Electron diffraction 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.* A**55**, 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'.

_diffrn_measurement.tracking (*Code*)

_diffrn_measurement_tracking

Yes or no flag indicating if a tracking method to follow the crystal was used in the data acquisition. Typically used to track very small crystals in electron diffraction experiments.

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

The data value must be one of the following:

yes	A crystal tracking method is used.
y	Abbreviation for 'yes'.
no	A crystal tracking method is not used.
n	Abbreviation for 'no'.

_diffrn_measurement.tracking_method (*Text*)

_diffrn_measurement_tracking_method

Description of the method used to follow the crystal during data collection.

Example: 'Electron-beam tracking by PyFast-ADT'

DIFFRN_RADIATION

_diffrn_radiation.illumination_mode (*Code*)

_diffrn_radiation

Code describing the optical configuration of the incident beam at the sample. For electron diffraction, parallel illumination is the normal mode in transmission electron microscopy (TEM), convergent-beam in scanning transmission electron microscopy (STEM).

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

The data value must be one of the following:

convergent	Convergent-beam illumination
parallel	Parallel illumination

DIFFRN_SOURCE

_diffrn_source.size (*Text*)

_diffrn_source_size

Description of the collimated source beam as viewed from the sample.

Examples: '8mm x 0.4 mm fine-focus', 'broad focus',
'300 nm electron beam in NBED (nano-beam electron diffraction)',
'1 micrometre aperture size in SAED (selected-aperture el. diffr.)'

REFINE

_refine.diffraction_theory (*Code*)

_refine_diffraction_theory

A code describing the approach to the calculation of the diffracted intensities. In the kinematical approximation, interactions of diffracted waves with matter are neglected, and integrated intensities of the Bragg reflections are proportional to the square of the modulus of the structure factor. In the dynamical calculation, interactions between diffracted waves are taken into account, and the proportionality of the intensities and the structure factors is not preserved.

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

The data value must be one of the following:

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

REFINE_DIFF

_refine_diff.density_max (*Real,* e $Å^{-1}$)

_refine_diff_density_max

_refine.diff_density_max

Maximum density value in a difference Fourier map.

The permitted range is $-100. \rightarrow \infty$.

_refine_diff.density_max_su (*Real,* e $Å^{-1}$)

_refine_diff_density_max_su

_refine.diff_density_max_esd

Standard uncertainty of the maximum density value in a difference Fourier map.

_refine_diff.density_min (*Real,* e $Å^{-1}$)

_refine_diff_density_min

_refine.diff_density_min

Minimum density value in a difference Fourier map.

The permitted range is $-\infty \rightarrow 100.$.

_refine_diff.density_min_su (*Real,* e $Å^{-1}$)

_refine_diff_density_min_su

_refine.diff_density_min_esd

Standard uncertainty of the minimum density value in a difference Fourier map.

_refine_diff.density_RMS (*Real,* e $Å^{-1}$)

_refine_diff_density_RMS

_refine.diff_density_RMS

Root mean square density value in a difference Fourier map. This 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.

The permitted range is $-100. \rightarrow 100.$.

_refine_diff.density_RMS_su (*Real,* e $Å^{-1}$)

_refine_diff_density_RMS_su

_refine.diff_density_RMS_esd

Standard uncertainty of the root mean square density value in a difference Fourier map.

REFINE_LS

_refine_ls.abs_structure_z-score (*Real*)

_refine_ls_abs_structure_z-score

The z-score is a measure of confidence in an absolute structure determination as described by Klar *et al.* (2023), based on the method of Le Page *et al.* (1990). For centrosymmetric structures, the only permitted value, if the data item is present, is 'inapplicable', represented by '.' .

References: Klar, P. B. *et al.* (2023). *Nature Chem.* **15**, 848–855. Le Page, Y., Gabe, E. J. & Gainsford, G. J. (1990). *J. Appl. Cryst.* **23**, 406–411.