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## `_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.

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

```
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_calc_flag
_atom_site_calc_attached_atom
O1   .4154(4)  .5699(1)  .3026(0)  .060(1)  Uani  ?    ?
C2   .5630(5)  .5087(2)  .3246(1)  .060(2)  Uani  ?    ?
C3   .5350(5)  .4920(2)  .3997(1)  .048(1)  Uani  ?    ?
N4   .3570(3)  .5558(1)  .4167(0)  .039(1)  Uani  ?    ?
# - - - - data truncated for brevity - - - -
H321C  .04(1)  .318(3)   .320(2)   .14000   Uiso  ?    ?
H322A  .25(1)  .272(4)   .475(3)   .19000   Uiso  ?    ?
H322B  .34976  .22118    .40954    .19000   Uiso  calc C322
```

*Example 2 - based on data set TOZ of Willis, Beckwith & Tozer [(1991). Acta Cryst. C47, 2276–2277].*

```
loop_
_atom_site_aniso_label
_atom_site_aniso_B_11  _atom_site_aniso_B_22
_atom_site_aniso_B_33  _atom_site_aniso_B_12
_atom_site_aniso_B_13  _atom_site_aniso_B_23
_atom_site_aniso_type_symbol
O1   .071(1) .076(1) .0342(9) .008(1)   .0051(9) -.0030(9) O
C2   .060(2) .072(2) .047(1)  .002(2)   .013(1)  -.009(1)  C
C3   .038(1) .060(2) .044(1)  .007(1)   .001(1)  -.005(1)  C
N4   .037(1) .048(1) .0325(9) .0025(9)  .0011(9) -.0011(9) N
# - - - - data truncated for brevity - - - -
```

*Example 3 - based on data set DPTD of Yamin, Suwandi, Fun, Sivakumar & bin Shawkataly [(1996). Acta Cryst. C52, 951–953].*

```
loop_
_atom_site_label
_atom_site_chemical_conn_number
_atom_site_fract_x  _atom_site_fract_y  _atom_site_fract_z
_atom_site_U_iso_or_equiv
S1  1  0.74799(9)  -0.12482(11)  0.27574(9)  0.0742(3)
S2  2  1.08535(10)  0.16131(9)   0.34061(9)  0.0741(3)
N1  3  1.0650(2)   -0.1390(2)    0.2918(2)   0.0500(5)
C1  4  0.9619(3)   -0.0522(3)    0.3009(2)   0.0509(6)
# - - - - data truncated for brevity - - - -
```

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

```
loop_
_atom_site_label
_atom_site_occupancy
_atom_site_disorder_assembly #
_atom_site_disorder_group    #   H11B    H11A      H13B
C1     1      .       .      #       .    |    .
H11A   .5     M       A      #         .  |  .
H12A   .5     M       A      #            C1 ---------C2---
H13A   .5     M       A      #          / .  \
H11B   .5     M       B      #        /   .    \
H12B   .5     M       B      #      /     .      \
H13B   .5     M       B      #   H12A    H12B    H13A
```

## `_atom_site_adp_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 $U$ |
| `Bani` | anisotropic $B^{ij}$ |
| `Biso` | isotropic $B$ |
| `Bovl` | overall $B$ |

Related item(s): `_atom_site_thermal_displace_type` (alternate). Appears in list containing `_atom_site_label`. `[atom_site]`

## `_atom_site_aniso_B_11`
## `_atom_site_aniso_B_12`
## `_atom_site_aniso_B_13`
## `_atom_site_aniso_B_22`
## `_atom_site_aniso_B_23`
## `_atom_site_aniso_B_33` (*numb*)

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

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

$h$ = the Miller indices, $a^*$ = the reciprocal-space cell lengths.

The unique elements of the real symmetric matrix are entered by row. 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_aniso_label`. Related item(s): `_atom_site_aniso_U_` (conversion). `[atom_site]`

## `_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`.

Appears in list as essential element of loop structure. **Must** match data name `_atom_site_label`. `[atom_site]`

## `_atom_site_aniso_ratio` (*numb*)

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

Appears in list containing `_atom_site_aniso_label`. The permitted range is 1.0→∞. `[atom_site]`

## `_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.

Appears in list containing `_atom_site_aniso_label`. **Must** match data name `_atom_site_type_symbol`. `[atom_site]`

### `_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 in ångströms squared which appear in the structure factor term:

$$T = \exp\left\{-2\pi^2 \sum_i \left[\sum_j (U^{ij} h_i h_j a_i^* a_j^*)\right]\right\}$$

$h$ = the Miller indices, $a^*$ = the reciprocal-space cell lengths.

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

Appears in list containing `_atom_site_aniso_label`. Related item(s): `_atom_site_aniso_B_` (conversion). `[atom_site]`

### `_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.

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

Example(s): `'2'` (water oxygen), `'1'` (hydroxyl oxygen), `'4'` (ammonium nitrogen) `[atom_site]`

### `_atom_site_B_equiv_geom_mean` (*numb*)

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

$$B_{\rm equiv} = (B_i B_j B_k)^{1/3}$$

$B_n$ = the principal components of the orthogonalised $B^{ij}$.

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→∞. Related item(s): `_atom_site_B_iso_or_equiv` (alternate), `_atom_site_U_equiv_geom_mean` (conversion). `[atom_site]`

### `_atom_site_B_iso_or_equiv` (*numb*)

Isotropic atomic displacement parameter, or equivalent isotropic atomic displacement parameter, $B_{\rm equiv}$, in ångströms squared, calculated from anisotropic temperature factor parameters.

$$B_{\rm equiv} = (1/3) \sum_i \left[\sum_j (B^{ij} a_i^* a_j^* a_i a_j)\right]$$

$a$ = the real-space cell lengths, $a^*$ = the reciprocal-space cell lengths, $B^{ij} = 8\pi^2 U^{ij}$.

Ref: Fischer, R. X. & Tillmanns, E. (1988). *Acta Cryst.* C**44**, 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→∞. Related item(s): `_atom_site_B_equiv_geom_mean` (alternate), `_atom_site_U_iso_or_equiv` (conversion). `[atom_site]`

### `_atom_site_calc_attached_atom` (*char*)

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

Appears in list containing `_atom_site_label`. Where no value is given, the assumed value is `'.'`. `[atom_site]`

### `_atom_site_calc_flag` (*char*)

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 |
| `c` | abbreviation for “calc” |
| `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]`

### `_atom_site_Cartn_x`
### `_atom_site_Cartn_y`
### `_atom_site_Cartn_z` (*numb*)

The atom site coordinates in ångströms 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_fract_` (alternate). Appears in list containing `_atom_site_label`. `[atom_site]`

### `_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`.

Appears in list containing `_atom_site_label`. **Must** match data name `_chemical_conn_atom_number`. The permitted range is 1→∞. `[atom_site]`

### `_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`.

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

Example(s): `'pop=1.0-pop(Zn3)'` `[atom_site]`

### `_atom_site_description` (*char*)

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

Appears in list containing `_atom_site_label`.

Example(s): `'Ag/Si disordered'` `[atom_site]`

### `_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), `‘B’` (disordered sites related by a mirror), `‘S’` (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_fract_x`
### `_atom_site_fract_y`
### `_atom_site_fract_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`. `[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 `*_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.

Appears in list as essential element of loop structure. May match subsidiary data name(s): `_atom_site_aniso_label`,
`_geom_angle_atom_site_label_1`,
`_geom_angle_atom_site_label_2`,
`_geom_angle_atom_site_label_3`,
`_geom_bond_atom_site_label_1`,
`_geom_bond_atom_site_label_2`,
`_geom_contact_atom_site_label_1`,
`_geom_contact_atom_site_label_2`,
`_geom_hbond_atom_site_label_D`,
`_geom_hbond_atom_site_label_H`,
`_geom_hbond_atom_site_label_A`,
`_geom_torsion_atom_site_label_1`,
`_geom_torsion_atom_site_label_2`,
`_geom_torsion_atom_site_label_3`,
`_geom_torsion_atom_site_label_4`.

Example(s): `‘C12’`, `‘Ca3g28’`, `‘Fe3+17’`, `‘H*251’`, `‘boron2a’`, `‘C_a_phe_83_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 $-3u \leq x \leq 1 + 3u$. The `_enumeration_range` of 0.0:1.0 is thus correctly interpreted as meaning $(0.0 - 3u) \leq x \leq (1.0 + 3u)$.

Appears in list containing `_atom_site_label`. Where no value is given, the assumed value is `‘1.0’`.The permitted range is 0.0→1.0. `[atom_site]`

### `_atom_site_refinement_flags` (*char*)

**This definition has been superseded and is retained here only for archival purposes. Use instead `_atom_site_refinement_flags_posn`, `*_adp` and `*_occupancy`.**

*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` | $U_{\mathrm{iso}}$ or $U^{ij}$ restraint (rigid bond) |
| `P` | partial occupancy constraint |

Appears in list containing `_atom_site_label`. `[atom_site]`

### _atom_site_refinement_flags_adp (*char*)

A code which indicates the refinement restraints or constraints applied to the atomic displacement parameters of this site.

| | |
|---|---|
| `.` | no constraints on atomic displacement parameters |
| `T` | special-position constraints on atomic displacement parameters |
| `U` | $U_{\text{iso}}$ or $U^{ij}$ restraint (rigid bond) |
| `TU` | Both constraints applied |

Appears in list containing `_atom_site_label`. Related item(s): `_atom_site_refinement_flags_posn` (alternate). `[atom_site]`

### _atom_site_refinement_flags_occupancy (*char*)

A code which indicates that refinement restraints or constraints were applied to the occupancy of this site.

| | |
|---|---|
| `.` | no constraints on site occupancy parameters |
| `P` | site occupancy constraint |

Appears in list containing `_atom_site_label`. Related item(s): `_atom_site_refinement_flags_posn` (alternate). `[atom_site]`

### _atom_site_refinement_flags_posn (*char*)

A code which indicates the refinement restraints or constraints applied to the positional coordinates of this site.

| | |
|---|---|
| `.` | no constraints on positional coordinates |
| `D` | distance or angle restraint on positional coordinates |
| `G` | rigid group refinement of positional coordinates |
| `R` | riding-atom site attached to non-riding atom |
| `S` | special position constraint on positional coordinates |
| `DG` | combination of the above constraints |
| `DR` | combination of the above constraints |
| `DS` | combination of the above constraints |
| `GR` | combination of the above constraints |
| `GS` | combination of the above constraints |
| `RS` | combination of the above constraints |
| `DGR` | combination of the above constraints |
| `DGS` | combination of the above constraints |
| `DRS` | combination of the above constraints |
| `GRS` | combination of the above constraints |
| `DGRS` | combination of the above constraints |

Appears in list containing `_atom_site_label`. Related item(s): `_atom_site_refinement_flags_posn` (alternate). `[atom_site]`

### _atom_site_restraints (*char*)

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

Appears in list containing `_atom_site_label`.

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

### _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).

Appears in list containing `_atom_site_label`. The permitted range is 1→192. `[atom_site]`

### _atom_site_thermal_displace_type (*char*)

**This definition has been superseded and is retained here only for archival purposes. Use instead `_atom_site_adp_type`**
*A standard code used to describe the type of atomic displacement parameters used for the site.*

`[atom_site]`

### _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(SDS)'`

`[atom_site]`

### _atom_site_U_equiv_geom_mean (*numb*)

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

$$U_{\text{equiv}} = (U_i U_j U_k)^{1/3}$$

$U_n$ = 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_U_iso_or_equiv` (alternate), `_atom_site_B_equiv_geom_mean` (conversion).

`[atom_site]`

### _atom_site_U_iso_or_equiv (*numb*)

Isotropic atomic displacement parameter, or equivalent isotropic atomic displacement parameter, $U_{\text{equiv}}$, in ångströms squared, calculated from anisotropic atomic displacement parameters.

$$U_{\text{equiv}} = (1/3) \sum_i \left[ \sum_j (U^{ij} a_i^* a_j^* a_i a_j) \right]$$

$a$ = the real-space cell lengths, $a^*$ = the reciprocal-space cell lengths.

Ref: Fischer, R. X. and Tillmanns, E. (1988). *Acta Cryst.* C**44**, 775–776.

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

`[atom_site]`

### _atom_site_Wyckoff_symbol (*char*)

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

Appears in list containing `_atom_site_label`. `[atom_site]`

## _atom_sites_[]

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

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

```
_atom_sites_Cartn_transform_axes
               'c along z, astar along x, b along y'
_atom_sites_Cartn_tran_matrix_11    58.39
_atom_sites_Cartn_tran_matrix_12     0.00
_atom_sites_Cartn_tran_matrix_13     0.00
_atom_sites_Cartn_tran_matrix_21     0.00
_atom_sites_Cartn_tran_matrix_22    86.70
_atom_sites_Cartn_tran_matrix_23     0.00
_atom_sites_Cartn_tran_matrix_31     0.00
_atom_sites_Cartn_tran_matrix_32     0.00
_atom_sites_Cartn_tran_matrix_33    46.27
```

`_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 in the ATOM_SITES category to Cartesian coordinates. The axial alignments of this transformation are described in `_atom_sites_Cartn_transform_axes`. The 3 × 1 translation is defined in `_atom_sites_Cartn_tran_vector_`.

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

`[atom_sites]`

`_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]`

`_atom_sites_Cartn_tran_vector_1`
`_atom_sites_Cartn_tran_vector_2`
`_atom_sites_Cartn_tran_vector_3` (*numb*)

Elements of a 3 × 1 translation vector used in the transformation of fractional coordinates in the ATOM_SITES category to Cartesian coordinates. The axial alignments of this transformation are described in `_atom_sites_Cartn_transform_axes`.

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

`[atom_sites]`

`_atom_sites_fract_tran_matrix_11`
`_atom_sites_fract_tran_matrix_12`
`_atom_sites_fract_tran_matrix_13`
`_atom_sites_fract_tran_matrix_21`
`_atom_sites_fract_tran_matrix_22`
`_atom_sites_fract_tran_matrix_23`
`_atom_sites_fract_tran_matrix_31`
`_atom_sites_fract_tran_matrix_32`
`_atom_sites_fract_tran_matrix_33` (*numb*)

Matrix elements used to transform Cartesian coordinates in the ATOM_SITES category to fractional coordinates. The axial alignments of this transformation are described in `_atom_sites_Cartn_transform_axes`. The 3 × 1 translation is defined in `_atom_sites_fract_tran_vector_`.

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

`[atom_sites]`

`_atom_sites_fract_tran_vector_1`
`_atom_sites_fract_tran_vector_2`
`_atom_sites_fract_tran_vector_3` (*numb*)

Elements of a 3 × 1 translation vector used in the transformation of Cartesian coordinates in the ATOM_SITES category to fractional coordinates. The axial alignments of this transformation are described in `_atom_sites_Cartn_transform_axes`.

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

`[atom_sites]`

`_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_sites]`

`_atom_sites_special_details` (*char*)

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

`[atom_sites]`

`_atom_type_[]`

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

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

```
loop_
_atom_type_symbol
_atom_type_oxidation_number
_atom_type_number_in_cell
_atom_type_scat_dispersion_real
_atom_type_scat_dispersion_imag
_atom_type_scat_source
C  0  72  .017  .009  International_Tables_Vol_IV_Table_2.2B
H  0  100  0     0    International_Tables_Vol_IV_Table_2.2B
O  0  12  .047  .032  International_Tables_Vol_IV_Table_2.2B
N  0  4   .029  .018  International_Tables_Vol_IV_Table_2.2B
```

`_atom_type_analytical_mass_%` (*numb*)

Mass percentage of this atom type derived from chemical analysis.

Appears in list containing `_atom_type_symbol`. The permitted range is 0.0→100.0. `[atom_type]` `_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.

Appears in list containing `_atom_type_symbol`.

Example(s): `‘deuterium’`, `‘0.34Fe+0.66Ni’` `[atom_type]`

`_atom_type_number_in_cell` (*numb*)

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

Appears in list containing `_atom_type_symbol`. The permitted range is $0\rightarrow\infty$. `[atom_type]`

`_atom_type_oxidation_number` (*numb*)

Formal oxidation state of this atom type in the structure.

Appears in list containing `_atom_type_symbol`. Where no value is given, the assumed value is `‘0’`.The permitted range is $-8\rightarrow8$. `[atom_type]`

`_atom_type_radius_bond`
`_atom_type_radius_contact` (*numb*)

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

Appears in list containing `_atom_type_symbol`. The permitted range is $0.0\rightarrow5.0$. `[atom_type]`

`_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.

Ref: *International Tables for X-ray Crystallography*, Vol. IV (1974) Table 2.2B, or *International Tables for Crystallography*, Vol. C (1991) Tables 6.1.1.4 and 6.1.1.5.

Appears in list containing `_atom_type_symbol`. `[atom_type]`

`_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`.

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

`_atom_type_scat_dispersion_source` (*char*)

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

Appears in list containing `_atom_type_symbol`.

Example(s):
`‘International Tables Vol. IV Table 2.3.1’` `[atom_type]`

`_atom_type_scat_length_neutron` (*numb*)

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

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

`_atom_type_scat_source` (*char*)

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

Appears in list containing `_atom_type_symbol`.

