

TOPAS-Academic, Version 9

Electron Diffraction

September 30, 2026

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working with Claude Opus 5.5, the AI model from Anthropic

www.topas-academic.com

1.... ELECTRON DIFFRACTION

```

[ed_crystal $file]... ' starts a crystal, the data of one .cif_pets file
[ed_g_max !E] ' default 1.9 Å-1
[ed_sg_max !E] ' default 0.05 Å-1
[ed_sg_bethe !E] ' Bethe potentials; default 0.008 Å-1 for frames > 80 beams, else 0
[ed_sg_max_refine !E] ' default 0.1 Å-1
[ed_rsg_max !E] ' default 0.75
[ed_dsg_min !E] ' default 0.0015 Å-1
[ed_num_integration_steps !E] ' default 15
[ed_num_precession_steps !E] ' default 24
[ed_max_beams !E] ' default 400
[ed_orient_search !E] ' orientation search range in degrees; default 0, no search
[ed_invert_hand !E] ' 1 fits the inverted structure; default 0
[ed_abs_symmetric !E] ' 0 always uses the general solver; default 1
[r_f #]
[xdd_ed $file]... ' one virtual frame
    [ed_frame_number !E] ' the frame in the file
    [ed_alpha !E] ' the goniometer angle of the frame; not used in the calculation
    [ed_thickness E] ' crystal thickness in Å; default 500
    [ed_absorption E] ' absorptive potential as a fraction of the potential; refinable; default 0
    [ed_frame_rotate_x E] ' orientation correction in degrees; default 0
    [ed_frame_rotate_y E] ' orientation correction in degrees; default 0
    [ed_data] ' electron scattering factors; implied by xdd_ed
[f0_f1_f11_atom $atom]... ' electron data: in the shared str_dets of the frames
    ' f1 is the charge q, f11 the absorption fraction kt
[ed_hand_out $file] ' writes the reflections of this refinement
[ed_hand_compare $file] ' the absolute structure against another refinement
[#inp_from_cif_pets $file] ' writes an ed_crystal and one xdd_ed for every frame

```

Examples: TEST_EXAMPLES\ED

GLYCINE\TOPAS\GLY-DYN-0.INP, GLY-DYN-1.INP

QUARTZ\TOPAS\QTZ-DYN-0.INP

The data and the Jana2020 refinements are those of Klar et al. (2021), doi 10.5281/zenodo.7185657, published under CC BY 4.0; the same deposit holds the albite data used below.

1.1.....Introduction

This chapter describes dynamical refinement of three-dimensional electron diffraction (3D ED) data in TOPAS, with intensities calculated by the Bloch wave form of the dynamical theory, following Palatinus, Petříček & Antunes Corrêa (2015) and Klar et al. (2023).

In 3D ED the crystal is rotated in the electron beam, and diffraction images, called frames, are recorded as it turns. With continuous rotation, each frame covers a small range of angles; with stepwise data, each frame is recorded at a single angle. For continuous-rotation data, PETS2 combines consecutive frames into virtual frames, and each `xdd_ed` corresponds to one virtual frame. Electrons scatter strongly, and an individual electron is scattered many times within the crystal. The resulting intensity depends on other reflections, on the crystal thickness, and on the orientation of the frame. The kinematical approximation, in which the intensity is proportional to the square of the structure factor, is therefore poor.

A kinematical refinement merges all frames into one list of reflections and fits a single structure. A dynamical refinement keeps each frame separate and fits all frames with one structure. Each data set is an `ed_crystal` and each of its virtual frames an `xdd_ed`. An `xdd_ed` uses a `str`, which can have its own sites and lattice parameters. Alternatively, a shared `str_dets` and a shared `lat_prms` can be used for all `xdd_ed`s, similar to what is done in XRD-CT refinements. For example:

```
str_dets s1 { space_group ... site ... }
lat_prms l1 { a 5.4 b 5.4 c 5.4 ... }
ed_crystal ...
  xdd_ed ... use { s1 l1 }
  xdd_ed ... use { s1 l1 }
  ...
```

Within the shared `str_dets`, keywords such as `rigid`, `occ_merge`, `penalty` etc... can all be used.

