, 517–525]. This symbol gives the space-group setting explicitly. Leave spaces between the separate components of the symbol.

Example(s): `'-P 2ac 2n'`, `'-R 3 2"'`, `'P 61 2 2 (0 0 -1)'`

**_symmetry_space_group_name_H-M** (*char*)

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 `*_Hall` 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)'`, `'R -3 2/m'`