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

`_atom_type_scat_versus_stol_list` (*char*)

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

Appears in list containing `_atom_type_symbol`. `[atom_type]`

`_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.

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

Example(s): `‘C’`, `‘Cu2+’`, `‘H(SDS)’`, `‘dummy’`, `‘FeNi’` `[atom_type]`

`_audit_[]`

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

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

```
_audit_block_code                TOZ_1991-03-20
_audit_creation_date             1991-03-20
_audit_creation_method
                 from_xtal_archive_file_using_CIFIO
_audit_update_record
;  1991-04-09   text and data added by Tony Willis.
   1991-04-15   rec'd by co-editor as manuscript HL0007.
   1991-04-17   adjustments based on first referee report.
   1991-04-18   adjustments based on second referee report.
;
```

`_audit_block_code` (*char*)

A code intended to identify uniquely the current data block.

Example(s): `‘TOZ_1991-03-20’` `[audit]`

`_audit_creation_date` (*char*)

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

Example(s): `‘1990-07-12’` `[audit]`

### `_audit_creation_method` (*char*)

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

Example(s): `'spawned by the program QBEE'` [audit]

### `_audit_update_record` (*char*)

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

Example(s): `'1990-07-15 Updated by the Co-editor'` [audit]

## `_audit_author_[]`

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

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

```
loop_
_audit_author_name
_audit_author_address
'Fitzgerald, Paula M. D.'
;   Department of Biophysical Chemistry
    Merck Research Laboratories
    PO Box 2000, Ry80M203
    Rahway
    New Jersey 07065
    USA
;
'Van Middlesworth, J. F.'
;   Department of Biophysical Chemistry
    Merck Research Laboratories
    PO Box 2000, Ry80M203
    Rahway
    New Jersey 07065
    USA
;
```

### `_audit_author_address` (*char*)

The address of an author of this data block. If there are multiple authors, `_audit_author_address` is looped with `_audit_author_name`.

Appears in list containing `_audit_author_name`.

Example(s):

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

[audit_author]

### `_audit_author_name` (*char*)

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

Appears in list as essential element of loop structure.

Example(s): `'Bleary, Percival R.'`, `'O'Neil, F. K.'`, `'Van den Bossche, G.'`, `'Yang, D.-L.'`, `'Simonov, Yu.A'`, `'M\"uller, H. A.'`, `'Ross II, C. R.'` [audit_author]

## `_audit_conform_[]`

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

*Example 1 - Any file conforming to the current CIF core dictionary.*

```
_audit_conform_dict_name        cif_core.dic
_audit_conform_dict_version     2.3
_audit_conform_dict_location
      ftp://ftp.iucr.org/pub/cif_core.2.3.dic
```

### `_audit_conform_dict_location` (*char*)

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

May appear in list containing `_audit_conform_dict_name`. [audit_conform]

### `_audit_conform_dict_name` (*char*)

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

May appear in list as essential element of loop structure. [audit_conform]

### `_audit_conform_dict_version` (*char*)

The version number of the conformant dictionary.

May appear in list containing `_audit_conform_dict_name`. [audit_conform]

## `_audit_contact_author_[]`

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

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

```
loop_
_audit_contact_author_name
_audit_contact_author_address
_audit_contact_author_email
_audit_contact_author_fax
_audit_contact_author_phone
'Fitzgerald, Paula M. D.'
;   Department of Biophysical Chemistry
    Merck Research Laboratories
    PO Box 2000, Ry80M203
    Rahway
    New Jersey 07065
    USA
;
'paula_fitzgerald@merck.com'
'1(908)5945510'
'1(908)5945510'
```

### `_audit_contact_author_address` (*char*)

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
;
```

[audit_contact_author]

### `_audit_contact_author_email` (*char*)

The electronic mail address of the author of the data block to whom correspondence should be addressed, in a form recognisable to international networks.

Example(s): `‘name@host.domain.country’`, `‘bm@iucr.org’`
`[audit_contact_author]`

### `_audit_contact_author_fax` (*char*)

The facsimile telephone number of the author of the data block to whom correspondence should be addressed. The recommended style includes the international dialing prefix, the area code in parentheses, followed by the local number with no spaces.

Example(s): `‘12(34)9477334’`, `‘12()349477334’`
`[audit_contact_author]`

### `_audit_contact_author_name` (*char*)

The name of the author of the data block to whom correspondence should be addressed. The family name(s), followed by a comma and including any dynastic components, precedes the first name(s) or initial(s).

Example(s): `‘Bleary, Percival R.’`, `‘O’Neil, F. K.’`, `‘Van den Bossche, G.’`, `‘Yang, D.-L.’`, `‘Simonov, Yu.A’`, `‘M\"uller, H. A.’`, `‘Ross II, C. R.’` `[audit_contact_author]`

### `_audit_contact_author_phone` (*char*)

The telephone number of the author of the data block to whom correspondence should be addressed. The recommended style 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()349477330’`, `‘12(34)9477330x5543’` `[audit_contact_author]`

## `_audit_link_[]`

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

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

```
loop_
_audit_link_block_code
_audit_link_block_description
.            'discursive text of paper with two structures'
morA_(1)     'structure 1 of 2'
morA_(2)     'structure 2 of 2'
```

*Example 2 - example file for the one-dimensional incommensurately modulated structure of $K_2SeO_4$.*

```
loop_
_audit_link_block_code
_audit_link_block_description
.        'publication details'
KSE_COM  'experimental data common to ref./mod. structures'
KSE_REF  'reference structure'
KSE_MOD  'modulated structure'
```

### `_audit_link_block_code` (*char*)

The value of `_audit_block_code` associated with a data block in the current file related to the current data block. The special value ‘.’ may be used to refer to the current data block for completeness.

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

### `_audit_link_block_description` (*char*)

A textual description of the relationship of the referenced data block to the current one.

Appears in list containing `_audit_link_block_code`.
`[audit_link]`

## `_cell_[]`

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

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

```
_cell_length_a                   5.959(1)
_cell_length_b                   14.956(1)
_cell_length_c                   19.737(3)
_cell_angle_alpha                90
_cell_angle_beta                 90
_cell_angle_gamma                90
_cell_volume                     1759.0(3)
_cell_measurement_temperature    293
_cell_measurement_reflns_used    25
_cell_measurement_theta_min      25
_cell_measurement_theta_max      31
```

### `_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_`.

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

### `_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]`

### `_cell_length_a`
### `_cell_length_b`
### `_cell_length_c` (*numb*)

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

The permitted range is 0.0→∞. `[cell]`

`_cell_measurement_pressure` (*numb*)

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→∞. `[cell]`

`_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]`

`_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]`

`_cell_measurement_temperature` (*numb*)

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

The permitted range is 0.0→∞. `[cell]`

`_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]`

`_cell_measurement_wavelength` (*numb*)

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

The permitted range is 0.0→∞. `[cell]`

`_cell_reciprocal_angle_alpha`
`_cell_reciprocal_angle_beta`
`_cell_reciprocal_angle_gamma` (*numb*)

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

$$\cos(\alpha_{\rm recip}) = [\cos(\beta)\cos(\gamma) - \cos(\alpha)]/[\sin(\beta)\sin(\gamma)]$$

$$\cos(\beta_{\rm recip}) = [\cos(\gamma)\cos(\alpha) - \cos(\beta)]/[\sin(\gamma)\sin(\alpha)]$$

$$\cos(\gamma_{\rm recip}) = [\cos(\alpha)\cos(\beta) - \cos(\gamma)]/[\sin(\alpha)\sin(\beta)]$$

Ref: Buerger, M. J. (1942). *X-ray Crystallography*, p. 360. New York: John Wiley & Sons Inc.

Where no value is given, the assumed value is `'90.0'`. The permitted range is 0.0→180.0. `[cell]`

`_cell_reciprocal_length_a`
`_cell_reciprocal_length_b`
`_cell_reciprocal_length_c` (*numb*)

The reciprocal cell lengths in inverse ångströms. These are related to the real cell by the following equation:

$$a_{\rm recip} = bc\sin(\alpha)/V$$

$$b_{\rm recip} = ca\sin(\beta)/V$$

$$c_{\rm recip} = ab\sin(\gamma)/V$$

where $V$ is the cell volume. Ref: Buerger, M. J. (1942). *X-ray Crystallography*, p. 360. New York: John Wiley & Sons Inc.

The permitted range is 0.0→∞. `[cell]`

`_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]`

`_cell_volume` (*numb*)

Cell volume $V$ in ångströms cubed.

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

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

The permitted range is 0.0→∞. `[cell]`

### `_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 $Rb_2S_2O_6$ 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
-2    4    1          8.67
 0    3    2          9.45
 3    0    2          9.46
-3    4    1          8.93
-2    1   -2          7.53
10    0    0         23.77
 0   10    0         23.78
-5    4    1         11.14
# - - - - data truncated for brevity - - - -
```

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

Miller indices of a reflection used for measurement of the unit cell.

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

`_cell_measurement_refln_theta` (*numb*)

$\theta$ 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. `[cell_measurement_refln]`

### `_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.

*Example 1 - based on data set 9597gaus of Alyea, Ferguson & Kannan [(1996). Acta Cryst. C52, 765–767].*

```
_chemical_name_systematic
 trans-bis(tricyclohexylphosphine)tetracarbonylmolybdenum(0)
```

### `_chemical_absolute_configuration` (*char*)

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

Ref: Flack, H. D. & Bernardinelli, G. (1999). *Acta Cryst.* A**55**, 908–915. (http://www.iucr.org/paper?sh0129) Flack, H. D. & Bernardinelli, G. (2000). *J. Appl. Cryst.* **33**, 1143–1148. (http://www.iucr.org/paper?ks0021)

| | |
|---|---|
| `rm` | absolute configuration established by the structure determination of a compound containing a chiral reference molecule of known absolute configuration |
| `ad` | absolute configuration established by anomalous dispersion effects in diffraction measurements on the crystal |
| `rmad` | absolute configuration established by the structure determination of a compound containing a chiral reference molecule of known absolute configuration and confirmed by anomalous dispersion effects in diffraction measurements on the crystal |
| `syn` | absolute configuration has not been established by anomalous dispersion effects in diffraction measurements on the crystal. The enantiomer has been assigned by reference to an unchanging chiral centre in the synthetic procedure |
| `unk` | absolute configuration is unknown, there being no firm chemical evidence for its assignment to hand and it having not been established by anomalous dispersion effects in diffraction measurements on the crystal. An arbitrary choice of enantiomer has been made |
| `.` | inapplicable |

`[chemical]`

### `_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]`

### `_chemical_melting_point` (*numb*)

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

The permitted range is 0.0→∞. `[chemical]`

### `_chemical_melting_point_gt`
### `_chemical_melting_point_lt` (*numb*)

A temperature in kelvins below which (`*_lt`) or above which (`*_gt`) the melting point, the temperature at which a crystalline solid changes to a liquid, lies. These items allow a range of temperatures to be given.

`_chemical_melting_point` should always be used in preference to these items whenever possible.

The permitted range is 0.0→∞. Related item(s): `_chemical_melting_point` (alternate). `[chemical]`

### `_chemical_name_common` (*char*)

Trivial name by which the compound is commonly known.

Example(s): `‘1-bromoestradiol’` `[chemical]`

### `_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]`

### `_chemical_name_structure_type` (*char*)

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

Example(s): `‘perovskite’`, `‘sphalerite’`, `‘A15’` `[chemical]`

### `_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’`
`[chemical]`

### `_chemical_optical_rotation` (*char*)

The optical rotation in solution of the compound is specified in the following format:

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

where *TEMP* is the temperature of the measurement in degrees Celsius, *WAVE* is an indication of the wavelength of the light used for the measurement, *CONC* is the concentration of the solution given as the mass of the substance in g in 100 ml of solution, *SORT* is the signed value (preceded by a + or a − sign) of $100\alpha/(lc)$, where $\alpha$ 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): `‘[\a]^25^~D~= +108 (c = 3.42, CHCl~3~)’`
`[chemical]`

### `_chemical_properties_biological` (*char*)

A free description of the biological properties of the material.

Example(s):

```
; diverse biological activities including use as a
  laxative and strong antibacterial activity against
  S. aureus and weak activity against
  cyclooxygenase-1 (COX-1)
;,
; antibiotic activity against Bacillus subtilis
  (ATCC 6051) but no significant activity against
  Candida albicans (ATCC 14053), Aspergillus flavus
  (NRRL 6541) and Fusarium verticillioides (NRRL
  25457)
;,
; weakly potent lipoxygenase nonredox inhibitor
;,
; no influenza A virus sialidase inhibitory and
  plaque reduction activities
;,
; low toxicity against Drosophila melanogaster
;
```

`[chemical]`

### _chemical_properties_physical (*char*)

A free description of the physical properties of the material.

Example(s): `'air-sensitive'`, `'moisture-sensitive'`, `'hygroscopic'`, `'deliquescent'`, `'oxygen-sensitive'`, `'photo-sensitive'`, `'pyrophoric'`, `'semiconductor'`, `'ferromagnetic at low temperature'`, `'paramagnetic and thermochromic'` `[chemical]`

### _chemical_temperature_decomposition (*numb*)

The temperature in kelvins at which a solid decomposes.

The permitted range is 0.0→∞.

Example(s): `'350'` `[chemical]`

### _chemical_temperature_decomposition_gt
### _chemical_temperature_decomposition_lt (*numb*)

A temperature in kelvins below which (`*_lt`) or above which (`*_gt`) the solid is known to decompose. These items allow a range of temperatures to be given.

`_chemical_temperature_decomposition` should always be used in preference to these items whenever possible.

The permitted range is 0.0→∞.

Example(s): `'350'`

Related item(s): `_chemical_temperature_decomposition` (alternate). `[chemical]`

### _chemical_temperature_sublimation (*numb*)

The temperature in kelvins at which a solid sublimes.

The permitted range is 0.0→∞.

Example(s): `'350'` `[chemical]`

### _chemical_temperature_sublimation_gt
### _chemical_temperature_sublimation_lt (*numb*)

A temperature in kelvins below which (`*_lt`) or above which (`*_gt`) the solid is known to sublime. These items allow a range of temperatures to be given.

`_chemical_temperature_sublimation` should always be used in preference to these items whenever possible.

The permitted range is 0.0→∞.

Example(s): `'350'`

Related item(s): `_chemical_temperature_sublimation` (alternate). `[chemical]`

## _chemical_conn_atom_[]

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

*Example 1 - based on data set DPTD of Yamin, Suwandi, Fun, Sivakumar & bin Shawkataly [(1996). Acta Cryst. C52, 951–953].*

```
loop_
_chemical_conn_atom_number
_chemical_conn_atom_type_symbol
_chemical_conn_atom_display_x
_chemical_conn_atom_display_y
_chemical_conn_atom_NCA
_chemical_conn_atom_NH
1   S    .39  .81   1   0
2   S    .39  .96   2   0
3   N    .14  .88   3   0
4   C    .33  .88   3   0
5   C    .11  .96   2   2
6   C    .03  .96   2   2
7   C    .03  .80   2   2
8   C    .11  .80   2   2
9   S    .54  .81   1   0
10  S    .54  .96   2   0
11  N    .80  .88   3   0
12  C    .60  .88   3   0
13  C    .84  .96   2   2
14  C    .91  .96   2   2
15  C    .91  .80   2   2
16  C    .84  .80   2   2
```

### _chemical_conn_atom_charge (*numb*)

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

Appears in list containing `_chemical_conn_atom_type_symbol`. 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]`

### _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 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.

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

### _chemical_conn_atom_NCA (*numb*)

The number of connected atoms excluding terminal hydrogen atoms.

Appears in list containing `_chemical_conn_atom_type_symbol`. The permitted range is 0→∞. [`chemical_conn_atom`]

### `_chemical_conn_atom_NH` (*numb*)

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

Appears in list containing `_chemical_conn_atom_type_symbol`. The permitted range is 0→∞. [`chemical_conn_atom`]

### `_chemical_conn_atom_number` (*numb*)

The chemical sequence number to be associated with this atom.

Appears in list containing `_chemical_conn_atom_type_symbol`. May match 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`]

### `_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 recognisable element symbol.

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

## `_chemical_conn_bond_[]`

Data items in the `_chemical_conn_atom_` and `_chemical_conn_bond_` 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 `_chemical_conn_bond_` data items specify the connections between the atoms in the `_chemical_conn_atom_` list and the nature of the chemical bond between these atoms.

*Example 1 - based on data set DPTD of Yamin, Suwandi, Fun, Sivakumar & bin Shawkataly [(1996). Acta Cryst. C52, 951–953].*

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

### `_chemical_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.

Appears in list. **Must** match data name `_chemical_conn_atom_number`. The permitted range is 1→∞. [`chemical_conn_bond`]

### `_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 |

Appears in list containing `_chemical_conn_bond_atom_`. Where no value is given, the assumed value is `'sing'`. [`chemical_conn_bond`]

## `_chemical_formula_[]`

`_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 cluster of (element symbol + 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 depends on whether or not carbon is present. If carbon is present, the order should be: C, then H, then the other elements in alphabetical order of their symbol. If carbon is not present, the elements are listed purely in alphabetic 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`.