1.2Nomenclature

Nomenclature	
λ	Electron wavelength (Å)
E	Accelerating voltage
m, m_0	Relativistic and rest mass of the electron
$\mathbf{K}$	Incident wave vector, along the beam; $K = 1/\lambda$ (Å ⁻¹)
$\mathbf{h}$	Miller indices (h, k, l) of a reflection
$\mathbf{g}$	Reciprocal lattice vector of reflection h; $ \mathbf{g} = 1/d$ (Å ⁻¹)
s	$\sin\theta/\lambda = \mathbf{g} /2$ (Å ⁻¹)
$f_e(s)$	Electron scattering factor (Å)
a_i, b_i	Gaussian coefficients of the electron scattering factor
f_x, Z	X-ray scattering factor and atomic number
f'	Absorptive form factor, the imaginary part of the electron scattering factor; not the anomalous dispersion term of X-ray diffraction
A, B	Geometric parts of the structure factor of a site
C, D	Scattering parts of the structure factor of a site; D is zero for electrons
F_g	Structure factor of reflection g computed with electron scattering factors

$F_{g, re}, F_{g, im}$	Real and imaginary parts of the structure factor
U_g	Fourier coefficient of the crystal potential for reflection g ($\text{\AA}^{-2}$)
V	Unit cell volume ($\text{\AA}^3$)
UB	Orientation matrix of a crystal, from the .cif_pets file
R	Rotation of a frame, including the refined corrections
s_g	Excitation error of reflection g ($\text{\AA}^{-1}$)
M	Structure matrix of a frame, one row and one column for each beam
$\mathbf{g}_m, \mathbf{g}_n$	Beams m and n of a frame
$\mathbf{C}^{(j)}$	Eigenvector j of M , the Bloch wave j
γ_j	Eigenvalue of Bloch wave j ($\text{\AA}^{-1}$)
ε_j	Excitation of Bloch wave j by the incident beam
t	Crystal thickness ($\text{\AA}$)
φ_g	Amplitude of beam g at the exit surface
I_g	Intensity of reflection g in a frame
S_f	Scale of frame f
k_f	Factor on the intensities of frame f , fixed at the first calculation
N_s	Number of integration steps across a virtual frame
R_{sg}, D_{sg}	Reflection selection ratio and distance from the limiting Ewald spheres
p	A refined parameter
$f_{x, ion}$	X-ray scattering factor of an ion
q	Charge of an ion (-2 for O^{2-}), or partial charge of an atom type (the f1 of f0_f1_f11_atom for electron data)
$\Delta(s)$	Change in f_e per unit charge ($\text{\AA}$)
w	A weak beam, included by Bethe potentials
I_o, I_c	Observed and calculated intensity of a reflection
F_o, F_c	$\sqrt{I_o}$ and $\sqrt{I_c}$
σ_{I_o}, σ_F	Standard uncertainties of I_o and F_o
w_F	Weight of a reflection in $wR(F)$
N, N_p	Number of reflections, and of refined parameters
N_+	Reflections nearer I_o with the hand refined than with the other hand
$I_{c, inv}$	Calculated intensity with the other hand
Z, Z_{adj}	z score of the absolute structure, and z adjusted for noise
W	Reduction of N for reflections that the two hands do not separate
Φ	Normal distribution function

κ	Absorptive potential as a fraction of the potential, ed_absorption
κ_t	Absorptive form factor of an atom type as a fraction of f_e , $f' = \kappa_t f_e$; the f11 of f0_f1_f11_atom

1.3Electron wavelength and scattering factors

The electron wavelength at an accelerating voltage E , with a relativistic correction, is defined as:

$$\lambda = \frac{h}{\sqrt{2m_0eE\left(1 + \frac{eE}{2m_0c^2}\right)}}$$

$$\frac{m}{m_0} = 1 + \frac{eE}{m_0c^2}$$

The electron scattering factors are sums of Gaussians, with coefficients from International Tables Vol. C, Table 4.3.2.2:

$$f_e(s) = \sum_{i=1}^5 a_i \exp(-b_i s^2)$$

The Mott formula gives the electron scattering factor as a function of the X-ray scattering factor:

