

Twinning dictionary

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This dictionary contains names and definitions of twinning data items recognized by the International Union of Crystallography for the exchange of data between laboratories and submissions to journals and databases.

TWIN

Data items in the TWIN category record general details about the nature of the twinning in the sample. Terminology for twin dataname definitions was taken directly from: "International Union of Crystallography Commission on Mathematical and Theoretical Crystallography Research themes: Crystal twinning" by Massimo Nespolo, February 3, 2009. <http://www.crystallography.fr/mathcryst/twins.htm>.

*The twinning example presented here shows twinning by merohedry for a trigonal crystal system. The simulated space group is $P3_221$, but the true space group is $P3_2$. The twin operation chosen is $2: x, x, 0$ in $P3_221$ corresponding to operation (by rows) $0, 1, 0/1, 0, 0/0, 0, -1$ [see Table 11.2.2.1 of *International Tables for Crystallography* (2005), Vol. A].*

The TWIN_REFLN loop gives the properties of each diffraction peak (identified by `_twin_reflndatum_id`) which is indexed to both the twin individuals.

In each of the loops shown in this example the first items on a line are the list reference. While the list reference must be present in every loop, it is not necessary that it should be declared as the first item in the loop.

```
_twin_formation_mechanism      gt
_twin_dimensionality           triperiodic
_twin_morphology               polysynthetic
_twin_special_details
;      This is an example of a twin in space group P 32
      by the 2 x,x,0 twin operation.
;
```

```
loop_
_twin_individual_id
_twin_individual_mass_fraction_refined
_twin_individual_twin_lattice_type
_twin_individual_twin_matrix_11
_twin_individual_twin_matrix_12
_twin_individual_twin_matrix_13
_twin_individual_twin_matrix_21
_twin_individual_twin_matrix_22
_twin_individual_twin_matrix_23
_twin_individual_twin_matrix_31
_twin_individual_twin_matrix_32
_twin_individual_twin_matrix_33
  1 0.545(2) ref  1 0 0 0 1 0 0 0 0 1
  2 0.455(2) mt_II 0 1 0 1 0 0 0 0 0 -1
```

```
loop_
_twin_reflndatum_id
_twin_reflndatum_individual_id
_twin_reflndatum_index_h
_twin_reflndatum_index_k
_twin_reflndatum_index_l
_twin_reflndatum_F_squared_calc
_twin_reflndatum_F_squared_meas
_twin_reflndatum_F_squared_sigma
_twin_reflndatum_include_status
  1  1 -1  1 -32  40.17  55.86  7.39 o
  1  2  1 -1  32  40.17  55.86  7.39 o
  2  1  0  1 -32 125.83 145.63  9.36 o
  2  2  1  0  32 125.83 145.63  9.36 o
  3  1  1  1 -32 10.33  30.89  7.39 o
  3  2  1  1  32 10.33  30.89  7.39 o
  4  1 -3  2 -32 28.26  26.84  9.47 o
  4  2  2 -3  32 28.26  26.84  9.47 o
# - - - - data truncated for brevity - - - -
```

`_twin_dimensionality` (char)

The degree of overlap between the twin lattices. Most twin lattice symmetry (TLS) and twin lattice quasi-symmetry (TLQS) twins as defined by Donnay and Donnay will be triperiodic.

Reference: Donnay, G. & Donnay, J. D. H. (1974). *Can. Mineral.* **12**, 422-425.

The data value must be one of the following:

triperiodic	common lattice in three dimensions
diperiodic	common lattice in two dimensions
monoperiodic	common lattice in one dimension

[twin]

`_twin_formation_mechanism` (char)

A description of the method of twin formation.

The data value must be one of the following:

gt	growth twin formed during crystal growth
tt	transformation twin formed during phase transition
mt	mechanical twin formed as a result of mechanical action

[twin]

`_twin_morphology` (char)

The physical relationship of the different twins to one another.

The data value must be one of the following:

contact	separated by a surface
penetration	sharing a volume
simple	individuals are not repeated
polysynthetic	individuals repeat in approximately linear arrangement
cyclic	individuals repeat in closed edifice

[twin]

`_twin_special_details` (char)

Information about twinning in the sample not contained in other data items.

Example:

```
; Individuals 3 and 4 arise from form (I) following an
enantiotropic phase transition by sudden cooling in
a cryostat to 173K.
```

[twin]

`_twin_individual_twin_lattice_type` (char)

Identification of the symmetry relationships between the twin lattices as described in *International Tables for Crystallography* (2004), Vol. C, Chapter 1.3. The twin with the identity matrix should be denoted as 'ref'.

Appears in list.