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

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

*Example 2 - based on data set 9597gaus of Alyea, Ferguson & Kannan [(1996). Acta Cryst. C52, 765–767].*

```
_chemical_formula_iupac      '[Mo (C O)4 (C18 H33 P)2]'
_chemical_formula_moiety     'C40 H66 Mo O4 P2'
_chemical_formula_structural '((C O)4 (P (C6 H11)3)2)Mo'
_chemical_formula_sum         'C40 H66 Mo O4 P2'
_chemical_formula_weight      768.81
```

### `_chemical_formula_analytical` (*char*)

Formula determined by standard chemical analysis including trace elements. See `_chemical_formula_[]` for rules for writing chemical formulae. Parentheses are used only for standard uncertainties (e.s.d.'s).

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

### `_chemical_formula_iupac` (*char*)

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

Ref: IUPAC (1990). *Nomenclature of Inorganic Chemistry.* Oxford: Blackwell Scientific Publications.

Example(s): `'[Co Re (C12 H22 P)2 (C O)6].0.5C H3 O H'` `[chemical_formula]`

### `_chemical_formula_moiety` (*char*)

Formula with each discrete bonded residue or ion shown as a separate moiety. See above `_chemical_formula_[]` 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_[]`.
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]`

### `_chemical_formula_structural` (*char*)

See `_chemical_formula_[]` 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 lists 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]`

### `_chemical_formula_sum` (*char*)

See `_chemical_formula_[]` 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_[]`. Parentheses are not normally used.

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

### `_chemical_formula_weight` (*numb*)

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

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

### `_chemical_formula_weight_meas` (*numb*)

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

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

## `_citation_[]`

Data items in the CITATION category record details about the literature cited relevant to the contents of the data block.

---

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

```
loop_
_citation_id
_citation_coordinate_linkage
_citation_title
_citation_country
_citation_page_first
_citation_page_last
_citation_year
_citation_journal_abbrev
_citation_journal_volume
_citation_journal_issue
_citation_journal_id_ASTM
_citation_journal_id_ISSN
_citation_book_title
_citation_book_publisher
_citation_book_id_ISBN
_citation_special_details
primary  yes
;  Crystallographic analysis of a complex between human
  immunodeficiency virus type 1 protease and
  acetyl-pepstatin at 2.0-Angstroms resolution.
;
US  14209  14219  1990  'J. Biol. Chem.'  265  .
HBCHA3  0021-9258  .  .  .
;  The publication that directly relates to this coordinate
  set.
;
2  no
;  Three-dimensional structure of aspartyl-protease from
  human immunodeficiency virus HIV-1.
;
UK  615  619  1989  'Nature'  337  .
NATUAS  0028-0836  .  .  .
;  Determination of the structure of the unliganded enzyme.
;
3 no
;  Crystallization of the aspartylprotease from human
  immunodeficiency virus, HIV-1.
;
US  1919  1921  1989  'J. Biol. Chem.'  264  .
HBCHA3  0021-9258  .  .  .
;  Crystallization of the unliganded enzyme.
;
```

`_citation_abstract` (*char*)

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

Appears in list containing `_citation_id`. `[citation]`

`_citation_abstract_id_CAS` (*char*)

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

Appears in list containing `_citation_id`. `[citation]`

`_citation_book_id_ISBN` (*char*)

The International Standard Book Number (ISBN) code assigned to the book cited; relevant for book chapters.

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`.

Example(s): `'John Wiley'` `[citation]`

`_citation_book_publisher_city` (*char*)

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

Appears in list containing `_citation_id`.

Example(s): `'New York'` `[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_CSD` (*char*)

Identifier ('refcode') of the database record in the Cambridge Structural Database containing details of the cited structure.

Appears in list containing `_citation_id`.

Example(s): `'LEKKUH'` `[citation]`

`_citation_database_id_Medline` (*numb*)

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

Appears in list containing `_citation_id`. The permitted range is $1 \rightarrow \infty$.

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`.

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`.

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]`

`_citation_journal_full` (*char*)

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

Appears in list containing `_citation_id`.

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`.

Example(s): `'2'` `[citation]`

`_citation_journal_volume` (*char*)

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

Appears in list containing `_citation_id`.

Example(s): `'174'` `[citation]`

`_citation_language` (*char*)

Language in which the citation appears.

Appears in list containing `_citation_id`.

Example(s): `'german'` `[citation]`

`_citation_page_first`
`_citation_page_last` (*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 relates to further refinement of structure
  reported in citation 2
;                                            [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 Duck Ovotransferrin at
  2.35 \%A Resolution.
;                                            [citation]
```

`_citation_year` (*numb*)

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

Appears in list containing `_citation_id`.

Example(s): `'1984'` `[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
primary  'Fitzgerald, P. M. D.'
primary  'McKeever, B. M.'
primary  'Van Middlesworth, J. F.'
primary  'Springer, J. P.'
primary  'Heimbach, J. C.'
primary  'Leu, C.-T.'
primary  'Herber, W. K.'
primary  'Dixon, R. A. F.'
primary  'Darke, P. L.'
2      'Navia, M. A.'      2      'Fitzgerald, P. M. D.'
2      'McKeever, B. M.'   2      'Leu, C.-T.'
2      'Heimbach, J. C.'   2      'Herber, W. K.'
2      'Sigal, I. S.'      2      'Darke, P. L.'
2      'Springer, J. P.'   3      'McKeever, B. M.'
3      'Navia, M. A.'      3      'Fitzgerald, P. M. D.'
3      'Springer, J. P.'   3      'Leu, C.-T.'
3      'Heimbach, J. C.'   3      'Herber, W. K.'
3      '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.

Example(s): `'Bleary, Percival R.'`, `'O'Neil, F. K.'`, `'Van den Bossche, G.'`, `'Yang, D.-L.'`, `'Simonov, Yu.A'`, `'M\"uller, H. A.'`, `'Ross II, C. R.'` `[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]`

### `_citation_editor_[]`

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

*Example 1 - hypothetical example.*

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

`_citation_editor_citation_id` (*char*)

The value of `_citation_editor_citation_id` must match an identifier specified by `_citation_id` in the `_citation_` list.

Appears in list as essential element of loop structure. **Must** match 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.

Example(s): `'Bleary, Percival R.'`, `'O'Neil, F. K.'`, `'Van den Bossche, G.'`, `'Yang, D.-L.'`, `'Simonov, Yu.A'`, `'M\"uller, H. A.'`, `'Ross II, C. R.'` `[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]`

### `_computing_[]`

Data items in the COMPUTING category record details about the computer programs used in the crystal structure analysis.

---

*Example 1 - Rodríguez-Romero, Ruiz-Pérez & Solans [(1996). Acta Cryst. C52, 1415–1417].*

```
_computing_data_collection     'CAD-4 (Enraf-Nonius, 1989)'
_computing_cell_refinement     'CAD-4 (Enraf-Nonius, 1989)'
_computing_data_reduction             'CFEO (Solans, 1978)'
_computing_structure_solution  'SHELXS86 (Sheldrick, 1990)'
_computing_structure_refinement
                               'SHELXL93 (Sheldrick, 1993)'
_computing_molecular_graphics     'ORTEPII (Johnson, 1976)'
_computing_publication_material    'PARST (Nardelli, 1983)'
```

`_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): `'CAD-4 (Enraf-Nonius, 1989)'`, `'DIFDAT, SORTRF, ADDREF (Hall & Stewart, 1990)'`, `'FRODO (Jones, 1986), ORTEP (Johnson, 1965)'`, `'CRYSTALS (Watkin, 1988)'`, `'SHELX85 (Sheldrick, 1985)'`
`[computing]`

### `_database_[]`

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

---

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

```
_database_code_CSD                  'VOBYUG'
```

`_database_code_CAS`
`_database_code_CSD`
`_database_code_ICSD`
`_database_code_MDF`
`_database_code_NBS`
`_database_code_PDB`
`_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); Protein Data Bank; and the Powder Diffraction File (JCPDS/ICDD).
`[database]`

`_database_code_depnum_ccdc_fiz` (*char*)

Deposition numbers assigned by the Fachinformatsionszentrum Karlsruhe (FIZ) to files containing structural information archived by the Cambridge Crystallographic Data Centre (CCDC).
`[database]`

`_database_code_depnum_ccdc_journal` (*char*)

Deposition numbers assigned by various journals to files containing structural information archived by the Cambridge Crystallographic Data Centre (CCDC).
`[database]`

`_database_code_depnum_ccdc_archive` (*char*)

Deposition numbers assigned by the Cambridge Crystallographic Data Centre (CCDC) to files containing structural information archived by the CCDC.
`[database]`

`_database_CSD_history` (*char*)

A history of changes made by the Cambridge Crystallographic Data Centre and incorporated into the Cambridge Structural Database (CSD).
`[database]`

`_database_journal_ASTM`
`_database_journal_CSD` (*char*)

The ASTM CODEN designator for a journal as given in the Chemical Source List maintained by the *Chemical Abstracts* Service, and the journal code used in the Cambridge Structural Database.
`[database]`

### `_diffrn_[]`

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

---

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

```
_diffrn_special_details
; \q scan width (1.0 + 0.14tan\q)\%, \q scan rate 1.2 \%
 min^-1^. Background counts for 5 s on each side every
  scan.
;
_diffrn_ambient_temperature        293
```

`_diffrn_ambient_environment` (*char*)

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

Example(s): `'He'`, `'vacuum'`, `'mother liquor'` `[diffrn]`

`_diffrn_ambient_pressure` (*numb*)

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

The permitted range is 0.0→∞. `[diffrn]`

`_diffrn_ambient_pressure_gt`
`_diffrn_ambient_pressure_lt` (*numb*)

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

The permitted range is 0.0→∞. Related item(s): `_diffrn_ambient_pressure` (alternate). `[diffrn]`

`_diffrn_ambient_temperature` (*numb*)

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

The permitted range is 0.0→∞. `[diffrn]`

`_diffrn_ambient_temperature_gt`
`_diffrn_ambient_temperature_lt` (*numb*)

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

The permitted range is 0.0→∞. Related item(s): `_diffrn_ambient_temperature` (alternate). `[diffrn]`

`_diffrn_crystal_treatment` (*char*)

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'` `[diffrn]`

`_diffrn_measured_fraction_theta_full` (*numb*)

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

Appears in list. The permitted range is 0→1.0. `[diffrn]`

`_diffrn_measured_fraction_theta_max` (*numb*)

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

Appears in list. The permitted range is 0→1.0. `[diffrn]`

`_diffrn_special_details` (*char*)

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.
;
```

`[diffrn]`

`_diffrn_symmetry_description` (*char*)

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

`[diffrn]`

`_diffrn_attenuator_[]`

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

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

```
loop_
_diffrn_attenuator_code
_diffrn_attenuator_scale       1     16.976
```

`_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 intensities. See `_diffrn_attenuator_scale`.

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

`_diffrn_attenuator_material` (*char*)

Material from which the attenuator is made.

Appears in list containing `_diffrn_attenuator_code`. `[diffrn_attenuator]`

`_diffrn_attenuator_scale` (*numb*)

The scale factor applied when an intensity measurement is reduced by an attenuator identified by `_diffrn_attenuator_code`. This scale must be multiplied by the measured intensity to convert it to the same scale as unattenuated intensities.

Appears in list containing `_diffrn_attenuator_code`. The permitted range is 1.0→∞. `[diffrn_attenuator]`

`_diffrn_detector_[]`

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

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

```
_diffrn_detector                   'multiwire'
_diffrn_detector_type              'Siemens'
```

`_diffrn_detector` (*char*)

The general class of the radiation detector.

Example(s): `'photographic film'`, `'scintillation counter'`, `'CCD plate'`, `'BF~3~ counter'`

Related item(s): `_diffrn_radiation_detector` (alternate). `[diffrn_detector]`

`_diffrn_detector_area_resol_mean` (*numb*)

The resolution of an area detector, in pixels/mm.

The permitted range is 0.0→∞. `[diffrn_detector]`

`_diffrn_detector_details` (*char*)

A description of special aspects of the radiation detector.

`[diffrn_detector]`

`_diffrn_detector_dtime` (*numb*)

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

Related item(s): `_diffrn_radiation_detector_dtime` (alternate). The permitted range is 0.0→∞. `[diffrn_detector]`

`_diffrn_detector_type` (*char*)

The make, model or name of the detector device used.

`[diffrn_detector]`

`_diffrn_radiation_detector` (*char*)

**This definition has been superseded and is retained here only for archival purposes. Use instead `_diffrn_detector`**
*The detector used to measure the diffraction intensities.*

`[diffrn_detector]`

### _diffrn_radiation_detector_dtime (*numb*)

**This definition has been superseded and is retained here only for archival purposes. Use instead `_diffrn_detector_dtime`**
*The deadtime in microseconds of the detector used to measure the diffraction intensities.*

`[diffrn_detector]`

## _diffrn_measurement_[]

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

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

```
_diffrn_measurement_device_type
                        'Philips PW1100/20 diffractometer'
_diffrn_measurement_method          \q/2\q
```

### _diffrn_measurement_details (*char*)

A description of special aspects of the intensity measurement.

Example(s): `'440 frames of 0.25\%'` `[diffrn_measurement]`

### _diffrn_measurement_device (*char*)

The general class of goniometer or device used to support and orient the specimen.

Example(s): `'three-circle diffractometer'`, `'four-circle diffractometer'`, `'\k-geometry diffractometer'`, `'oscillation camera'`, `'precession camera'` `[diffrn_measurement]`

### _diffrn_measurement_device_details (*char*)

A description of special aspects of the device used to measure the diffraction intensities.

Example(s):

```
; commercial goniometer modified locally to
  allow for 90\% \t arc
;
```

`[diffrn_measurement]`

### _diffrn_measurement_device_type (*char*)

The make, model or name of the measurement device (goniometer) used.

`[diffrn_measurement]`

### _diffrn_measurement_method (*char*)

Method used to measure intensities.

Example(s): `'profile data from \q/2\q scans'` `[diffrn_measurement]`

### _diffrn_measurement_specimen_support (*char*)

The physical device used to support the crystal during data collection.

Example(s): `'glass capillary'`, `'quartz capillary'`, `'fiber'`, `'metal loop'` `[diffrn_measurement]`

## _diffrn_orient_matrix_[]

Data items in the DIFFRN_ORIENT_MATRIX category record details about the orientation matrix used in data measurement.

*Example 1 - data set n-alkylation_C-4 of Hussain, Fleming, Norman & Chang [(1996). Acta Cryst. C52, 1010–1012].*

```
_diffrn_orient_matrix_UB_11          -0.04170
_diffrn_orient_matrix_UB_12          -0.01429
_diffrn_orient_matrix_UB_13          -0.02226
_diffrn_orient_matrix_UB_21          -0.00380
_diffrn_orient_matrix_UB_22          -0.05578
_diffrn_orient_matrix_UB_23          -0.05048
_diffrn_orient_matrix_UB_31           0.00587
_diffrn_orient_matrix_UB_32          -0.13766
_diffrn_orient_matrix_UB_33           0.02277
_diffrn_orient_matrix_type  'TEXSAN convention (MSC, 1989)'
```

### _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]`

### _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_matrix]`

## _diffrn_orient_refln_[]

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

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

```
loop_
_diffrn_orient_refln_index_h
_diffrn_orient_refln_index_k
_diffrn_orient_refln_index_l
_diffrn_orient_refln_angle_theta
_diffrn_orient_refln_angle_phi
_diffrn_orient_refln_angle_omega
_diffrn_orient_refln_angle_kappa
-3   2   3    7.35   44.74   2.62    17.53
-4   1   0    9.26   83.27   8.06     5.79
 0   0   6    5.85  -43.93 -25.36    86.20
 2   1   3    7.36  -57.87   6.26     5.42
 0   0  -6    5.85 -161.59  36.96   -86.79
-3   1   0    6.74   80.28   5.87     2.60
 2   0   3    5.86  -76.86  -0.17    21.34
 0   0  12   11.78  -44.02 -19.51    86.41
 0   0 -12   11.78 -161.67  42.81   -86.61
-5   1   0   11.75   86.24   9.16     7.44
 0   4   6   11.82  -19.82  10.45     4.19
 5   0   6   14.13  -77.28  10.17    15.34
 8   0   0   20.79  -77.08  25.30   -13.96
```

### `_diffrn_orient_refln_angle_chi`
### `_diffrn_orient_refln_angle_kappa`
### `_diffrn_orient_refln_angle_omega`
### `_diffrn_orient_refln_angle_phi`
### `_diffrn_orient_refln_angle_psi`
### `_diffrn_orient_refln_angle_theta` (*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`.

Appears in list containing `_diffrn_orient_refln_index_`. `[diffrn_orient_refln]`

### `_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_`.

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

### `_diffrn_radiation_[]`

Data items in the DIFFRN_RADIATION category describe the radiation used in measuring diffraction intensities, its collimation and monochromatisation before the sample. Post-sample treatment of the beam is described by data items in the DIFFRN_DETECTOR category.