$$f_e(s) = 0.023934 \frac{Z - f_x(s)}{s^2}$$

ed_data selects these scattering factors. The coefficients are read from the file EDSCAT.TXT. The electron scattering factor of an ion, named with the sign first as in O-2 or Si+4, is defined as:

$$f_{e,ion}(s) = f_e(s) + 0.023934 \frac{q + f_x(s) - f_x(0) - f_{x,ion}(s) + f_{x,ion}(0)}{s^2}$$

where f_e is the electron scattering factor of the neutral atom, f_x and $f_{x,ion}$ the X-ray scattering factors of the atom and the ion respectively, and q the charge in the name of the ion (-2 for O-2). The charge dominates at small s . Beyond about $0.25 \text{ \AA}^{-1}$ the ion and the neutral atom have nearly the same electron scattering factor. These quantities can be refined as follows:

```
prm qf 0.1 min -0.5 max 1.5
site Si1 x 1.000000 y 0.470511 z = 5/6;
  occ Si = 1 - qf; ADPs { 0.005939 0.006824 0.002087 0.002969 0.001812 0.000906 }
  occ Si+4 = qf; ADPs { 0.005939 0.006824 0.002087 0.002969 0.001812 0.000906 }
' and the same for O1, with 0 and 0-2
```

1.4Structure factors and the crystal potential

The structure factor of a site is written as a geometric part ($A+iB$) times a scattering part ($C+iD$):

$$F = (A + iB)(C + iD)$$

For electrons D is zero; C carries the occupancy, the Debye Waller factor and the electron scattering factor. The structure factor of reflection $\mathbf{g}$ is the sum over the sites:

$$F_{\mathbf{g}} = F_{\mathbf{g},re} + iF_{\mathbf{g},im}, \quad F_{\mathbf{g},re} = \sum_s A_s C_s, \quad F_{\mathbf{g},im} = \sum_s B_s C_s$$

The Fourier coefficient of the crystal potential is defined as:

$$U_{\mathbf{g}} = \frac{m}{m_0} \frac{1}{\pi V} F_{\mathbf{g}}^*$$

The structure factors do not depend on the orientation of a frame. They are calculated once for the shared `str_dets` and used by every frame.

1.5The geometry of a frame

Reflection $\mathbf{h}$ of a crystal with orientation matrix $\mathbf{UB}$, in a frame with rotation $\mathbf{R}$, lies at:

$$\mathbf{g} = \mathbf{R} \mathbf{U} \mathbf{B} \mathbf{h}$$

The excitation error of reflection $\mathbf{g}$ is defined as:

$$s_{\mathbf{g}} = \frac{K^2 - |\mathbf{K} + \mathbf{g}|^2}{2K}$$

The beam travels against the zone axis (u v w) of the frame. $\mathbf{UB}$ is written in laboratory coordinates, whose x-axis is the goniometer axis. `ed_frame_rotate_x` corrects the goniometer angle of a frame by rotating the crystal about the goniometer axis. `ed_frame_rotate_y` rotates the crystal about the axis perpendicular to both the beam and the goniometer axis. Both parameters are in degrees and can be refined for each frame. They correct the beam direction at the centre of the frame, and the integration steps are distributed around this corrected direction. Calculated intensities are independent of rotation of the crystal around the beam.

Two sign choices determine the hand of an acentric structure. One choice is whether $U_{\mathbf{g}}$ uses the structure factor or its conjugate; the other is the direction of the beam. Changing the conjugate reverses the structure. The beam direction is fixed by the data, because the beam must travel against the zone axis; only then do the recorded reflections lie two to three times closer to the Ewald sphere than they would with the beam along the zone axis. Once the beam direction is set, quartz confirms the correct conjugate, since the published absolute structure gives the lower Rwp, as shown in the examples.

