

CIF dictionary

ED_GROUP

The ED_GROUP data items describe atomic information specific to crystallographic structure determination using electron diffraction.

CHEMICAL

`_chemical.absolute_configuration` (Text)

`_chemical_absolute_configuration`

Necessary conditions for this assignment are given by Flack, H. D. & Bernardinelli, G. (1999). *Acta Cryst.* A55, 908-915. Flack, H. D. & Bernardinelli, G. (2000). *J. Appl. Cryst.* 33, 1143-1148.

The data value must be one of the following:

rm	'reference molecule' Absolute configuration established by the structure determination of a compound containing a chiral reference molecule of known absolute configuration.
ad	'anomalous dispersion' Absolute configuration established by a-d effects in diffraction measurements on the crystal.
dyn	Absolute configuration determined directly from dynamical refinement.
rmad	'rm + ad' Absolute configuration established by the structure determination of a compound containing a chiral reference molecule of known absolute configuration and confirmed by a-d effects in diffraction measurements on the crystal.
syn	'synthetic' 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	'unknown' No firm chemical or a-d evidence for an assignment is available. An arbitrary choice of enantiomer has been made.
.	Inapplicable.

DIFFRN

`_diffrn.precession_angle` (Real; °)

`_diffrn_precession_angle`

Angle at the sample of tilt from the normal direction of a radiation beam moved in a precessional scan.

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

`_diffrn.precession_angle_su` (Real; °)

`_diffrn_precession_angle_su`

Standard uncertainty of `_diffrn.precession_angle`.

DIFFRN_MEASUREMENT

`_diffrn_measurement.integration` (Code)

`_diffrn_measurement_integration`

Code describing the technique used to sample as completely as possible the accessible range of reciprocal space.

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

The data value must be one of the following:

beam-tilt	The radiation beam is tilted in order to collect intensities in different regions of reciprocal space while the sample remains stationary.
continuous	Synonym for 'rotation' commonly used in 3D electron diffraction.
rotation	The detector records diffracted intensities continuously while the sample is rotated. This is the usual mode for X-ray crystallography.
stepwise	The detector records diffracted intensities at intervals while the sample is panned or tilted in discrete steps. Often used in 3D electron diffraction.

`_diffrn_measurement.method_precession` (Code)

`_diffrn_measurement_method_precession`

Yes or no flag indicating if the radiation beam illuminates the sample at an angle that is rotated about a precession axis.

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

The data value must be one of the following:

yes	Precession method is used.
y	Abbreviation for 'yes'.
no	Precession method is not used.
n	Abbreviation for 'no'.

REFINE

`_refine.diffraction_theory` (Code)

`_refine_diffraction_theory`

A code describing the approach to summation of diffracted beams from scattering layers of the sample. In the kinematical approximation the integrated intensities of the Bragg reflections are proportional to the square of the modulus of the structure factor.

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

The data value must be one of the following:

dynamical	Interactions between propagating waves and matter are taken into account when calculating the amplitudes of diffracted beams.
kinematical	Interactions between propagating waves and matter are ignored when calculating the amplitudes of diffracted beams.