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

```
_diffrn_radiation_type           'Cu K\a'
_diffrn_radiation_monochromator  'graphite'
```

### `_diffrn_radiation_collimation` (*char*)

The collimation or focusing applied to the radiation.

Example(s): `'0.3 mm double-pinhole'`, `'0.5 mm'`, `'focusing mirrors'` `[diffrn_radiation]`

### `_diffrn_radiation_filter_edge` (*numb*)

Absorption edge in ångströms of the radiation filter used.

The permitted range is 0.0→∞. `[diffrn_radiation]`

### `_diffrn_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→∞. `[diffrn_radiation]`

### `_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.

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

### `_diffrn_radiation_polarisn_norm` (*numb*)

The angle in degrees, as viewed from the specimen, between the perpendicular component of the polarisation and the diffraction plane. See `_diffrn_radiation_polarisn_ratio`.

The permitted range is $-180.0 \rightarrow 180.0$. `[diffrn_radiation]`

### `_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).

The permitted range is 0.0→∞. `[diffrn_radiation]`

### `_diffrn_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`

`[diffrn_radiation]`

### `_diffrn_radiation_type` (*char*)

The type of the radiation. This represents a finer-grained level of description than `_diffrn_radiation_probe` and is typically a description of the X-ray wavelength in Siegbahn notation.

Example(s): `'Cu K\a'`, `'Cu K\a~1~'`, `'Cu K-L~2,3~'`, `'white-beam'` `[diffrn_radiation]`

### `_diffrn_radiation_xray_symbol` (*char*)

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

| | |
|---|---|
| `K-L~3~` | K$\alpha_1$ in older Siegbahn notation |
| `K-L~2~` | K$\alpha_2$ in older Siegbahn notation |
| `K-M~3~` | K$\beta_1$ in older Siegbahn notation |
| `K-L~2,3~` | use where K-L$_3$ and K-L$_2$ are not resolved |

`[diffrn_radiation]`

### `_diffrn_radiation_wavelength_[]`

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

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

```
_diffrn_radiation_wavelength      1.5418
```

### `_diffrn_radiation_wavelength` (*numb*)

The radiation wavelength in ångströms.

May appear in list containing `_diffrn_radiation_wavelength_id`. The permitted range is 0.0→∞. `[diffrn_radiation_wavelength]`

### `_diffrn_radiation_wavelength_id` (*char*)

An arbitrary code identifying each value of `_diffrn_radiation_wavelength`. Items in the DIFFRN_RADIATION category are looped when multiple wavelengths are used. This code is used to link with the `_diffrn_refln_` list. It must match with one of the `_diffrn_refln_wavelength_id` codes.

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

Example(s): `‘x1’`, `‘x2’`, `‘neut’`

[`diffrn_radiation_wavelength`]

### `_diffrn_radiation_wavelength_wt` (*numb*)

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

Appears in list containing `_diffrn_radiation_wavelength_id`. Where no value is given, the assumed value is `‘1.0’`. The permitted range is 0.0→1.0. [`diffrn_radiation_wavelength`]

## `_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 $Tl_2Cd_2(SO_4)_3$ at 85 K (unpublished).*

```
loop_
_diffrn_refln_index_h
_diffrn_refln_index_k
_diffrn_refln_index_l
_diffrn_refln_angle_chi
_diffrn_refln_scan_rate
_diffrn_refln_counts_bg_1
_diffrn_refln_counts_total
_diffrn_refln_counts_bg_2
_diffrn_refln_angle_theta
_diffrn_refln_angle_phi
_diffrn_refln_angle_omega
_diffrn_refln_angle_kappa
_diffrn_refln_scan_width
_diffrn_refln_elapsed_time
0  0 -16  0. 4.12  28 127  36  33.157  -75.846  16.404
50.170  1.516 19.43
0  0 -15  0. 4.12  38 143  28  30.847  -75.846  14.094
50.170  1.516 19.82
0  0 -14  0. 1.03 142 742 130  28.592  -75.846  11.839
50.170  1.516 21.32
0  0 -13  0. 4.12  26 120  37  26.384  -75.846   9.631
50.170  1.450 21.68
0  0 -12  0. 0.97 129 618 153  24.218  -75.846   7.464
50.170  1.450 23.20
0  0 -11  0. 4.12  33 107  38  22.087  -75.846   5.334
50.170  1.384 23.55
0  0 -10  0. 4.12  37 146  33  19.989  -75.846   3.235
50.170  1.384 23.90
0  0  -9  0. 4.12  50 179  49  17.918  -75.846   1.164
50.170  1.384 24.25
# - - - - data truncated for brevity - - - -
3  4  -4  0. 1.03  69 459  73  30.726  -53.744  46.543
-47.552  1.516 2082.58
3  4  -5  0. 1.03  91 465  75  31.407  -54.811  45.519
-42.705  1.516 2084.07
3 14  -6  0. 1.03  84 560  79  32.228  -55.841  44.745
-38.092  1.516 2085.57
# - - - - data truncated for brevity - - - -
```

### `_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.

Appears in list containing `_diffrn_refln_index_`.

[`diffrn_refln`]

### `_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.

Appears in list containing `_diffrn_refln_index_`. **Must** match data name `_diffrn_attenuator_code`. [`diffrn_refln`]

### `_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 $m = \sum |m_i|$, 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 cell.

Appears in list containing `_diffrn_refln_index_`. **Must** match data name `_diffrn_reflns_class_code`. [`diffrn_refln`]

### `_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).

Appears in list containing `_diffrn_refln_index_`.

[`diffrn_refln`]

### `_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.

Appears in list containing `_diffrn_refln_index_`. **Must** match data name `_exptl_crystal_id`. [`diffrn_refln`]

### `_diffrn_refln_detect_slit_horiz`
### `_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`]

### `_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 $0.0 \rightarrow \infty$. `[diffrn_refln]`

### `_diffrn_refln_index_h`
### `_diffrn_refln_index_k`
### `_diffrn_refln_index_l` (*numb*)

Miller indices of a measured 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_`.

Appears in list as essential element of loop structure. `[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 $0 \rightarrow \infty$. `[diffrn_refln]`

### `_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 (e.s.d.) of the net intensity calculated from the diffraction counts after the attenuator and standard scales have been applied.*

`[diffrn_refln]`

### `_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 $0 \rightarrow \infty$. `[diffrn_refln]`

### `_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]`

### `_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 |
| `q` | $Q$-scans (arbitrary reciprocal directions) |

Appears in list containing `_diffrn_refln_index_`.
`[diffrn_refln]`

### `_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 |

Appears in list containing `_diffrn_refln_index_`.
`[diffrn_refln]`

### `_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 $0 \rightarrow \infty$. `[diffrn_refln]`

### `_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 $0 \rightarrow \infty$. `[diffrn_refln]`

### `_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 $0.0 \rightarrow 90.0$. `[diffrn_refln]`

### `_diffrn_refln_sint/lambda` (*numb*)

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

Appears in list containing `_diffrn_refln_index_`. The permitted range is $0.0 \rightarrow \infty$. `[diffrn_refln]`

### `_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`.

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

### `_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 $0.0 \rightarrow \infty$. `[diffrn_refln]`

### `_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]`

### `_diffrn_reflns_[]`

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

---

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

```
_diffrn_reflns_number             1592
_diffrn_reflns_av_R_equivalents   0
_diffrn_reflns_av_unetI/netI      .027
_diffrn_reflns_limit_h_min        0
_diffrn_reflns_limit_h_max        6
_diffrn_reflns_limit_k_min       -17
_diffrn_reflns_limit_k_max        0
_diffrn_reflns_limit_l_min        0
_diffrn_reflns_limit_l_max        22
_diffrn_reflns_theta_min          3.71
_diffrn_reflns_theta_max          61.97
```

### `_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 absolute difference between $av(I)$ and the individual symmetry-equivalent intensities.

The permitted range is 0.0→∞. `[diffrn_reflns]`

### `_diffrn_reflns_av_sigmaI/netI` (*numb*)

**This definition has been superseded and is retained here only for archival purposes. Use instead `_diffrn_reflns_av_unetI/netI`**
*Measure* $[\sum|u(netI)|/\sum|netI|]$ *for all measured reflections.*

`[diffrn_reflns]`

### `_diffrn_reflns_av_unetI/netI` (*numb*)

Measure $[\sum|u(netI)|/\sum|netI|]$ for all measured reflections.

Related item(s): `_diffrn_reflns_av_sigmaI/netI` (alternate). The permitted range is 0.0→∞. `[diffrn_reflns]`

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

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

`[diffrn_reflns]`

### `_diffrn_reflns_number` (*numb*)

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

The permitted range is 0→∞. `[diffrn_reflns]`

### `_diffrn_reflns_reduction_process` (*char*)

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

Example(s):
`'data averaged using Fisher test'` `[diffrn_reflns]`

### `_diffrn_reflns_resolution_full` (*numb*)

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

The permitted range is 0.0→∞. Related item(s): `_diffrn_reflns_theta_full` (alternate). `[diffrn_reflns]`

### `_diffrn_reflns_resolution_max` (*numb*)

Maximum resolution in reciprocal ångströms of the measured diffraction pattern.

The permitted range is 0.0→∞. Related item(s): `_diffrn_reflns_theta_max` (alternate). `[diffrn_reflns]`

### `_diffrn_reflns_theta_full` (*numb*)

The $\theta$ angle (in degrees) at which the measured reflection count is close to complete. The fraction of unique reflections measured out to this angle is given by `_diffrn_measured_fraction_theta_full`.

The permitted range is 0.0→90.0. `[diffrn_reflns]`

### `_diffrn_reflns_theta_max` (*numb*)

Maximum $\theta$ angle in degrees for the measured intensities.

The permitted range is 0.0→90.0. `[diffrn_reflns]`

### `_diffrn_reflns_theta_min` (*numb*)

Minimum $\theta$ angle in degrees for the measured intensities.

The permitted range is 0.0→90.0. `[diffrn_reflns]`

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

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

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

`[diffrn_reflns]`

### `_diffrn_reflns_class_[]`

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

*Example 1 - example corresponding to the one-dimensional incommensurately modulated structure of* $K_2SeO_4$*. 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_
_diffrn_reflns_class_number
_diffrn_reflns_class_d_res_high
_diffrn_reflns_class_d_res_low
_diffrn_reflns_class_av_R_eq
_diffrn_reflns_class_code
_diffrn_reflns_class_description
1580 0.551 6.136 0.015 'Main' 'm=0;  main reflections'
1045 0.551 6.136 0.010 'Sat1' 'm=1;  first-order satellites'
```

### `_diffrn_reflns_class_av_R_eq` (*numb*)

For each reflection class, 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 absolute difference between $av(I)$ and the individual symmetry-equivalent intensities.

Appears in list containing `_diffrn_reflns_class_code`. The permitted range is 0.0→∞. `[diffrn_reflns_class]`

### `_diffrn_reflns_class_av_sgI/I` (*numb*)

**This definition has been superseded and is retained here only for archival purposes. Use instead** `_diffrn_reflns_class_av_uI/I`
*Measure* $[\sum|u(netI)|/\sum|netI|]$ *for all measured intensities in a reflection class.*

`[diffrn_reflns_class]`

### `_diffrn_reflns_class_av_uI/I` (*numb*)

Measure $[\sum|u(netI)|/\sum|netI|]$ for all measured intensities in a reflection class.

Related item(s): `_diffrn_reflns_class_av_sgI/I` (alternate). Appears in list containing `_diffrn_reflns_class_code`. The permitted range is 0.0→∞. `[diffrn_reflns_class]`

### `_diffrn_reflns_class_code` (*char*)

The code identifying a certain reflection class.

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

Example(s): `'1'`, `'m1'`, `'s2'` `[diffrn_reflns_class]`

### `_diffrn_reflns_class_description` (*char*)

Description of each reflection class.

Appears in list containing `_diffrn_reflns_class_code`.

Example(s): `'m=1 first order satellites'`,
`'H0L0 common projection reflections'`
`[diffrn_reflns_class]`

### `_diffrn_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 `_diffrn_reflns_class_code`. The permitted range is 0.0→∞. `[diffrn_reflns_class]`

### `_diffrn_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 `_diffrn_reflns_class_code`. The permitted range is 0.0→∞. `[diffrn_reflns_class]`

### `_diffrn_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 `_diffrn_reflns_class_code`. The permitted range is 0→∞. `[diffrn_reflns_class]`

### `_diffrn_scale_group_[]`

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

*Example 1 - hypothetical example.*

```
loop_
_diffrn_scale_group_code
_diffrn_scale_group_I_net
1    .86473
2   1.0654
```

### `_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.

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

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

### `_diffrn_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 `_diffrn_refln_` or `_refln_` list on a common scale.

Appears in list containing `_diffrn_scale_group_code`. The permitted range is 0.0→∞. `[diffrn_scale_group]`

### `_diffrn_source_[]`

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

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

```
_diffrn_source                 'rotating anode X-ray tube'
_diffrn_source_type            'Rigaku RU-200'
_diffrn_source_power           50
_diffrn_source_current         180
_diffrn_source_size            '8 mm x 0.4 mm broad focus'
```

### `_diffrn_radiation_source` (*char*)

**This definition has been superseded and is retained here only for archival purposes. Use instead** `_diffrn_source`
*The source of radiation.*

`[diffrn_source]`

### `_diffrn_source` (*char*)

The general class of the source of radiation.

Related item(s): `_diffrn_radiation_source` (alternate).

Example(s): `'sealed X-ray tube'`, `'nuclear reactor'`, `'spallation source'`, `'electron microscope'`, `'rotating-anode X-ray tube'`, `'synchrotron'`

`[diffrn_source]`

### `_diffrn_source_current` (*char*)

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

The permitted range is 0.0→∞. `[diffrn_source]`

### `_diffrn_source_details` (*char*)

A description of special aspects of the source used.

`[diffrn_source]`

### `_diffrn_source_power` (*numb*)

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

The permitted range is 0.0→∞. `[diffrn_source]`

### `_diffrn_source_size` (*char*)

The dimensions of the source as viewed from the sample.

Example(s): `'8mm x 0.4 mm fine-focus'`, `'broad focus'`

`[diffrn_source]`

### `_diffrn_source_take-off_angle` (*numb*)

The complement of the angle in degrees between the normal to the surface of the X-ray tube target and the primary X-ray beam for beams generated by traditional X-ray tubes.

The permitted range is 0→90.

Example(s): `'1.53'` `[diffrn_source]`

### `_diffrn_source_target` (*char*)

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.

```
H    He   Li   Be   B    C    N    O    F    Ne   Na
Mg   Al   Si   P    S    Cl   Ar   K    Ca   Sc   Ti
V    Cr   Mn   Fe   Co   Ni   Cu   Zn   Ga   Ge   As
Se   Br   Kr   Rb   Sr   Y    Zr   Nb   Mo   Tc   Ru
Rh   Pd   Ag   Cd   In   Sn   Sb   Te   I    Xe   Cs
Ba   La   Ce   Pr   Nd   Pm   Sm   Eu   Gd   Tb   Dy
Ho   Er   Tm   Yb   Lu   Hf   Ta   W    Re   Os   Ir
Pt   Au   Hg   Tl   Pb   Bi   Po   At   Rn   Fr   Ra
Ac   Th   Pa   U    Np   Pu   Am   Cm   Bk   Cf   Es
Fm   Md   No   Lr
```

`[diffrn_source]`

### `_diffrn_source_type` (*char*)

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

Example(s): `'NSLS beamline X8C'`, `'Rigaku RU200'`

`[diffrn_source]`

### `_diffrn_source_voltage` (*numb*)

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

The permitted range is 0.0→∞. `[diffrn_source]`

## `_diffrn_standard_refln_[]`

Data items in the DIFFRN_STANDARD_REFLN category record details about the reflections treated as standards during the measurement of diffraction intensities. Note that these are the individual standard reflections, not the results of the analysis of the standard reflections.

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

```
loop_
_diffrn_standard_refln_index_h
_diffrn_standard_refln_index_k
_diffrn_standard_refln_index_l
3 2 4    1 9 1    3 0 10
```

### `_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.

Appears in list containing `_diffrn_standard_refln_index_`. May match subsidiary data name(s): `_diffrn_refln_standard_code`.

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

`[diffrn_standard_refln]`

### `_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.

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

## `_diffrn_standards_[]`

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

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

```
_diffrn_standards_number           3
_diffrn_standards_interval_time    120
_diffrn_standards_decay_%          0
```

### `_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.

The permitted range is $-\infty \rightarrow 100$. `[diffrn_standards]`

### `_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 $0 \rightarrow \infty$. `[diffrn_standards]`

### `_diffrn_standards_number` (*numb*)

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

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

### `_diffrn_standards_scale_sigma` (*numb*)

**This definition has been superseded and is retained here only for archival purposes. Use instead `_diffrn_standards_scale_u`**
*The standard uncertainty (e.s.d.) of the individual mean standard scales applied to the intensity data.*

`[diffrn_standards]`

### `_diffrn_standards_scale_u` (*numb*)

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

Related item(s): `_diffrn_standards_scale_sigma` (alternate).
The permitted range is $0.0 \rightarrow \infty$. `[diffrn_standards]`

### `_exptl_[]`

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

*Example 1 - based on a paper by Steiner [(1996). Acta Cryst. C52, 2554–2556].*