1.6The Bloch wave equations

For beams m and n of a frame the structure matrix is defined as:

$$M_{mm} = 2K s_{\mathbf{g}_m}, \quad M_{mn} = U_{\mathbf{g}_m - \mathbf{g}_n}$$

An off-diagonal element uses the structure factor of the reflection $g_m - g_n$, which means structure factors are required up to twice `ed_g_max`; TOPAS calculates them to 2.1 `ed_g_max`; The Bloch waves are the eigenvectors of the structure matrix.

$$\mathbf{M} \mathbf{C}^{(j)} = 2K\gamma_j \mathbf{C}^{(j)}$$

The amplitude of beam g at the exit surface of a crystal of thickness t is:

$$\varphi_g(t) = \sum_j C_g^{(j)} \varepsilon_j \exp(2\pi i \gamma_j t), \quad \varepsilon_j = C_0^{(j)*}$$

$$I_g = |\varphi_g(t)|^2$$

A new thickness needs no new eigenvectors. For a thin crystal the result reduces to the kinematical intensity:

$$I_g \propto |U_g|^2 \propto |F_g|^2$$

1.7Integration over a virtual frame

A virtual frame covers a range of orientations, and the calculated intensity is defined as:

$$I_{g,calc} = S_f k_f \frac{1}{N_s} \sum_{k=1}^{N_s} |\varphi_g(t, \mathbf{R}_k)|^2$$

The virtual frame spans a range of angles, and TOPAS divides this range into N_s equal parts and calculates the intensity at the centre of each part. N_s is controlled by `ed_num_integration_steps`, which defaults to 15. For continuous-rotation data, PETS2 (Palatinus et al., 2019) writes the half-width of each virtual frame into the precession-angle column of the CIF_PETS file. For precession data, an average over azimuths around the precession cone is taken, and `ed_num_precession_steps` sets how many azimuths are used, the default is 24.

Fifteen integration steps are fast, but they are not always sufficient. In glycine, refining the frame orientations required the 42 steps used in the Jana2020 refinement; with only 15, the calculated intensities do not vary smoothly with orientation.

1.8Selection of beams and reflections

For each frame TOPAS chooses the beams of the calculation and the measured reflections to fit. A reflection is a beam when $|g| \leq \text{ed_g_max}$ and it comes close to the Ewald sphere within the frame. Close means an excitation error within $\pm \text{ed_sg_max}$ at one or more of the integration steps, or a crossing of the Ewald sphere within the frame. A measured reflection is fitted when it passes three tests: $|g| \leq \text{ed_g_max}$; its excitation error at the centre of the frame is within $\pm \text{ed_sg_max_refine}$; and it crosses the Ewald sphere well inside the frame. The last test uses two quantities:

For each frame, beams and measured reflections are selected to be fitted. A reflection is treated as a beam when $|g| \leq \text{ed_g_max}$ and it approaches the Ewald sphere within the frame. “Close” means that its excitation error falls within $\pm \text{ed_sg_max}$ at one or more integration steps, or that it crosses the Ewald sphere somewhere inside the frame. A measured reflection is fitted when it passes three tests: $|g| \leq \text{ed_g_max}$; its excitation error at the centre of the frame lies within $\pm \text{ed_sg_max_refine}$; and it crosses the Ewald sphere well inside the frame. The last test uses two quantities.

$$R_{sg} = \frac{|s_g|}{D_{sg} + |s_g|} \leq \text{ed_rsg_max}, \quad D_{sg} \geq \text{ed_dsg_min}$$

D_{sg} is the distance of the reflection from the Ewald sphere at the nearer of the two ends of the frame. D_{sg} is positive when the reflection crosses the Ewald sphere within the frame and negative when it does not. The examples use the Jana2020 values for `ed_g_max`, `ed_sg_max`, `ed_sg_max_refine`, `ed_dsg_min` and `ed_rsg_max`.

A frame contains at most `ed_max_beams` beams. These include the incident beam, all reflections fitted in the frame, and any additional reflections that satisfy the `ed_g_max` and `ed_sg_max` tests. When more reflections qualify than the limit allows, the ones closest to the Ewald sphere is kept. If the incident beam and the fitted reflections already exceed `ed_max_beams`, TOPAS retains all of them and prints a warning. The beams are selected when the data are loaded, and again for the orientation found by `ed_orient_search`. They are chosen before refinement begins and remain fixed throughout refinement. This ensures that the calculated intensities vary smoothly as `ed_frame_rotate_x` and `ed_frame_rotate_y` are refined.

