Electron diffraction CIF dictionary

This dictionary defines data items used to specify the aspects of crystal structures determined by electron diffraction specific to that technique.

CIF_ED_HEAD

This category is the Head category for an extension dictionary used for 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.

COMPUTING

_computing.sample_tracking (*Text*)

Reference to software used to track the position of a sample with respect to the diffraction source beam. Typically used in 3D electron diffraction. More details of the tracking method may be provided in **_diffrn_measurement.sample_tracking_method**.

Example: 'PyFast-ADT (Santucci, 2024)'

DIFFRN

_diffrn.precession_semi_angle (*Real*; °)

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

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

_diffrn.precession_semi_angle_su (*Real*; °)

Standard uncertainty of **_diffrn.precession_semi_angle**.

DIFFRN_MEASUREMENT

_diffrn_measurement.method_precession (*Code*)

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

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.rotation_mode (*Code*)

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

The data value must be one of the following:

rotation	The detector records diffracted intensities continuously while the sample is rotated.
stepwise	The detector records diffracted intensities while the sample is stationary and the beam is either steady or performing a defined motion, typically precessing around a conical surface normal to the sample (precession electron diffraction).

_diffrn_measurement.sample_tracking (*Code*)

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.

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.sample_tracking_method (*Text*)

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*)

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).

The data value must be one of the following:

convergent	Convergent-beam illumination
parallel	Parallel illumination

DIFFRN_SOURCE

_diffrn_source.convergence_angle (*Real*; °)

The angle of convergence of the source beam (for example in convergent-beam electron diffraction). The convergence angle is the angular spread of the cone of illumination (*i.e.* 2α, where the semi-angle α is measured from the axis defining the beam direction).

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

_diffrn_source.ed_diffracting_area_selection (*Text*)

Enumerated code for the technique in electron diffraction used to select the region of the sample from which the diffraction pattern is obtained.

The data value must be one of the following:

`probe`	Diffraction region selected by the size of the probe (= beam)
`SAED`	Selected-area electron diffraction

_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.)`'

EXPTL_CRYSTAL

_exptl_crystal.mosaic_block_size (*Real*; Å)

Isotropic and resolution-independent term representing the average size of mosaic domains in the crystal specified in ångströms. Larger size indicates better ordered crystals.

The permitted range is $0. \rightarrow \infty$.

_exptl_crystal.mosaic_block_size_su (*Real*; Å)

Standard uncertainty of **_exptl_crystal.mosaic_block_size**.

_exptl_crystal.mosaic_method (*Text*)

How parameters derived from the spot shape (such as mosaic block size and rotation, beam divergence, and crossfire) and their errors were estimated. This can be a written description or a citation to a specific software package that determined these parameters.

Example: '`Determined from rocking curve.`'

_exptl_crystal.mosaicity (*Real*; °)

Isotropic approximation of the distribution of mis-orientation angles specified in degrees of all the mosaic domain blocks in the crystal, represented as a standard deviation. Here, a mosaic block is a set of contiguous unit cells assumed to be perfectly aligned. Lower mosaicity indicates better ordered crystals. See for example: Nave, C. (1998). *Acta Cryst.* D**54**, 848–853. Note that many software packages estimate the mosaic rotation distribution differently and may combine several physical properties of the experiment into a single mosaic term. This term will help fit the modelled spots to the observed spots without necessarily being directly related to the physics of the crystal itself.

The permitted range is $0. \rightarrow \infty$.

_exptl_crystal.mosaicity_su (*Real*; °)

Standard uncertainty of **_exptl_crystal.mosaicity**.

REFINE

_refine.diffraction_theory (*Code*)

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.

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.diffraction_theory_details (*Text*)

Details needed to characterize the approach to the calculation of the diffracted intensities, such as a description of the parameters that were refined dynamically.

REFINE_DIFF

_refine_diff.potential_max (*Real*; e Å^{-1})

Maximum electrostatic potential value in a difference Fourier map.

_refine_diff.potential_max_su (*Real*; e Å^{-1})

Standard uncertainty of **_refine_diff.potential_max**.

_refine_diff.potential_min (*Real*; e Å^{-1})

Minimum electrostatic potential value in a difference Fourier map.

_refine_diff.potential_min_su (*Real*; e Å^{-1})

Standard uncertainty of **_refine_diff.potential_min**.

_refine_diff.potential_RMS (*Real*; e Å^{-1})

Root mean square electrostatic potential value in a difference Fourier map. This value is measured with respect to the arithmetic mean potential 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_diff.potential_RMS_su (*Real*; e Å^{-1})

Standard uncertainty of **_refine_diff.potential_RMS**.

REFINE_LS

_refine_ls.abs_structure_z-score (*Real*)

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.

_refine_ls.sample_shape_details (*Text*)

Additional details describing the sample thickness when calculated during dynamical refinement where this cannot be defined completely by the formula given in **_refine_ls.sample_shape_expression**.

Reference: Palatinus, L., Petricek, V. & Correa, C. A. (2015). *Acta Cryst.* A**71**, 235–244.

_refine_ls.sample_shape_expression (*Text*)

Formula for the sample thickness distribution when the sample thickness is considered during dynamical refinement.

Reference: Palatinus, L., Petricek, V. & Correa, C. A. (2015). *Acta Cryst.* A**71**, 235–244.

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;
  F(\t) = 1 - ( 1 - \t^2^)^1/2^
;
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(The cumulative distribution function in terms of the reduced thickness τ of a sample treated as a cylinder. $\tau = t/t_m$, where t is the thickness at the point illuminated and t_m the maximum thickness of the cylinder (*i.e.* its diameter).)

_refine_ls.sample_thickness (*Real*; nanometres)

The refined sample thickness as determined by dynamical refinement.

Reference: Palatinus, L., Petricek, V. & Correa, C. A. (2015). *Acta Cryst.* A**71**, 235–244.

The permitted range is $0. \rightarrow \infty$.

Example: '35(2)'

_refine_ls.sample_thickness_su (*Real*; nanometres)

Standard uncertainty of **_refine_ls.sample_thickness**.