```
_exptl_absorpt_coefficient_mu     0.962
_exptl_absorpt_correction_type    psi-scan
_exptl_absorpt_process_details
                'North, Phillips & Mathews (1968)'
_exptl_absorpt_correction_T_min   0.929
_exptl_absorpt_correction_T_max   0.997
```

### `_exptl_absorpt_coefficient_mu` (*numb*)

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

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

### `_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 $0.0 \rightarrow 1.0$. `[exptl]`

### `_exptl_absorpt_correction_type` (*char*)

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

| | |
|---|---|
| `analytical` | analytical from crystal shape |
| `cylinder` | cylindrical |
| `empirical` | empirical from intensities |
| `gaussian` | Gaussian from crystal shape |
| `integration` | integration from crystal shape |
| `multi-scan` | symmetry-related measurements |
| `none` | no absorption correction applied |
| `numerical` | numerical from crystal shape |
| `psi-scan` | $\psi$-scan corrections |
| `refdelf` | refined from $\Delta F$ |
| `sphere` | spherical |

`[exptl]`

### `_exptl_absorpt_process_details` (*char*)

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

Example(s): `'Tompa analytical'`, `'MolEN (Fair, 1990)'`, `'(North, Phillips & Mathews, 1968)'` `[exptl]`

### `_exptl_crystals_number` (*numb*)

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

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

### `_exptl_special_details` (*char*)

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

`[exptl]`

### `_exptl_crystal_[]`

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

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

```
_exptl_crystal_description          prism
_exptl_crystal_colour               colourless
_exptl_crystal_size_max             0.32
_exptl_crystal_size_mid             0.27
_exptl_crystal_size_min             0.10
_exptl_crystal_density_diffrn       1.146
_exptl_crystal_density_meas         ?
_exptl_crystal_density_method       'not measured'
_exptl_crystal_F_000                656
```

### `_exptl_crystal_colour` (*char*)

The colour of the crystal.

May appear in list containing `_exptl_crystal_id`.

Example(s): `'dark green'`

Related item(s): `_exptl_crystal_colour_lustre` (alternate), `_exptl_crystal_colour_modifier` (alternate), `_exptl_crystal_colour_primary` (alternate). `[exptl_crystal]`

### `_exptl_crystal_colour_lustre` (*char*)

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

```
metallic
dull
clear
```

May appear in list containing `_exptl_crystal_id`. Related item(s): `_exptl_crystal_colour` (alternate). `[exptl_crystal]`

### `_exptl_crystal_colour_modifier` (*char*)

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

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

May appear in list containing `_exptl_crystal_id`. Related item(s): `_exptl_crystal_colour` (alternate). `[exptl_crystal]`

### `_exptl_crystal_colour_primary` (*char*)

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

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

May appear in list containing `_exptl_crystal_id`. Related item(s): `_exptl_crystal_colour` (alternate). `[exptl_crystal]`

### `_exptl_crystal_density_diffrn` (*numb*)

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

May appear in list containing `_exptl_crystal_id`. The permitted range is 0.0→$\infty$. `[exptl_crystal]`

### `_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).

May appear in list containing `_exptl_crystal_id`. The permitted range is 0.0→$\infty$. `[exptl_crystal]`

### `_exptl_crystal_density_meas_gt`
### `_exptl_crystal_density_meas_lt` (*numb*)

The value above which (`*_gt`) or below which (`*_lt`) the density measured using standard chemical and physical methods lies. The units are megagrams per cubic metre (grams per cubic centimetre). These items should not be used to report new experimental work where `_exptl_crystal_density_meas` should be used. They are intended for use in reporting information in existing databases and archives which would be misleading if reported under `_exptl_crystal_density_meas`.

May appear in list containing `_exptl_crystal_id`. The permitted range is 0.0→$\infty$.

Example(s): `'_exptl_crystal_density_meas_lt 1.0'` (specimen floats in water),

```
; _exptl_crystal_density_meas_gt 2.5
  _exptl_crystal_density_meas_lt 5.0
;
```

(Only the range within which the density lies was given in the original paper)

Related item(s): `_exptl_crystal_density_meas` (alternate). `[exptl_crystal]`

### `_exptl_crystal_density_meas_temp` (*numb*)

Temperature in kelvins at which `_exptl_crystal_density_meas` was determined.

May appear in list containing `_exptl_crystal_id`. The permitted range is 0.0→$\infty$. `[exptl_crystal]`

### `_exptl_crystal_density_meas_temp_gt`
### `_exptl_crystal_density_meas_temp_lt` (*numb*)

Temperature in kelvins above which (`*_gt`) or below which (`*_lt`) `_exptl_crystal_density_meas` was determined. These items should not be used for reporting new work where the correct temperature of measurement should be given. They are intended for use in reporting information stored in databases or archives which would be misleading if reported under `_exptl_crystal_density_meas_temp`.

May appear in list containing `_exptl_crystal_id`. The permitted range is 0.0→$\infty$.

Example(s): `'_exptl_crystal_density_meas_temp_lt 300'` (The density was measured at some unspecified temperature below room temperature.)

Related item(s): `_exptl_crystal_density_meas_temp` (alternate). `[exptl_crystal]`

### `_exptl_crystal_density_method` (*char*)

The method used to measure `_exptl_crystal_density_meas`.

May appear in list containing `_exptl_crystal_id`.

Example(s): `'flotation in aqueous KI'`, `'not measured'`, `'Berman density torsion balance'` `[exptl_crystal]`

### `_exptl_crystal_description` (*char*)

A description of the quality and habit of the crystal. The crystal dimensions should not normally be reported here; use instead `_exptl_crystal_size_` for the gross dimensions of the crystal, and `_exptl_crystal_face_` to describe the relationship between individual faces.

May appear in list containing `_exptl_crystal_id`. `[exptl_crystal]`

### `_exptl_crystal_F_000` (*numb*)

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

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

$f_r$ = real part of the scattering factors at $\theta = 0$, $f_i$ = 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→∞. `[exptl_crystal]`

### `_exptl_crystal_id` (*char*)

Code identifying each crystal if multiple crystals are used. It is used to link with `_diffrn_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): `_diffrn_refln_crystal_id`, `_refln_crystal_id`. `[exptl_crystal]`

### `_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]`

### `_exptl_crystal_pressure_history` (*char*)

Relevant details concerning the pressure history of the sample.

May appear in list containing `_exptl_crystal_id`. `[exptl_crystal]`

### `_exptl_crystal_recrystallization_method` (*char*)

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

`[exptl_crystal]`

### `_exptl_crystal_size_length`
### `_exptl_crystal_size_max`
### `_exptl_crystal_size_mid`
### `_exptl_crystal_size_min`
### `_exptl_crystal_size_rad` (*numb*)

The maximum, medial and minimum dimensions in millimetres of the crystal. If the crystal is a sphere then the `*_rad` item is its radius. If the crystal is a cylinder then the `*_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]`

### `_exptl_crystal_thermal_history` (*char*)

Relevant details concerning the thermal history of the sample.

May appear in list containing `_exptl_crystal_id`. `[exptl_crystal]`

## `_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    .18274      1    0   -2    .17571
-1    1   -2    .17845     -2    1    0    .21010
-1    0    2    .18849      1   -1    2    .20605
 2   -1    0    .24680     -1    2    0    .19688
 0    1    2    .15206
```

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

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

Appears in list containing `_exptl_crystal_face_index_`. `[exptl_crystal_face]`

### `_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`.

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

### `_exptl_crystal_face_perp_dist` (*numb*)

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

Appears in list containing `_exptl_crystal_face_index_`. The permitted range is 0.0→∞. `[exptl_crystal_face]`

### `_geom_[]`

Data items in the GEOM and related (GEOM_ANGLE, GEOM_BOND, GEOM_CONTACT, GEOM_HBOND and GEOM_TORSION) categories record details about the molecular and crystal geometry, as calculated from the contents of the ATOM, CELL, and SYMMETRY data. Geometry data are usually redundant, in that they can be calculated from other more fundamental quantities in the data block. They serve, however, the dual purpose of providing a check on the correctness of both sets of data, and of enabling the most important geometric data to be identified for publication by setting the appropriate publication flag.

---

*Example 1 - based on data set bagan of Yamane & DiSalvo [(1996). Acta Cryst. C52, 760–761].*

```
_geom_special_details
; All esds (except the esd in the dihedral angle between
  two l.s. planes) are estimated using the full covariance
  matrix. The cell esds are taken into account individually
  in the estimation of esds in distances, angles and
  torsion angles;  correlations between esds in cell
  parameters are only used when they are defined by crystal
  symmetry. An approximate (isotropic) treatment of cell
  esds is used for estimating esds involving l.s. planes.
;
```

### `_geom_special_details` (*char*)

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

`[geom]`

### `_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.

---

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

```
loop_
_geom_angle_atom_site_label_1
_geom_angle_atom_site_label_2
_geom_angle_atom_site_label_3
_geom_angle
_geom_angle_site_symmetry_1
_geom_angle_site_symmetry_2
_geom_angle_site_symmetry_3
_geom_angle_publ_flag
C2  O1  C5   111.6(2)  1_555  1_555  1_555  yes
O1  C2  C3   110.9(2)  1_555  1_555  1_555  yes
O1  C2  O21  122.2(3)  1_555  1_555  1_555  yes
C3  C2  O21  127.0(3)  1_555  1_555  1_555  yes
C2  C3  N4   101.3(2)  1_555  1_555  1_555  yes
C2  C3  C31  111.3(2)  1_555  1_555  1_555  yes
C2  C3  H3   107(1)    1_555  1_555  1_555  no
N4  C3  C31  116.7(2)  1_555  1_555  1_555  yes
# - - - - data truncated for brevity - - - -
```

### `_geom_angle` (*numb*)

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

Appears in list containing `_geom_angle_atom_site_label_`. `[geom_angle]`

### `_geom_angle_atom_site_label_1`
### `_geom_angle_atom_site_label_2`
### `_geom_angle_atom_site_label_3` (*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.

Appears in list as essential element of loop structure. **Must** match data name `_atom_site_label`. `[geom_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.

| | |
|---|---|
| `no` | do not include angle in special list |
| `n` | abbreviation for “no” |
| `yes` | do include angle in special list |
| `y` | abbreviation for “yes” |

Appears in list containing `_geom_angle_atom_site_label_`. Where no value is given, the assumed value is `'no'`. `[geom_angle]`

### `_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 ‘*klm*’. These numbers are combined to form the code ‘*n klm*’ or *n_klm*. The character string *n_klm* is composed as follows: *n* refers to the symmetry operation that is applied to the coordinates stored in `_atom_site_fract_x`, `_atom_site_fract_y` and `_atom_site_fract_z`. It must match a number given in `_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 angle. These translations $(x, y, z)$ are related to $(k, l, m)$ by the relations $k = 5 + x$, $l = 5 + y$, $m = 5 + z$. By adding 5 to the translations, the use of negative numbers is avoided.

Appears in list containing `_geom_angle_atom_site_label_`.

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_angle]`

### `_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.

---

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

```
loop_
_geom_bond_atom_site_label_1
_geom_bond_atom_site_label_2
_geom_bond_distance
_geom_bond_site_symmetry_1
_geom_bond_site_symmetry_2
_geom_bond_publ_flag
O1  C2   1.342(4)  1_555  1_555  yes
O1  C5   1.439(3)  1_555  1_555  yes
C2  C3   1.512(4)  1_555  1_555  yes
C2  O21  1.199(4)  1_555  1_555  yes
C3  N4   1.465(3)  1_555  1_555  yes
C3  C31  1.537(4)  1_555  1_555  yes
C3  H3   1.00(3)   1_555  1_555  no
N4  C5   1.472(3)  1_555  1_555  yes
# - - - - data truncated for brevity - - - -
```

`_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.

Appears in list as essential element of loop structure. **Must** match data name `_atom_site_label`. `[geom_bond]`

`_geom_bond_distance` (*numb*)

The intramolecular bond distance in ångströms.

Appears in list containing `_geom_bond_atom_site_label_`. The permitted range is 0.0→∞. `[geom_bond]`

`_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.

| | |
|---|---|
| `no` | do not include bond in special list |
| `n` | abbreviation for “no” |
| `yes` | do include bond in special list |
| `y` | abbreviation for “yes” |

Appears in list containing `_geom_bond_atom_site_label_`. Where no value is given, the assumed value is `‘no’`. `[geom_bond]`

`_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 ‘*klm*’. These numbers are combined to form the code ‘*n klm*’ or *n_klm*. The character string *n_klm* is composed as follows: *n* refers to the symmetry operation that is applied to the coordinates stored in `_atom_site_fract_x`, `_atom_site_fract_y` and `_atom_site_fract_z`. It must match a number given in `_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 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_bond_atom_site_label_`.

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]`

`_geom_bond_valence` (*numb*)

The bond valence calculated from `_geom_bond_distance`

Appears in list containing `_geom_bond_atom_site_label_`. `[geom_bond]`

## `_geom_contact_[]`

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

*Example 1 - based on data set CLPHO6 of Ferguson, Ruhl, McKervey & Browne [(1991). Acta Cryst. C48, 2262–2264].*

```
loop_
_geom_contact_atom_site_label_1
_geom_contact_atom_site_label_2
_geom_contact_distance
_geom_contact_site_symmetry_1
_geom_contact_site_symmetry_2
_geom_contact_publ_flag
O(1)  O(2)     2.735(3)  .  .  yes
H(O1) O(2)     1.82      .  .  no
```

`_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.

Appears in list as essential element of loop structure. **Must** match data name `_atom_site_label`. `[geom_contact]`

`_geom_contact_distance` (*numb*)

The interatomic contact distance in ångströms.

Appears in list containing `_geom_contact_atom_site_label_`. The permitted range is 0.0→∞. `[geom_contact]`

`_geom_contact_publ_flag` (*char*)

This code signals if the contact distance is referred to in a publication or should be placed in a list of significant contact distances.

| | |
|---|---|
| `no` | do not include distance in special list |
| `n` | abbreviation for “no” |
| `yes` | do include distance in special list |
| `y` | abbreviation for “yes” |

Appears in list containing `_geom_contact_atom_site_label_`. Where no value is given, the assumed value is `‘no’`. `[geom_contact]`

`_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 ‘*klm*’. These numbers are combined to form the code ‘*n klm*’ or *n_klm*. The character string *n_klm* is composed as follows: *n* refers to the symmetry operation that is applied to the coordinates stored in `_atom_site_fract_x`, `_atom_site_fract_y` and `_atom_site_fract_z`. It must match a number given in `_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 contact. These translations $(x, y, z)$ are related to $(k, l, m)$ by the relations $k = 5 + x$, $l = 5 + y$, $m = 5 + z$. By adding 5 to the translations, the use of negative numbers is avoided.

Appears in list containing `_geom_contact_atom_site_label_`.

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]`

## `_geom_hbond_[]`

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

*Example 1 - based on $C_{14}H_{13}ClN_2O.H_2O$, reported by Palmer, Puddle & Lisgarten [(1993). Acta Cryst. C49, 1777–1779].*

```
loop_
_geom_hbond_atom_site_label_D
_geom_hbond_atom_site_label_H
_geom_hbond_atom_site_label_A
_geom_hbond_distance_DH
_geom_hbond_distance_HA
_geom_hbond_distance_DA
_geom_hbond_angle_DHA
_geom_hbond_publ_flag
N6   HN6  OW   0.888(8)  1.921(12)  2.801(8)  169.6(8)  yes
OW   HO2  O7   0.917(6)  1.923(12)  2.793(8)  153.5(8)  yes
OW   HO1  N10  0.894(8)  1.886(11)  2.842(8)  179.7(9)  yes
```

### `_geom_hbond_angle_DHA` (*numb*)

Angle in degrees defined by the three sites `_geom_hbond_atom_site_label_D`, `*_H` and `*_A`. Site at `*_D` (the hydrogen atom participating in the interaction) is at the apex of the angle.

Appears in list containing `_geom_hbond_atom_site_label_`. [`geom_hbond`]

### `_geom_hbond_atom_site_label_D`
### `_geom_hbond_atom_site_label_H`
### `_geom_hbond_atom_site_label_A` (*char*)

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

Appears in list as essential element of loop structure. **Must** match data name `_atom_site_label`. [`geom_hbond`]

### `_geom_hbond_distance_DH`
### `_geom_hbond_distance_HA`
### `_geom_hbond_distance_DA` (*numb*)

Distances in ångströms between the donor and hydrogen (`*_DH`), hydrogen and acceptor (`*_HA`) and donor and acceptor (`*_DA`) sites in a hydrogen bond.