A reflection whose excitation error $|S_g|$ at the centre of a frame exceeds `ed_sg_max_refine` is removed. The `ed_sg_max_refine` test is performed after `ed_g_max` and `ed_dsg_min`, and before `ed_rsg_max`.

Negative measured intensities are set to zero. When the data are loaded, a line is printed for each frame with the number of reflections kept, beams, structure factors used and integration steps. Frames with no reflections are removed.

1.9Bethe potentials

At each step of the integration, a beam is strong if it is the incident beam or a fitted reflection, or if its excitation error is within $\pm \text{ed_sg_bethe}$. The other beams are weak, and enter the structure matrix of the strong beams as Bethe potentials (Bethe, 1928):

$$M_{mn,eff} = M_{mn} - \sum_w \frac{M_{mw} M_{wn}}{M_{ww}}$$

m and n are strong beams, and only the matrix of the strong beams is diagonalised, so a large `ed_sg_max` adds little cost. The derivatives, however, still include the weak beams. The division into strong and weak beams is made when the beams are chosen, and it is repeated if a change in the frame rotations brings the excitation error of a weak beam within $\pm \text{ed_sg_bethe}/2$ at any integration step. With `ed_sg_bethe` set to zero, every beam is strong and the calculation is exact. `ed_sg_bethe`

may be an equation of `ed_num_beams`, the number of beams in the frame. This equation is evaluated for each frame at the start, and the default is:

```
ed_sg_bethe = If(Get(ed_num_beams) > 80, 0.008, 0);
```

This approach uses Bethe potentials for frames with more than 80 beams and calculates smaller frames exactly. Without Bethe potentials, refining the structure of glycine on 74 frames with an `ed_sg_max` of 0.05 took 652s. With `ed_sg_bethe` set to 0.008, the time drops to 19.6s. The change in Rwp is negligible, and the coordinates agree to within 10^{-5} . At `ed_sg_max` 0.05, the frames of glycine and albite reach the `ed_max_beams` limit of four hundred.

1.10Absorption

`ed_absorption` κ is frame dependent and sets the absorptive potential to κ times the potential. κ is written in the `xdd_ed` of the frame and can be refined. Every U_g then becomes

$$U_g \rightarrow (1 + i\kappa) U_g$$

A frame with absorption takes 2 to 3 times longer to calculate. On quartz, in QTZ-DYN-0.INP with the coordinates of O1 refined, κ increased from zero to 0.087 and Rwp changed from 13.18 to 13.02. Colmey et al. (2026) found that absorption is important for heavy atoms in thick crystals but negligible for quartz.

For electron data, `f0_f1_f11_atom` defines `f0`, `f1` and `f11` for a single atom type. `f0_f1_f11_atom` must be written inside the shared `str_dets` used by the frames. `f0` replaces the electron scattering factor f_e . `f1` is q , the partial charge of the atom type, in units of the electron charge. A positive q removes electrons from the atom. `f11` is κ_t , the absorption of the atom type, a dimensionless fraction of its scattering factor. q and κ_t can be refined. With $\kappa_t = \kappa$ for every atom type and `ed_absorption` 0, the result is that of `ed_absorption` κ . `f11` cannot be used with layers, modulation, magnetism, protein sites or `scale_occ`. A `str_dets` with `f11` cannot also be used by X-ray or neutron data. A `scale_occ` that changes from reflection to reflection cannot be used with `xdd_ed` frames or other single crystal data. With `f1`, the electron scattering factor of the atom type is replaced by

$$f_e(s) \rightarrow f_e(s) + q\Delta(s)$$

$\Delta(s)$ is the change in f_e per unit charge, taken from the ion scattering factors of section 1.3. $\Delta(s)$ is largest at small s . For `ed_data`, use the neutral atom name with `f1`: O, not O-2. `f1` cannot be used for C, N, P, S, B and Se, which have no ion in ATMSCAT.TXT.

On 20 frames of quartz, neutral atoms gave Rwp = 15.373. Fixed formal charges, +4 for Si and -2 for O, gave Rwp = 16.584. q for Si refined to 0.43, giving Rwp = 15.347. A neutral cell then sets q for O to -0.22.