The data value must be one of the following:

ref	reference twin
mt_I	merohedral class I (simple inversion)
mt_II	merohedral class II (mirror or twofold)
mt_I+II	class I and II simultaneously present
rmt	reticular merohedral
pmt	pseudo-merohedral
rpmt	reticular pseudo-merohedral
nmt	non-merohedral

[twin]

TWIN_INDIVIDUAL

Data items in the TWIN_INDIVIDUAL category describe properties of each twinned individual, and the symmetry relationships between the individuals.

_twin_individual_id (char)

The unique identifier for this twin individual. The twin for which **_twin_individual_twin_matrix** is the identity matrix is called the reference twin. It is recommended that the reference twin be labelled '1'.

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

_twin_refl_individual_id [twin_individual]

_twin_individual_mass_fraction_refined (numb, su)

The refined mass fraction of this twin individual; the sum of all mass fractions must equal unity within the limits of experimental uncertainty.

Appears in list containing **_twin_individual_id**.

The permitted range is 0 → 1.0. [twin_individual]

_twin_individual_twin_matrix_11

_twin_individual_twin_matrix_12

_twin_individual_twin_matrix_13

_twin_individual_twin_matrix_21

_twin_individual_twin_matrix_22

_twin_individual_twin_matrix_23

_twin_individual_twin_matrix_31

_twin_individual_twin_matrix_32

_twin_individual_twin_matrix_33 (numb)

Elements of the matrix U that multiplies the Miller indices h, k, l of the reference twin to give the Miller indices h', k', l' , of the twin specified by **_twin_individual_id**

$$\begin{pmatrix} h' & k' & l' \end{pmatrix} = U \begin{pmatrix} h & k & l \end{pmatrix}$$

It follows that the reference twin must have $U = I$, the identity matrix.

Appears in list containing **_twin_individual_id**. [twin_individual]

This example is taken from Colombo, Young & Gladfelter [Inorg. Chem. (2000), 39, 4621–4624]. Two structures of nitronium tetranitratogallate are reported as a result of an enantiotropic phase transition. The higher-temperature phase is in the tetragonal space group $I\bar{4}$, while the lower-temperature phase is a twin by non-merohedry in space group $I2$. The individuals are enantiomorphic as a result of the phase transition. In the listing it is clear that datums 620–624 do not contain overlapping reflections, whereas datums 625–629 contain contributions from both twins.

```
loop_
_twin_refl_datum_id
_twin_refl_individual_id
_twin_refl_index_h
_twin_refl_index_k
_twin_refl_index_l
_twin_refl_F_squared_calc
_twin_refl_F_squared_meas
_twin_refl_F_squared_sigma
_twin_refl_include_status
```

620	1	1	-6	-3	200.22	207.88	3.35	o
621	1	-1	6	3	225.34	224.15	3.62	o
622	2	-1	6	3	184.64	196.34	3.95	o
623	1	-1	-6	-3	173.28	181.13	3.06	o
624	2	-1	-6	-3	143.40	152.05	2.78	o
625	1	1	6	3	204.45	204.38	4.48	o
625	2	3	-6	1	204.45	204.38	4.48	o
626	1	3	-6	-3	240.97	241.19	3.75	o
626	2	-3	6	3	240.97	241.19	3.75	o
627	1	3	6	3	288.54	281.53	4.31	o
627	2	-3	-6	-3	288.54	281.53	4.31	o
628	1	-5	-6	-3	179.56	176.35	5.36	o
628	2	-3	6	5	179.56	176.35	5.36	o
629	1	5	6	3	235.04	238.84	4.06	o
629	2	-5	-6	-3	235.04	238.84	4.06	o

TWIN_REFLN

Items in the TWIN_REFLN category tabulate the calculated values of F^2 for each peak observed in the diffraction pattern, together with the measured value of F^2 . The calculated F^2 for an observed peak is a weighted sum of the contribution of all the twin components. The calculated structure factor for each twin contribution can also be given.

This partial listing describes seven observed diffraction peaks in a four-individual twin by non-merohedry. The reference individual is 1. Reflections from the other three individuals 2, 3 and 4 are present only if these cannot be experimentally separated from the reference individual.

```
loop_
_twin_refl_datum_id
_twin_refl_individual_id
_twin_refl_index_h
_twin_refl_index_k
_twin_refl_index_l
_twin_refl_F_squared_meas
_twin_refl_F_squared_sigma
_twin_refl_include_status
```