Appears in list containing `_geom_hbond_atom_site_label_`. The permitted range is 0.0→∞. [`geom_hbond`]

### `_geom_hbond_publ_flag` (*char*)

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

| | |
|---|---|
| `no` | do not include bond in special list |
| `n` | abbreviation for "no" |
| `yes` | do include bond in special list |
| `y` | abbreviation for "yes" |

Appears in list containing `_geom_hbond_atom_site_label_`. Where no value is given, the assumed value is `'no'`. [`geom_hbond`]

### `_geom_hbond_site_symmetry_D`
### `_geom_hbond_site_symmetry_H`
### `_geom_hbond_site_symmetry_A` (*char*)

The symmetry code of each atom site as the symmetry-equivalent position number '*n*' and the cell translation number '*klm*'. These numbers are combined to form the code '*n klm*' or *n_klm*. The character string *n_klm* is composed as follows: *n* refers to the symmetry operation that is applied to the coordinates stored in `_atom_site_fract_x`, `_atom_site_fract_y` and `_atom_site_fract_z`. It must match a number given in `_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): `'.'` (no symmetry or translation to site), `'4'` (4th symmetry operation applied), `'7_645'` (7th symm. posn.; $+a$ on $x$; $-b$ on $y$) [`geom_hbond`]

## `_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 & Browne [(1991). Acta Cryst. C48, 2262–2264].*

```
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
_geom_torsion_site_symmetry_1
_geom_torsion_site_symmetry_2
_geom_torsion_site_symmetry_3
_geom_torsion_site_symmetry_4
_geom_torsion_publ_flag
C(9)  O(2)  C(7)   C(2)    71.8(2)  .  .  .  .      yes
C(7)  O(2)  C(9)   C(10) -168.0(3)  .  .  .  2_666  yes
C(10) O(3)  C(8)   C(6)  -167.7(3)  .  .  .  .      yes
C(8)  O(3)  C(10)  C(9)   -69.7(2)  .  .  .  2_666  yes
O(1)  C(1)  C(2)   C(3)  -179.5(4)  .  .  .  .      no
O(1)  C(1)  C(2)   C(7)    -0.6(1)  .  .  .  .      no
```

### `_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 and Prelog.

Ref: Klyne, W. & Prelog, V. (1960). *Experientia*, **16**, 521–523.

Appears in list containing `_geom_torsion_atom_site_label_`. [`geom_torsion`]

### `_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 and Prelog. 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 site2–site1 onto the projection of the vector site3–site4. Clockwise torsions are positive, anticlockwise torsions are negative.

Ref: Klyne, W. & Prelog, V. (1960). *Experientia*, **16**, 521–523.

Appears in list as essential element of loop structure. **Must** match data name `_atom_site_label`. [`geom_torsion`]

### `_geom_torsion_publ_flag` (*char*)

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

| | |
|---|---|
| `no` | do not include angle in special list |
| `n` | abbreviation for "no" |
| `yes` | do include angle in special list |
| `y` | abbreviation for "yes" |

Appears in list containing `_geom_torsion_atom_site_label_`. Where no value is given, the assumed value is `'no'`. [`geom_torsion`]

`_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 '*klm*'. These numbers are combined to form the code '*n klm*' or *n_klm*. The character string *n_klm* is composed as follows: *n* refers to the symmetry operation that is applied to the coordinates stored in `_atom_site_fract_x`, `_atom_site_fract_y` and `_atom_site_fract_z`. It must match a number given in `_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 angle. These translations $(x, y, z)$ are related to $(k, l, m)$ by the relations $k = 5 + x$, $l = 5 + y$, $m = 5 + z$. By adding 5 to the translations, the use of negative numbers is avoided.

Appears in list containing `_geom_torsion_atom_site_label_`.

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_torsion`]

## _journal_[]

Data items in the JOURNAL category record details about the book keeping entries used by the journal staff when processing a CIF submitted for publication. 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 1 - based on Acta Cryst. file for entry HL0007 [Willis, Beckwith & Tozer (1991). Acta Cryst. C47, 2276–2277].*

```
_journal_date_recd_electronic     91-04-15
_journal_date_from_coeditor       91-04-18
_journal_date_accepted            91-04-18
_journal_date_printers_first      91-08-07
_journal_date_proofs_out          91-08-07
_journal_coeditor_code            HL0007
_journal_techeditor_code          C910963
_journal_coden_ASTM               ACSCEE
_journal_name_full   'Acta Crystallographica Section C'
_journal_year                     1991
_journal_volume                   47
_journal_issue                    NOV91
_journal_page_first               2276
_journal_page_last                2277
```

`_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_data_validation_number`
`_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_language`
`_journal_name_full`
`_journal_page_first`
`_journal_page_last`
`_journal_paper_category`
`_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.

[`journal`]

## _journal_index_[]

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.

*Example 1 - based on a paper by Zhu, Reynolds, Klein & Trudell [(1994). Acta Cryst. C50, 2067–2069].*

```
loop_
_journal_index_type
_journal_index_term
_journal_index_subterm
O   C16H19NO4           .
S   alkaloids           (-)-norcocaine
S   (-)-norcocaine      .
S
; [2R,3S-(2\b,3\b)]-methyl
   3-(benzoyloxy)-8-azabicyclo[3.2.1]octane-2-carboxylate
;                          .
```

`_journal_index_subterm`
`_journal_index_term`
`_journal_index_type` (*char*)

Indexing terms supplied by journals staff.

[`journal_index`]

### _publ_[]

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

---

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

```
_publ_section_title
; trans-3-Benzoyl-2-(tert-butyl)-4-(iso-butyl)-
  1,3-oxazolidin-5-one
;
_publ_section_abstract
;  The oxazolidinone ring is a shallow envelope
   conformation with the tert-butyl and iso-butyl groups
   occupying trans-positions with respect to the ring. The
   angles at the N atom sum to 356.2\%, indicating a very
   small degree of pyramidalization at this atom. This is
   consistent with electron delocalization between the N
   atom and the carbonyl centre [N--C=O = 1.374(3)\%A].
;
```

---

*Example 2 - based on $C_{31}H_{48}N_4O_4$, reported by Coleman, Patrick, Andersen & Rettig [(1996). Acta Cryst. C52, 1525–1527.*

```
_publ_section_title
;    Hemiasterlin Methyl Ester
;
_publ_section_title_footnote
;   IUPAC name: methyl 2,5-dimethyl-4-{2-[3-methyl-
    2-methylamino-3-(N-methylbenzo[b]pyrrol-
    3-yl)butanamido]-3,3-dimethyl-N-methyl-
    butanamido}-2-hexenoate.
;
```

### _publ_contact_author (*char*)

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

Example(s):

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

[publ]

### _publ_contact_author_address (*char*)

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

Example(s):

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

[publ]

### _publ_contact_author_email (*char*)

Email address in a form recognisable to international networks.

Example(s): `'name@host.domain.country'`, `'bm@iucr.org'`

[publ]

### _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()349477334'` [publ]

### _publ_contact_author_id_iucr (*char*)

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

Example(s): `'2985'` [publ]

### _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]

### _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 '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()349477330'`, `'12(34)9477330x5543'` [publ]

### _publ_contact_letter (*char*)

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

[publ]

### _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]

### _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]

### _publ_manuscript_text (*char*)

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

[publ]

### `_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*) |
| `FO` | Full submission - organic (*Acta C*) |
| `FM` | 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`]

### `_publ_requested_coeditor_name` (*char*)

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

[`publ`]

### `_publ_requested_journal` (*char*)

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

[`publ`]

### `_publ_section_title`
### `_publ_section_title_footnote`
### `_publ_section_synopsis`
### `_publ_section_abstract`
### `_publ_section_comment`
### `_publ_section_introduction`
### `_publ_section_experimental`
### `_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` (*char*)

The sections of a manuscript if submitted in parts. As an alternative see `_publ_manuscript_text` and `_publ_manuscript_processed`. The `_publ_section_exptl_prep`, `_publ_section_exptl_refinement` and `_publ_section_exptl_solution` items are preferred for separating the chemical preparation, refinement and structure solution aspects of the experimental description.

[`publ`]

## `_publ_author_[]`

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

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

```
loop_
_publ_author_name
_publ_author_address
'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`.

May appear in list containing `_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.

May appear in list containing `_publ_author_name`.

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

### `_publ_author_id_iucr` (*char*)

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

Appears in list.

Example(s): `‘2985’` [`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.

May appear in list as essential element of loop structure.

Example(s): `‘Bleary, Percival R.’`, `‘O'Neil, F. K.’`, `‘Van den Bossche, G.’`, `‘Yang, D.-L.’`, `‘Simonov, Yu.A’`, `‘M\"uller, H. A.’`, `‘Ross II, C. R.’` [`publ_author`]

## _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.

*Example 1 - based on a paper by R. Restori & D. Schwarzenbach (1996), Acta Cryst. A52, 369–378.*

```
loop_
_publ_body_element
_publ_body_label
_publ_body_title
_publ_body_format
_publ_body_contents
section   1         Introduction
cif
; X-ray diffraction from a crystalline material provides
  information on the thermally and spatially averaged
  electron density in the crystal...
;
section   2         Theory
tex
; In the rigid-atom approximation, the dynamic electron
  density of an atom is described by the convolution
  product of the static atomic density and a probability
  density function,
  $\rho_{dyn}(\bf r)=\rho_{stat}(\bf r)*P(\bf r).
  \eqno(1)$
;
```

*Example 2 - based on a paper by R. J. Papoular, Y. Vekhter & P. Coppens (1996), Acta Cryst. A52, 397–407.*

```
loop_
_publ_body_element
_publ_body_label
_publ_body_title
_publ_body_contents
   section       3
; The two-channel method for retrieval of the deformation
  electron density
;
     .
   subsection    3.1   ’The two-channel entropy S[\D\r(r)]’
; As the wide dynamic range involved in the total electron
  density...
;
   subsection    3.2
   ’Uniform vs informative prior model densities’     .
   subsubsection 3.2.1 ’Use of uniform models’
; Straightforward algebra leads to expressions analogous
  to...
;
```

### `_publ_body_contents` (*char*)

A text section of a submitted paper.

Appears in list containing `_publ_body_label`. [`publ_body`]

### `_publ_body_element` (*char*)

The functional role of the associated text section.

- `section`
- `subsection`
- `subsubsection`
- `appendix`
- `footnote`

Appears in list containing `_publ_body_label`. [`publ_body`]

### `_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`]

### `_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`]

### `_publ_body_title` (*char*)

Title of the associated section of text.

Appears in list containing `_publ_body_label`. [`publ_body`]

## _publ_manuscript_incl_[]

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

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

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

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

```
loop_
_publ_manuscript_incl_extra_item
_publ_manuscript_incl_extra_info
_publ_manuscript_incl_extra_defn
’_atom_site_symmetry_multiplicity’
                      ’to emphasise special sites’      yes
’_chemical_compound_source’
                      ’rare material, unusual source’   yes
’_reflns_d_resolution_high’
                      ’limited data is a problem here’  yes
’_crystal_magnetic_permeability’
                      ’unusual value for this material’  no
```

### `_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 |
| `n` | abbreviation for “no” |
| `yes` | 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]`

### `_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]`

### `_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. `[publ_manuscript_incl]`

## `_refine_[]`

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

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

```
_refine_special_details
           sfls: _F_calc_weight_full_matrix
_refine_ls_structure_factor_coef   F
_refine_ls_matrix_type             full
_refine_ls_weighting_scheme        calc
_refine_ls_weighting_details
                        ’w=1/(u^2^(F)+0.0004F^2^)’
_refine_ls_hydrogen_treatment      refxyz
_refine_ls_extinction_method       Zachariasen
_refine_ls_extinction_coef         3514(42)
_refine_ls_extinction_expression
; Larson, A. C. (1970). "Crystallographic Computing",
  edited by F. R. Ahmed. Eq. (22) p. 292. Copenhagen:
  Munksgaard.
;
_refine_ls_abs_structure_details
; The absolute configuration was assigned to agree
  with that of its precursor l-leucine at the chiral
  centre C3.
;
_refine_ls_number_reflns           1408
_refine_ls_number_parameters       272
_refine_ls_number_restraints       0
_refine_ls_number_constraints      0
_refine_ls_R_factor_all            .038
_refine_ls_R_factor_gt             .034
_refine_ls_wR_factor_all           .044
_refine_ls_wR_factor_gt            .042
_refine_ls_goodness_of_fit_all    1.462
_refine_ls_goodness_of_fit_gt     1.515
_refine_ls_shift/su_max            .535
_refine_ls_shift/su_mean           .044
_refine_diff_density_min          -.108
_refine_diff_density_max           .131
```

### `_refine_diff_density_max`
### `_refine_diff_density_min`
### `_refine_diff_density_rms` (*numb*)

The largest, smallest and root-mean-square-deviation, in electrons per ångström cubed, of the final difference electron density. The `*_rms` value is measured with respect to the arithmetic mean density, and is derived from summations over each grid point in the asymmetric unit of the cell. This quantity is useful for assessing the significance of `*_min` and `*_max` values, and also for defining suitable contour levels.

`[refine]`

### `_refine_ls_abs_structure_details` (*char*)

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

`[refine]`

### `_refine_ls_abs_structure_Flack` (*numb*)

The measure of absolute structure as defined 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 $-3u \leq x \leq 1 + 3u$ and a standard uncertainty (e.s.d.) $u$ must be supplied. The `_enumeration_range` of 0.0:1.0 is correctly interpreted as meaning $(0.0 - 3u) \leq x \leq (1.0 + 3u)$.

Ref: Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.

The permitted range is 0.0→1.0. `[refine]`

### `_refine_ls_abs_structure_Rogers` (*numb*)

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

Ref: Rogers, D. (1981). *Acta Cryst.* A**37**, 734–741.

The permitted range is -1.0→1.0. `[refine]`

### `_refine_ls_d_res_high` (*numb*)

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

The permitted range is 0.0→∞. `[refine]`

### `_refine_ls_d_res_low` (*numb*)

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

The permitted range is 0.0→∞. `[refine]`

### `_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 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 ‘$\rho$’ value. Note that the magnitude of these values is usually of the order of 10000.

Ref: Becker, P. J. & Coppens, P. (1974). *Acta Cryst.* A**30**, 129–153. Zachariasen, W. H. (1967). *Acta Cryst.* **23**, 558–564. Larson, A. C. (1967). *Acta Cryst.* **23**, 664–665.

Example(s): `‘3472(52)’` (Zachariasen coefficient $r^* = 0.347(5) \times 10^4$) `[refine]`

### `_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):