Refined independently, q reached +0.66 for Si and -1.89 for O. To keep the cell neutral, the charges must be equations of a single refined `prm`.

For quartz, with one Si and two O atoms per formula unit, κ_i is refined for Si and O, and q for Si. The charge of O is minus half that of Si, which keeps the cell neutral:

```
prn q_Si 0.4 min -2 max 4
str_dets ed_str_dets {
  space_group P3221
  f0_f1_f11_atom Si f1 = q_Si;      f11 @ 0.1
  f0_f1_f11_atom O f1 = -q_Si / 2; f11 @ 0.1
  site Si1 x 1.000000 y 0.470511 z = 5/6; occ Si 1
    ADPs { 0.005939 0.006824 0.002087 0.002969 0.001812 0.000906 }
  site O1 x 0.852633 y 0.586703 z 0.619428 occ O 1
    ADPs { 0.004981 0.016649 0.013874 0.005758 -0.002919 0.003662 }
}
```

1.11Scale

A calculated intensity is a fraction of the incident beam, many orders of magnitude below the measured counts. On the first calculation, the intensities are multiplied for each frame by a factor that brings the refined **scale** of the frame close to one. This factor is computed once and then kept fixed. The factor is defined as follows.

$$k_f = \frac{\sum_r w_r I_r y_r}{\sum_r w_r I_r^2}, \quad w_r = \frac{1}{\sigma_r^2}$$

where I_r is the calculated intensity of reflection r of frame f before any **scale**, y_r the measured intensity and σ_r its standard uncertainty.

1.12.....Refinement and derivatives

Refined parameters can include structural parameters, two rotation parameters for each frame, thickness and absorption parameters for each crystal, and κ_i for each atom type. Lattice parameters are not refined. **bkg** and **fit_obj** are operational in ED data. A structure can be defined under a **str**, or, within a named **str_dets** object for shared use. **rigid** bodies, **occ_merge**, **scale_pks**, and penalties can all be used in the normal TOPAS manner. Additionally, electron diffraction data can be refined with X-ray or neutron single crystal or powder data.

The derivatives of the intensities with respect to a structural parameter is:

$$\frac{dI_r}{dp} = \sum_{\mathbf{g}} \frac{\partial I_r}{\partial F_{\mathbf{g},re}} \frac{\partial F_{\mathbf{g},re}}{\partial p} + \frac{\partial I_r}{\partial F_{\mathbf{g},im}} \frac{\partial F_{\mathbf{g},im}}{\partial p}$$

The sum runs over the structure factors in the structure matrix of the frame. A frame rotation θ changes only the diagonal of the structure matrix, so the derivative of an eigenvalue with respect to θ comes entirely from the eigenvectors that have already been calculated:

$$\frac{\partial 2K\gamma_j}{\partial \theta} = \sum_{\mathbf{g}} |C_{\mathbf{g}}^{(j)}|^2 \frac{\partial M_{\mathbf{g}\mathbf{g}}}{\partial \theta}$$

$$\frac{\partial \varphi_{\mathbf{g}}}{\partial t} = \sum_j 2\pi i \gamma_j C_{\mathbf{g}}^{(j)} \varepsilon_j \exp(2\pi i \gamma_j t)$$

All derivatives are analytical, and the structural derivatives are exact for both acentric and centrosymmetric structures. They were checked against finite differences for coordinates, occupancy, and beq, and in a separate test program for thickness, absorption, the absorptive structure factors, and the frame rotations. The results agree to one part in a million. In an acentric structure that uses **layers**, magnetism, modulation, or **scale_occ**, the structural derivatives are approximate. TOPAS prints a warning, and coordinates may converge more slowly.

1.13.....Frame orientations

The frame orientations from PETS2 are often wrong by 0.1 to 0.25°, and because reflections enter and leave the frame, the calculated intensities do not vary smoothly with orientation. Least-squares refinement of **ed_frame_rotate_x** and **ed_frame_rotate_y** is therefore slow. **ed_orient_search** instead searches for the best orientation of each frame, in the same way that Jana2020 uses a simplex.

