Electron diffraction extension 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:

continuous	The detector collects a sequence of diffraction patterns from a crystal at different tilt angles by rotating the goniometer. This is commonly used with a transmission electron microscope 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 beam path through the specimen.

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.