```
; Larson, A. C. (1970). "Crystallographic Computing",
  edited by F. R. Ahmed. Eq. (22) p. 292.
  Copenhagen: Munksgaard.
;
```

`[refine]`

### `_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, either ‘Becker–Coppens’ or ‘Zachariasen’. The latter is sometimes referred to as the ‘Larson’ method 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 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 multiple coefficients cannot be contained in `*_extinction_coef` and must be listed in `_refine_special_details`.

Ref: Becker, P. J. & Coppens, P. (1974). *Acta Cryst.* A**30**, 129–153. Zachariasen, W. H. (1967). *Acta Cryst.* **23**, 558–564. Larson, A. C. (1967). *Acta Cryst.* **23**, 664–665.

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

Example(s): `'B-C type 2 Gaussian isotropic'`, `'none'`

`[refine]`

### `_refine_ls_goodness_of_fit_all` (*numb*)

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 $(1/u^2)$, $u$ = 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→∞. `[refine]`

### `_refine_ls_goodness_of_fit_gt` (*numb*)

The least-squares goodness-of-fit parameter $S$ for significantly intense reflections, (see `_reflns_threshold_expression`), 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 $(1/u^2)$, $u$ = 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.

Related item(s): `_refine_ls_goodness_of_fit_obs` (alternate). The permitted range is 0.0→∞. `[refine]`

### `_refine_ls_goodness_of_fit_obs` (*numb*)

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

*The least-squares goodness-of-fit parameter S for observed reflections (see* `_reflns_observed_criterion`*), after the final cycle of refinement. Ideally, account should be taken of parameters restrained in the least squares. 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 $(1/u^2)$, $u$ = 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.*

`[refine]`

### `_refine_ls_goodness_of_fit_ref` (*numb*)

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.

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

$Y(obs)$ = 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 $(1/u^2)$, $u$ = 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→∞. `[refine]`

### `_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 |
| `constr` | H parameters constrained |
| `mixed` | some constrained, some independent |
| `undef` | H-atom parameters not defined |

Where no value is given, the assumed value is `'undef'`. `[refine]`

`_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`]

`_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`]

`_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`]

`_refine_ls_number_reflns` (*numb*)

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

The permitted range is 0→∞. [`refine`]

`_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`]

`_refine_ls_R_factor_all` (*numb*)

Residual factor for all reflections satisfying the resolution limits established by `_refine_ls_d_res_high` and `_refine_ls_d_res_low`. This is the conventional *R* factor. See also `_refine_ls_wR_factor_` definitions.

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

$F(obs)$ = the observed structure-factor amplitudes, $F(calc)$ = the calculated structure-factor amplitudes, and the sum $\sum$ is taken over the specified reflections.

The permitted range is 0.0→∞. [`refine`]

`_refine_ls_R_factor_gt` (*numb*)

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

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

$F(obs)$ = the observed structure-factor amplitudes, $F(calc)$ = the calculated structure-factor amplitudes, and the sum $\sum$ is taken over the specified reflections.

Related item(s): `_refine_ls_R_factor_obs` (alternate). The permitted range is 0.0→∞. [`refine`]

`_refine_ls_R_factor_obs` (*numb*)

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

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

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

*$F(obs)$ = the observed structure-factor amplitudes, $F(calc)$ = the calculated structure-factor amplitudes, and the sum $\sum$ is taken over the specified reflections.*

[`refine`]

`_refine_ls_R_Fsqd_factor` (*numb*)

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

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

$F(obs)^2$ = squares of the observed structure-factor amplitudes, $F(calc)^2$ = squares of the calculated structure-factor amplitudes, and the sum $\sum$ is taken over the specified reflections.

The permitted range is 0.0→∞. [`refine`]

`_refine_ls_R_I_factor` (*numb*)

Residual factor $R(I)$ for significantly intense reflections (satisfying `_reflns_threshold_expression`) and included in the refinement. This is most often calculated in Rietveld refinements of powder data, where it is referred to as $R_B$ or $R_{\rm Bragg}$.

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

$I(obs)$ = the net observed intensities, $I(calc)$ = the net calculated intensities, and the sum $\sum$ is taken over the specified reflections.

The permitted range is 0.0→∞. [`refine`]

`_refine_ls_restrained_S_all` (*numb*)

The least-squares goodness-of-fit parameter $S'$ for all reflections after the final cycle of least squares. This parameter explicitly includes the restraints applied in the least-squares process. See also `_refine_ls_goodness_of_fit_` definitions.

$$S' = \left(\frac{\sum\{w[Y(obs) - Y(calc)]^2\} + \sum_r\{w_r[P(calc) - P(targ)]^2\}}{N_{ref} + N_{restr} - N_{param}}\right)^{1/2}$$

$Y(obs)$ = the observed coefficients (see `_refine_ls_structure_factor_coef`), $Y(calc)$ = the observed coefficients (see `_refine_ls_structure_factor_coef`), $w$ = the least-squares reflection weight [1/square of standard uncertainty (e.s.d.)], $P(calc)$ = the calculated restraint values, $P(targ)$ = the target restraint values, $w_r$ = the restraint weight, $N_{ref}$ = the number of reflections used in the refinement (see `_refine_ls_number_reflns`), $N_{restr}$ = the number of restraints (see `_refine_ls_number_restraints`), $N_{param}$ = the number of refined parameters (see `_refine_ls_number_parameters`), the sum $\sum$ is taken over the specified reflections, and the sum $\sum_r$ is taken over the restraints.

The permitted range is 0.0→∞. `[refine]`

### `_refine_ls_restrained_S_gt` (*numb*)

The least-squares goodness-of-fit parameter $S'$ for significantly intense reflections (satisfying `_reflns_threshold_expression`) after the final cycle of least squares. This parameter explicitly includes the restraints applied in the least-squares process. See also `_refine_ls_goodness_of_fit_` definitions.

$$S' = \left(\frac{\sum\{w[Y(obs) - Y(calc)]^2\} + \sum_r\{w_r[P(calc) - P(targ)]^2\}}{N_{ref} + N_{restr} - N_{param}}\right)^{1/2}$$

$Y(obs)$ = the observed coefficients (see `_refine_ls_structure_factor_coef`), $Y(calc)$ = the observed coefficients (see `_refine_ls_structure_factor_coef`), $w$ = the least-squares reflection weight [1/square of standard uncertainty (e.s.d.)], $P(calc)$ = the calculated restraint values, $P(targ)$ = the target restraint values, $w_r$ = the restraint weight, $N_{ref}$ = the number of reflections used in the refinement (see `_refine_ls_number_reflns`), $N_{restr}$ = the number of restraints (see `_refine_ls_number_restraints`), $N_{param}$ = the number of refined parameters (see `_refine_ls_number_parameters`), the sum $\sum$ is taken over the specified reflections, and the sum $\sum_r$ is taken over the restraints.

Related item(s): `_refine_ls_restrained_S_obs` (alternate). The permitted range is 0.0→∞. `[refine]`

### `_refine_ls_restrained_S_obs` (*numb*)

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

*The least-squares goodness-of-fit parameter $S'$ for observed reflections, after the final cycle of least squares. This parameter explicitly includes the restraints applied in the least-squares process. See also* `_refine_ls_goodness_of_fit_` *definitions.*

$$S' = \left(\frac{\sum\{w[Y(obs) - Y(calc)]^2\} + \sum_r\{w_r[P(calc) - P(targ)]^2\}}{N_{ref} + N_{restr} - N_{param}}\right)^{1/2}$$

*$Y(obs)$ = the observed coefficients (see* `_refine_ls_structure_factor_coef`*), $Y(calc)$ = the observed coefficients (see* `_refine_ls_structure_factor_coef`*), $w$ = the least-squares reflection weight [1/square of standard uncertainty (e.s.d.)], $P(calc)$ = the calculated restraint values, $P(targ)$ = the target restraint values, $w_r$ = the restraint weight, $N_{ref}$ = the number of reflections used in the refinement (see* `_refine_ls_number_reflns`*), $N_{restr}$ = the number of restraints (see* `_refine_ls_number_restraints`*), $N_{param}$ = the number of refined parameters (see* `_refine_ls_number_parameters`*), the sum $\sum$ is taken over the specified reflections, and the sum $\sum_r$ is taken over the restraints.*

`[refine]`

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

**This definition has been superseded and is retained here only for archival purposes. Use instead** `_refine_ls_shift/su_max`

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

`[refine]`

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

**This definition has been superseded and is retained here only for archival purposes. Use instead** `_refine_ls_shift/su_mean`

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

`[refine]`

### `_refine_ls_shift/su_max` (*numb*)

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

Related item(s): `_refine_ls_shift/esd_max` (alternate). `[refine]`

### `_refine_ls_shift/su_max_lt` (*numb*)

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

The permitted range is 0.0→∞. Related item(s): `_refine_ls_shift/su_max` (alternate). `[refine]`

### `_refine_ls_shift/su_mean` (*numb*)

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

The permitted range is 0.0→∞. Related item(s): `_refine_ls_shift/esd_mean` (alternate). `[refine]`

### `_refine_ls_shift/su_mean_lt` (*numb*)

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

The permitted range is 0.0→∞. Related item(s): `_refine_ls_shift/su_mean` (alternate). `[refine]`

### `_refine_ls_structure_factor_coef` (*char*)

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

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

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

### `_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 `_refine_ls_weighting_scheme` is specified as 'calc'.

Example(s):

```
; Sigdel model of Konnert-Hendrickson:
  Sigdel = Afsig + Bfsig*(sin(\q)/\l - 1/6)
  Afsig = 22.0, Bfsig = 150.0 at the beginning of
refinement.
  Afsig = 16.0, Bfsig = 60.0 at the end of
refinement.
;
```

`[refine]`

### `_refine_ls_weighting_scheme` (*char*)

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

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

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

### `_refine_ls_wR_factor_all` (*numb*)

Weighted residual factors for all reflections. The reflections also satisfy the resolution limits established by `_refine_ls_d_res_high` and `_refine_ls_d_res_low`. See also the `_refine_ls_R_factor_` definitions.

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

$Y(obs)$ = the observed amplitude specified by `_refine_ls_structure_factor_coef`, $Y(calc)$ = the calculated amplitude specified by `_refine_ls_structure_factor_coef`, $w$ = the least-squares weight, and the sum $\sum$ is taken over the specified reflections.

The permitted range is 0.0→∞. `[refine]`

### `_refine_ls_wR_factor_gt` (*numb*)

Weighted residual factors for significantly intense reflections (satisfying `_reflns_threshold_expression`) included in the refinement. The reflections also satisfy the resolution limits established by `_refine_ls_d_res_high` and `_refine_ls_d_res_low`. See also the `_refine_ls_R_factor_` definitions.

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

$Y(obs)$ = the observed amplitude specified by `_refine_ls_structure_factor_coef`, $Y(calc)$ = the calculated amplitude specified by `_refine_ls_structure_factor_coef`, $w$ = the least-squares weight, and the sum $\sum$ is taken over the specified reflections.

Related item(s): `_refine_ls_wR_factor_obs` (alternate). The permitted range is 0.0→∞. `[refine]`

### `_refine_ls_wR_factor_obs` (*numb*)

**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 `_reflns_observed_criterion`) and included in the refinement. The reflections also satisfy the resolution limits established by `_refine_ls_d_res_high` and `_refine_ls_d_res_low`. See also the `_refine_ls_R_factor_` definitions.*

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

*$Y(obs)$ = the observed amplitude specified by `_refine_ls_structure_factor_coef`, $Y(calc)$ = the calculated amplitude specified by `_refine_ls_structure_factor_coef`, $w$ = the least-squares weight, and the sum $\sum$ is taken over the specified reflections.*

`[refine]`

### `_refine_ls_wR_factor_ref` (*numb*)

Weighted residual factors for all reflections included in the refinement. The reflections also satisfy the resolution limits established by `_refine_ls_d_res_high` and `_refine_ls_d_res_low`. See also the `_refine_ls_R_factor_` definitions.

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

$Y(obs)$ = the observed amplitude specified by `_refine_ls_structure_factor_coef`, $Y(calc)$ = the calculated amplitude specified by `_refine_ls_structure_factor_coef`, $w$ = the least-squares weight, and the sum $\sum$ is taken over the specified reflections.

The permitted range is 0.0→∞. `[refine]`

### `_refine_special_details` (*char*)

Description of special aspects of the refinement process.

`[refine]`

## `_refine_ls_class_[]`

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

*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_gt
_refine_ls_class_code
0.057    'Main'
0.074    'Com'
0.064    'NbRefls'
0.046    'LaRefls'
0.112    'Sat1'
0.177    'Sat2'
```

`_refine_ls_class_code` (*char*)

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

Appears in list. **Must** match data name `_reflns_class_code`.

Example(s): `'1'`, `'m1'`, `'s2'` `[refine_ls_class]`

`_refine_ls_class_d_res_high` (*numb*)

For each reflection class, the highest resolution in ångströms for the spacing in 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]`

`_refine_ls_class_d_res_low` (*numb*)

For each reflection class, the lowest resolution in ångströms for the spacing in 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]`

`_refine_ls_class_R_factor_all`
`_refine_ls_class_R_factor_gt` (*numb*)

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 `_refine_ls_class_d_res_high` and `_refine_ls_class_d_res_low`. This is the conventional *R* factor.

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

$F(obs)$ = the observed structure-factor amplitudes, $F(calc)$ = the calculated structure-factor amplitudes, and the sum $\sum$ is taken over the reflections of this class. See also `_refine_ls_class_wR_factor_all` definitions.

Appears in list containing `_refine_ls_class_code`. The permitted range is 0.0→∞. `[refine_ls_class]`

`_refine_ls_class_R_Fsqd_factor` (*numb*)

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

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

$F(obs)^2$ = squares of the observed structure-factor amplitudes, $F(calc)^2$ = 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→∞. `[refine_ls_class]`

`_refine_ls_class_R_I_factor` (*numb*)

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

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

$I(obs)$ = the net observed intensities, $I(calc)$ = the net calculated intensities, 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→∞. `[refine_ls_class]`

`_refine_ls_class_wR_factor_all` (*numb*)

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

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

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

Appears in list containing `_refine_ls_class_code`. The permitted range is 0.0→∞. `[refine_ls_class]`

`_refln_[]`

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

*Example 1 - based on data set fetod of Todres, Yanovsky, Ermekov & Struchkov [(1993). Acta Cryst. C49, 1352–1354].*

```
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 - - - -
```

*Example 2 - based on standard test data set p6122 of the Xtal distribution [Hall, King & Stewart (1995). Xtal3.4 User's Manual. Univ. Western Australia].*

```
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    .895  <  1
# - - - - data truncated for brevity - - - -
```

### `_refln_A_calc`
### `_refln_A_meas` (*numb*)

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

$$A = |F| \cos(phase)$$

Appears in list containing `_refln_index_`. [`refln`]

### `_refln_B_calc`
### `_refln_B_meas` (*numb*)

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

$$B = |F| \sin(phase)$$

Appears in list containing `_refln_index_`. [`refln`]

### `_refln_class_code` (*char*)

The code identifying the class to which this reflection has been assigned. This code must match a value of `_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 $m = \sum |m_i|$, 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 `_reflns_class_code`. [`refln`]

### `_refln_d_spacing` (*numb*)

The *d* spacing in ångströms for this reflection. It is related to the $(\sin\theta)/\lambda$ value by the expression `_refln_d_spacing` = 2/(`_refln_sint/lambda`)

Appears in list containing `_refln_index_`. The permitted range is 0.0→∞. [`geom_bond`]

### `_refln_crystal_id` (*char*)

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

Appears in list containing `_refln_index_`. **Must** match data name `_exptl_crystal_id`. [`refln`]

### `_refln_F_calc`
### `_refln_F_meas`
### `_refln_F_sigma` (*numb*)

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_`. [`refln`]

### `_refln_F_squared_calc`
### `_refln_F_squared_meas`
### `_refln_F_squared_sigma` (*numb*)

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

Appears in list containing `_refln_index_`. [`refln`]

### `_refln_include_status` (*char*)

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’)<br>satisfies `_refine_ls_d_res_high`<br>satisfies `_refine_ls_d_res_low`<br>exceeds `_reflns_threshold_expression` |
| `<` | satisfies `_refine_ls_d_res_high`<br>satisfies `_refine_ls_d_res_low`<br>does not exceed `_reflns_threshold_expression` |
| `-` | systematically absent reflection |
| `x` | unreliable measurement – not used |
| `h` | does not satisfy `_refine_ls_d_res_high` |
| `l` | does not satisfy `_refine_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`]

### `_refln_index_h`
### `_refln_index_k`
### `_refln_index_l` (*numb*)

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`]

### `_refln_intensity_calc`
### `_refln_intensity_meas`
### `_refln_intensity_sigma` (*numb*)

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

Appears in list containing `_refln_index_`. [`refln`]

### `_refln_mean_path_length_tbar` (*numb*)

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

Appears in list containing `_refln_index_`. [`refln`]

### `_refln_observed_status` (*char*)

**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`]

### `_refln_phase_calc` (*numb*)

The calculated structure-factor phase in degrees.

Appears in list containing `_refln_index_`. [`refln`]

### `_refln_phase_meas` (*numb*)

The measured structure-factor phase in degrees.

Appears in list containing `_refln_index_`. [`refln`]

### `_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 |

Appears in list containing `_refln_index_`. Where no value is given, the assumed value is ‘`incl`’. [`refln`]

### `_refln_scale_group_code` (*char*)

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

Appears in list containing `_refln_index_`. **Must** match data name `_reflns_scale_group_code`.

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

`_refln_sint/lambda` (*numb*)

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

Appears in list containing `_refln_index_`. The permitted range is 0.0→∞. [refln]

`_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.

Appears in list containing `_refln_index_`. The permitted range is 1→48. [refln]

`_refln_symmetry_multiplicity` (*numb*)

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

Appears in list containing `_refln_index_`. The permitted range is 1→48. [refln]

`_refln_wavelength` (*numb*)

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→∞. [refln]

`_refln_wavelength_id` (*char*)

Code identifying the wavelength in the `_diffrn_radiation_` list. See `_diffrn_radiation_wavelength_id`.

Appears in list containing `_refln_index_`. **Must** match data name `_diffrn_radiation_wavelength_id`. [refln]

`_reflns_[]`

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

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

```
_reflns_limit_h_min                 0
_reflns_limit_h_max                 6
_reflns_limit_k_min                 0
_reflns_limit_k_max                 17
_reflns_limit_l_min                 0
_reflns_limit_l_max                 22
_reflns_number_total                1592
_reflns_number_gt                   1408
_reflns_threshold_expression        'F > 6.0u(F)'
_reflns_d_resolution_high           0.8733
_reflns_d_resolution_low            11.9202
```

`_reflns_d_resolution_high`
`_reflns_d_resolution_low` (*numb*)

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]

`_reflns_Friedel_coverage` (*numb*)

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_refln_` list, $N$(Crystal class) is the number of reflections obtained on averaging under the symmetry of the crystal class, $N$(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 $hkl$ is equivalent to $-h-k-l$ in the crystal class and all Friedel pairs $\{hkl; -h-k-l\}$ have been measured. (*c*) For whole-sphere data in space group $Pmm2$, the value will be $< 1.0$ because although reflections $hkl$ and $-h-k-l$ are not equivalent when $hkl$ indices are non-zero, they are when $l = 0$. (*d*) For a crystal in the group $Pmm2$ measurements of the two inequivalent octants $h \geq 0, k \geq 0, l$ lead to the same value as in (*c*), whereas measurements of the two equivalent octants $h \geq 0, k, l \geq 0$ will lead to a zero value for `_reflns_Friedel_coverage`.

The permitted range is 0.0→1.0. [reflns]

`_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 reported reflections. These need not be the same as the `_diffrn_reflns_limit_` values.

[reflns]

`_reflns_number_gt` (*numb*)

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`.