1	1	1	0	0	1.03	0.18	o
1	3	1	0	0	1.03	0.18	o
2	1	2	0	0	1290.01	55.59	o
2	3	2	0	0	1290.01	55.59	o
3	1	3	0	0	2.59	0.42	o
3	3	3	0	0	2.59	0.42	o
4	1	4	0	0	30.98	1.47	o
4	3	4	0	0	30.98	1.47	o
5	1	5	0	0	1.97	0.96	o
5	3	5	0	0	1.97	0.96	o
6	1	6	0	0	1.55	1.14	o
6	2	6	1	2	1.55	1.14	o
6	3	6	0	0	1.55	1.14	o
6	4	6	1	2	1.55	1.14	o
7	1	-6	1	0	0.47	1.06	o
7	2	6	2	2	0.47	1.06	o

_twin_refl_datum_id (char)

This item serves to identify an observed diffraction peak. It may include contributions from one or more twin components and so may appear more than once in the list. The values of **_twin_refl_F_squared_calc** and **_twin_refl_F_squared_meas** indexed by **_twin_refl_datum_id** include the contributions from all the twins. The diffraction peak is indexed by **_twin_refl_index_h**, ***_k** and ***_l** referred to the cell of the twin component identified by **_twin_refl_individual_id**. The list reference includes both **_twin_refl_datum_id** and **_twin_refl_individual_id**. The combination of these two items may only appear once in a list.

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

_twin_refl_F_squared_calc (numb)

Calculated value for the overall squared structure factors (in electrons squared for X-ray diffraction) arising from all the twin contributions to the peak defined by **_twin_refl_datum_id**. The total contribution from all twins to a single observed reflection is modelled according to the method of Pratt, Coyle and Ibers as follows:

$$\text{_twin_refln_F_squared_calc} = \text{osf} \times \sum(m_f \times \text{_refln_F_squared_calc})$$

where osf is the overall scale factor, m_f is the mass fraction, and the sum is taken over all the twin components that contribute to this diffraction peak.

Reference: Pratt, C. S., Coyle, B. A. & Ibers, J. A. (1971). *J. Chem. Soc. A*, pp. 2146–2151.

Appears in list containing **_twin_refl_datum_id**,

_twin_refl_individual_id. [twin_refl]

_twin_refl_n_F_squared_calc_individual (numb)
Contribution of the twin identified by **_twin_refl_n_individual_id** to **_twin_refl_n_F_squared_calc**.

$$\text{_twin_refln_F_squared_calc_individual} = \text{osf} \times \text{mf} \times \text{_refln_F_squared_calc}$$

where *osf* is the overall scale factor, *mf* is the mass factor. For X-ray diffraction the units are electrons squared.

Appears in list containing **_twin_refl_n_datum_id**,
_twin_refl_n_individual_id.

[twin_refl_n]

_twin_refl_n_F_squared_meas (numb)
The observed value F^2 of the peak referenced by **_twin_refl_n_datum_id**. This is typically the observed peak intensity after Lorentz and polarization corrections.

Appears in list containing **_twin_refl_n_datum_id**,
_twin_refl_n_individual_id.

[twin_refl_n]

_twin_refl_n_F_squared_sigma (numb)
Standard uncertainty of **_twin_refl_n_F_squared_meas**
Appears in list containing **_twin_refl_n_datum_id**,
_twin_refl_n_individual_id.

[twin_refl_n]

_twin_refl_n_include_status (char)
A symbol indicating how the reflection is treated during refinement.

Appears in list containing **_twin_refl_n_datum_id**,
_twin_refl_n_individual_id.

The data value must be one of the following:

o (lower-case letter o for 'observed') satisfies **_refine_ls_d_res_high**, satisfies **_refine_ls_d_res_low** and exceeds **_reflns_threshold_expression**
< satisfies **_refine_ls_d_res_high**, satisfies **_refine_ls_d_res_low** and does not exceed **_reflns_threshold_expression**
- systematically absent reflection
x unreliable measurement – not used
r removed from the refinement for other reasons
h does not satisfy **_refine_ls_d_res_high**
l does not satisfy **_refine_ls_d_res_low**

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

[twin_refl_n]

_twin_refl_n_index_h

_twin_refl_n_index_k

_twin_refl_n_index_l

(numb)

Miller indices of a reflection from the twin component labelled by **_twin_refl_n_individual_id**. The values of the Miller indices must correspond to the cell defined for this twin component.

Appears in list containing **_twin_refl_n_datum_id**,

_twin_refl_n_individual_id.

[twin_refl_n]

_twin_refl_n_individual_id

(char)

The unique identifier of the twin individual whose Miller indices are given in **_twin_refl_n_index_**. The ID must match a **_twin_individual_id** in the TWIN_INDIVIDUAL category. The list reference includes both **_twin_refl_n_datum_id** and **_twin_refl_n_individual_id**. The combination of these two items may only appear once in a list.

Appears in list as essential element of loop structure. containing

_twin_refl_n_datum_id, **_twin_refl_n_individual_id**. Must match parent

data name **_twin_individual_id**.

[twin_refl_n]