Related item(s): `_reflns_number_observed` (alternate). The permitted range is 0→∞. [reflns]

### `_reflns_number_observed` (*numb*)

**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_observed_criterion`). 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]`

### `_reflns_number_total` (*numb*)

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]`

### `_reflns_observed_criterion` (*char*)

**This definition has been superseded and is retained here only for archival purposes. Use instead `_reflns_threshold_expression`**
*The criterion used to classify a reflection as 'observed'. This criterion is usually expressed in terms of a $\sigma(I)$ or $\sigma(F)$ threshold.*

`[reflns]`

### `_reflns_special_details` (*char*)

Description of the properties of the reported reflection list that is not given in other data items. In particular it should include information about the averaging (or not) of symmetry-equivalent reflections including Friedel pairs.

`[reflns]`

### `_reflns_threshold_expression` (*char*)

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 `_refine_ls_R_factor_gt`.

Related item(s): `_reflns_observed_criterion` (alternate).

Example(s): `'I>2u(I)'` `[reflns]`

### `_reflns_class_[]`

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

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

```
loop_
_reflns_class_number_gt
_reflns_class_code
584     'Main'
226     'Sat1'
50      'Sat2'
```

### `_reflns_class_code` (*char*)

The code identifying a certain reflection class.

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

Example(s): `'1'`, `'m1'`, `'s2'` `[reflns_class]`

### `_reflns_class_description` (*char*)

Description of each reflection class.

Appears in list containing `_reflns_class_code`.

Example(s): `'m=1 first order satellites'`,
`'H0L0 common projection reflections'` `[reflns_class]`

### `_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]`

### `_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]`

### `_reflns_class_number_gt` (*numb*)

For each reflection class, the number of significantly intense reflections (see `_reflns_threshold_expression`) 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`.

Appears in list containing `_reflns_class_code`. The permitted range is 0.0→∞. `[reflns_class]`

### `_reflns_class_number_total` (*numb*)

For each reflection class, 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`.

Appears in list containing `_reflns_class_code`. The permitted range is 0.0→∞. `[reflns_class]`

### `_reflns_class_R_factor_all`
### `_reflns_class_R_factor_gt` (*numb*)

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.

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

$F(obs)$ = the observed structure-factor amplitudes, $F(calc)$ = the calculated structure-factor amplitudes, and the sum $\sum$ is taken over the reflections of this class. See also `_reflns_class_wR_factor_all` definitions.

Appears in list containing `_reflns_class_code`. The permitted range is 0.0→∞. `[reflns_class]`

### `_reflns_class_R_Fsqd_factor` (*numb*)

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

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

$F(obs)^2$=squares of the observed structure-factor amplitudes, $F(calc)^2$=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_R_I_factor` (*numb*)

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

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

$I(obs)$ = the net observed intensities, $I(calc)$ = the net calculated intensities, 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`.

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

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

Appears in list containing `_reflns_class_code`. The permitted range is 0.0→∞. `[reflns_class]`

## `_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 `_refln_scale_group_code`.

*Example 1 - based on standard test data set p6122 of the Xtal distribution [Hall, King & Stewart (1995). Xtal3.4 User's Manual. Univ. Western Australia]*

```
loop_
_reflns_scale_group_code
_reflns_scale_meas_F
1  .895447
```

### `_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`. These codes need not correspond to those in the `_diffrn_scale_` list.

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

### `_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_scale]`

## `_reflns_shell_[]`

Data items in the REFLNS_SHELL category record details about the reflections used to determine the ATOM_SITE data items, as broken down by shells of resolution.

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

```
loop_
_reflns_shell_d_res_high
_reflns_shell_d_res_low
_reflns_shell_meanI_over_uI_gt
_reflns_shell_number_measured_gt
_reflns_shell_number_unique_gt
_reflns_shell_percent_possible_gt
_reflns_shell_Rmerge_F_gt
31.38  3.82  69.8  9024  2540  96.8   1.98
3.82  3.03  26.1  7413  2364  95.1   3.85
3.03  2.65  10.5  5640  2123  86.2   6.37
2.65  2.41   6.4  4322  1882  76.8   8.01
2.41  2.23   4.3  3247  1714  70.4   9.86
2.23  2.10   3.1  1140   812  33.3  13.99
```

### `_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]`

### `_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]`

### `_reflns_shell_meanI_over_sigI_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 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]`

### `_reflns_shell_meanI_over_sigI_gt` (*numb*)

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

### `_reflns_shell_meanI_over_sigI_obs` (*numb*)

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

`[reflns_shell]`

### `_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.

Related item(s): `_reflns_shell_meanI_over_sigI_all` (alternate). Appears in list. `[reflns_shell]`

### `_reflns_shell_meanI_over_uI_gt` (*numb*)

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

Related item(s): `_reflns_shell_meanI_over_sigI_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 $R_{\rm merge}(F)$ for all reflections in a given shell.

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

$F_j$ = the amplitude of the *j*th observation of reflection *i*, $\langle F\rangle$ = the mean of the amplitudes of all observations of reflection *i*, 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 $R_{\rm merge}(F)$ for significantly intense reflections (see `_reflns_threshold_expression`) in a given shell.

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

$F_j$ = the amplitude of the *j*th observation of reflection *i*, $\langle F\rangle$ = the mean of the amplitudes of all observations of reflection *i*, 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 $R_{\rm merge}(F)$ for reflections classified as 'observed' (see `_reflns_observed_criterion`) in a given shell.*

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

*$F_j$ = the amplitude of the jth 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]`

`_reflns_shell_Rmerge_I_all` (*numb*)

The value of $R_{\rm merge}(I)$ for all reflections in a given shell.

$$R_{\rm merge}(I) = \frac{\sum_i(\sum_j |I_j - \langle I\rangle|)}{\sum_i(\sum_j \langle I\rangle)}$$

$I_j$ = the intensity of the *j*th observation of reflection *i*, $\langle I\rangle$ = the mean of the intensities of all observations of reflection *i*, 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_I_gt` (*numb*)

The value of $R_{\rm merge}(I)$ for significantly intense reflections (see `_reflns_threshold_expression`) in a given shell.

$$R_{\rm merge}(I) = \frac{\sum_i(\sum_j |I_j - \langle I\rangle|)}{\sum_i(\sum_j \langle I\rangle)}$$

$I_j$ = the intensity of the *j*th observation of reflection *i*, $\langle I\rangle$ = the mean of the intensities of all observations of reflection *i*, 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_I_obs` (alternate). Appears in list. The permitted range is 0.0→∞. `[reflns_shell]`

`_reflns_shell_Rmerge_I_obs` (*numb*)

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

*The value of $R_{\rm merge}(I)$ for reflections classified as 'observed' (see `_reflns_observed_criterion`) in a given shell.*

$$R_{\rm merge}(I) = \frac{\sum_i(\sum_j |I_j - \langle I\rangle|)}{\sum_i(\sum_j \langle I\rangle)}$$

*$I_j$ = the intensity of the jth observation of reflection i, $\langle I\rangle$ = the mean of the intensities 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→∞. Related item(s): `_reflns_shell_Rmerge_I_obs` (replace). `[reflns_shell]`

### `_space_group_[]`

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

*Example 1 - The monoclinic space group no. 15 with unique axis b.*

```
_space_group_id                 1
_space_group_name_H-M_alt       'C 2/c'
_space_group_IT_number          15
_space_group_name_Hall          '-C 2yc'
_space_group_crystal_system     monoclinic
```

`_space_group_crystal_system` (*char*)

The name of the system of geometric crystal classes of space groups (crystal system) to which the space group belongs. Note that rhombohedral space groups belong to the trigonal system.

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

May appear in list containing `_space_group_id`. Related item(s): `_symmetry_cell_setting` (alternate). `[space_group]`

`_space_group_id` (*char*)

This is an identifier needed if `_space_group_` items are looped.

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

### `_space_group_IT_number` (*numb*)

The number as assigned in *International Tables for Crystallography Vol A*, specifying the proper affine class (*i.e.* the orientation preserving affine class) of space groups (crystallographic space group type) to which the space group belongs. This number defines the space group type but not the coordinate system in which it is expressed.

May appear in list containing `_space_group_id`. The permitted range is 1→230. Related item(s): `_symmetry_Int_Tables_number` (alternate). `[space_group]`

### `_space_group_name_Hall` (*char*)

Space group symbol defined by Hall. Each component of the space group name is separated by a space or an underscore. The use of space is strongly recommended. The underscore is only retained because it was used in earlier archived files. It should not be used in new CIFs. `_space_group_name_Hall` uniquely defines the space group and its reference to a particular coordinate system.

Ref: Hall, S. R. (1981). *Acta Cryst.* A**37**, 517–525. [See also *International Tables for Crystallography, Vol. B* (1993) 1.4 Appendix B]

May appear in list containing `_space_group_id`.

Example(s): `‘P 2c -2ac’` (equivalent to *Pca*21), `‘-I 4bd 2ab 3’` (equivalent to *Ia*3*d*)

Related item(s): `_symmetry_space_group_name_Hall` (alternate). `[space_group]`

### `_space_group_name_H-M_alt` (*char*)

`_space_group_name_H-M_alt` allows for any Hermann–Mauguin symbol to be given. The way in which this item is used is determined by the user and in general is not intended to be interpreted by computer. It may, for example, be used to give one of the extended Hermann–Mauguin symbols given in Table 4.3.1 of *International Tables for Crystallography Vol. A* (1995) or a Hermann–Mauguin symbol for a conventional or unconventional setting. Each component of the space group name is separated by a space or underscore. The use of space is strongly recommended. The underscore is only retained because it was used in earlier archived files. It should not be used in new CIFs. Subscripts should appear without special symbols. Bars should be given as negative signs before the numbers to which they apply. The commonly used Hermann–Mauguin symbol determines the space group type uniquely but a given space group type may be described by more than one Hermann–Mauguin symbol. The space group type is best described using `_space_group_IT_number`. The Hermann–Mauguin symbol may contain information on the choice of basis though not on the choice of origin. To define the setting uniquely use `_space_group_name_Hall` or list the symmetry operations.

May appear in list containing `_space_group_id`.

Example(s):

```
; loop_
  _space_group_name_H-M_alt
  'C m c m'
  'C 2/c 2/m 21/m'
  'A m a m'
;
```

(three examples for the space group number 63)

Related item(s): `_symmetry_space_group_name_H-M` (alternate). `[space_group]`

### `_space_group_symop_[]`

Contains information about the symmetry operations of the space group.

*Example 1 - The symmetry operations for the space group P21/c.*

```
loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1    x,y,z
2   -x,-y,-z
3   -x,1/2+y,1/2-z
4    x,1/2-y,1/2+z
```

### `_space_group_symop_id` (*char*)

An arbitrary identifier that uniquely labels each symmetry operation in the list.

Appears in list as essential element of loop structure.
Related item(s): `_symmetry_equiv_pos_site_id` (alternate). `[space_group_symop]`

### `_space_group_symop_operation_xyz` (*char*)

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

$$X' = WX + w$$

(Note: $X$ is used to represent $\mathbf{x}$ in *International Tables for Crystallography Vol. A*, Section 5) When a list of symmetry operations is given, it must contain a complete set of coordinate representatives which generates all the operations of the space group by the addition of all primitive translations of the space group. Such representatives are to be found as the coordinates of the general-equivalent position in *International Tables for Crystallography Vol. A*, to which it is necessary to add any centring translations shown above the general-equivalent position. That is to say, it is necessary to list explicity all the symmetry operations required to generate all the atoms in the unit cell defined by the setting used.

May appear in list containing `_space_group_symop_id`. Where no value is given, the assumed value is `‘x,y,z’`.

Example(s): `‘x,1/2-y,1/2+z’` (glide reflection through the plane (x,1/4,z),with glide vector 1/2 c)

Related item(s): `_symmetry_equiv_pos_as_xyz` (alternate). `[space_group_symop]`

### `_space_group_symop_sg_id` (*numb*)

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

May appear in list containing `_space_group_symop_id`. **Must** match data name `_space_group_id`. `[space_group_symop]`

### `_symmetry_[]`

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

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

```
_symmetry_cell_setting            orthorhombic
_symmetry_space_group_name_H-M    'P 21 21 21'
_symmetry_space_group_name_Hall   'P 2ac 2ab'
```

### `_symmetry_cell_setting` (*char*)

**This definition has been superseded and is retained here only for archival purposes. Use instead** `_space_group_crystal_system`
*The cell settings for this space-group symmetry.*

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

[`symmetry`]

### `_symmetry_Int_Tables_number` (*numb*)

**This definition has been superseded and is retained here only for archival purposes. Use instead** `_space_group_IT_number`
*Space-group number from International Tables for Crystallography, Vol. A (1987).*

The permitted range is 1→230. [`symmetry`]

### `_symmetry_space_group_name_Hall` (*char*)

**This definition has been superseded and is retained here only for archival purposes. Use instead** `_space_group_name_Hall`
*Space-group symbol as described by Hall. This symbol gives the space-group setting explicitly. Leave spaces between the separate components of the symbol.*

*Ref: Hall, S. R. (1981). Acta Cryst. A***37***, 517–525.*

Example(s): `‘-P 2ac 2n’`, `‘-R 3 2"’`, `‘P 61 2 2 (0 0 -1)’`
[`symmetry`]

### `_symmetry_space_group_name_H-M` (*char*)

**This definition has been superseded and is retained here only for archival purposes. Use instead** `_space_group_name_H-M_alt`
*Hermann–Mauguin space-group symbol. Note that the 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’` [`symmetry`]

## `_symmetry_equiv_[]`

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

---

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

```
loop_
_symmetry_equiv_pos_as_xyz
+x,+y,+z  1/2-x,-y,1/2+z  1/2+x,1/2-y,-z  -x,1/2+y,1/2-z
```

*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.*

```
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1     x,y,z
2     1/2-x,-y,1/2+z
3     1/2+x,1/2-y,-z
4     -x,1/2+y,1/2-z
```

### `_symmetry_equiv_pos_as_xyz` (*char*)

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

May appear in list.

Example(s): `‘-y+x,-y,1/3+z’` [`symmetry_equiv`]

### `_symmetry_equiv_pos_site_id` (*numb*)

**This definition has been superseded and is retained here only for archival purposes. Use instead** `_space_group_symop_id`
*A code identifying each entry in the* `_symmetry_equiv_pos_as_xyz` *list. It is normally the sequence number of the entry in that list, and should be identified with the code ‘n’ in* `_geom_*_symmetry_` *codes of the form ‘n_klm’.*

Appears in list containing `_symmetry_equiv_pos_as_xyz`.
[`symmetry_equiv`]

## `_valence_param_[]`

Data items in the VALENCE_PARAM category define the parameters used for calculating bond valences from bond lengths. In addition to the parameters, a pointer is given to the reference (in VALENCE_REF) where the parameters have been published.

---

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

```
loop_
_valence_param_atom_1
_valence_param_atom_1_valence
_valence_param_atom_2
_valence_param_atom_2_valence
_valence_param_Ro
_valence_param_B
_valence_param_ref_id
_valence_param_details
Cu 2 O -2 1.679 0.37 a .
Cu 2 O -2 1.649 0.37 j .
Cu 2 N -3 1.64  0.37 m '2-coordinate N'
Cu 2 N -3 1.76  0.37 m '3-coordinate N'
loop_
_valence_ref_id
_valence_ref_reference
a  'Brown & Altermatt (1985), Acta Cryst. B41, 244-247'
j  'Liu & Thorp (1993), Inorg. Chem. 32, 4102-4205'
m  'See, Krause & Strub (1998), Inorg. Chem. 37, 5369-5375'
```

### `_valence_param_atom_1` (*char*)

The element symbol of the first atom forming the bond whose bond valence parameters are given in this category.

Appears in list. [`valence_param`]

### `_valence_param_atom_1_valence` (*numb*)

The valence (formal charge) of the first atom whose bond valence parameters are given in this category.

Appears in list. [`valence_param`]

`_valence_param_atom_2` (*char*)

The element symbol of the second atom forming the bond whose bond valence parameters are given in this category.

Appears in list. [`valence_param`]

`_valence_param_atom_2_valence` (*numb*)

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

Appears in list. [`valence_param`]

`_valence_param_B` (*numb*)

The bond valence parameter $B$ used in the expression

$$s = \exp[(R_o - R)/B]$$

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

Appears in list. [`valence_param`]

`_valence_param_details` (*char*)

Details or comments on the bond valence parameters.

Appears in list. [`valence_param`]

`_valence_param_id` (*char*)

An identifier for the valence parameters of a bond between the given atoms.

Appears in list. [`valence_param`]

`_valence_param_ref_id` (*char*)

An identifier which links to the reference to the source from which the bond valence parameters are taken. A child of `_valence_ref_id` which it must match.

Appears in list. **Must** match data name `_valence_ref_id`. . [`valence_param`]

`_valence_param_Ro` (*numb*)

The bond valence parameter $R_o$ used in the expression

$$s = \exp[(R_o - R)/B]$$

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

Appears in list. [`valence_param`]

`_valence_ref_[]`

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

`_valence_ref_id` (*char*)

An identifier for items in this category. Parent of `_valence_param_ref_id` which must have the same value.

Appears in list containing `_valence_ref_id`. May match subsidiary data name(s): `_valence_param_ref_id`. [`valence_ref`]

`_valence_ref_reference` (*char*)

Literature reference from which the valence parameters identified by `_valence_param_id` were taken.

Appears in list containing `_valence_ref_id`. [`valence_ref`]