At the first calculation, approximate rotations are determined for each frame. Any rotation defined by an equation is excluded from the search. The search begins on a coarse grid over ±R degrees and then proceeds more finely around the best grid points. The finer search can shift a rotation by as much as 1.25 R from its starting value. Each orientation tested is scored by the weighted sum of squares of the frame, with the frame **scale** fitted. The best orientation is kept, and the beams are reselected for that orientation. A rotation that is not refined keeps the value found, and the OUT file records it.

On the 74 glycine frames at forty-two steps, with the thickness fixed at 399 Å and the scales refined, Rwp reduced from 16.09 to 14.85 in twelve cycles. An **ed_orient_search** of 0.4 reaches 12.18 in 20s, and refinement after the search reaches an Rwp of 12.175.

1.14Input

PETS2 writes a CIF_PETS file for each crystal. It includes the cell, the wavelength, the orientation matrix **UB**, the zone axis, the angles of each frame, and the reflections, each tagged with its frame number. **#inp_from_cif_pets** reads this file and writes an **ed_crystal** followed by one **xdd_ed** for every frame. The generated frames use a **str_dets** named **ed_str_dets** and a **lat_prms** named **ed_lat_prms**, both of which must be defined in the INP file. Any settings such as **ed_g_max** that appear after **#inp_from_cif_pets** apply to the crystal it creates. The quartz example is:

```

iters 10
str_dets ed_str_dets {
  space_group P3221
  site Si1 x 1.000000 y 0.470511 z = 5/6; occ Si 1
    ADPs { 0.005939 0.006824 0.002087 0.002969 0.001812 0.000906 }
  site O1 x 0.852633 y 0.586703 z 0.619428 occ O 1
    ADPs { 0.004981 0.016649 0.013874 0.005758 -0.002919 0.003662 }
}
lat_prms ed_lat_prms { a 4.9226 b 4.9226 c 5.4003 al 90 be 90 ga 120 }
'-----
#inp_from_cif_pets "../quartz_dyn/200603-02-iEDT-1.00_dyn_s1m2.cif_pets"
ed_g_max 2
ed_sg_max 0.01
ed_sg_max_refine 0.1
ed_rsg_max 0.85
ed_dsg_min 0.0014
ed_num_integration_steps 42

```

For this file, `#inp_from_cif_pets` writes a thickness parameter and an absorption parameter, both named after the file, then the `ed_crystal` line, then the `xdd_ed` for frame 1:

```

prm ed_t_200603_02_iEDT_1_00_dyn_s1m2 500 min 20 max 5000
prm !ed_a_200603_02_iEDT_1_00_dyn_s1m2 0 min 0 max 1
ed_crystal "../quartz_dyn/200603-02-iEDT-1.00_dyn_s1m2.cif_pets"
xdd_ed "../quartz_dyn/200603-02-iEDT-1.00_dyn_s1m2.cif_pets"
  lam la 1 lo 0.0251
  ed_frame_number 1
  ed_alpha -49.197
  ed_thickness = ed_t_200603_02_iEDT_1_00_dyn_s1m2;
  ed_absorption = ed_a_200603_02_iEDT_1_00_dyn_s1m2;
  ed_frame_rotate_x 0
  ed_frame_rotate_y 0
  str use { ed_str_dets ed_lat_prms }
  scale @ 1
' and so on for the other frames

```

1.15.....Crystals

Several crystals can refine together by writing more than one `#inp_from_cif_pets`. Crystals that share a `str_dets` must share `lat_prms` and have the same wavelength and the same `ed_g_max`, or TOPAS stops with an error. Other `xdds`, such as X-ray powder data, can be refined with the crystals.

Several crystals can be refined together by writing more than one `#inp_from_cif_pets`. Crystals that share a `str_dets` must also share `lat_prms` and must have the same wavelength and the same `ed_g_max`, otherwise an error is thrown. Other `xdds`, such as X-ray powder data, can be refined together with the crystals.

1.16Agreement factors

At the end of a refinement TOPAS reports the agreement factors quoted in published dynamical refinements, for each crystal and, with several crystals, for all crystals together. They are calculated on $F = \sqrt{I}$, once for all reflections and once for the observed reflections, those with $I > 3\sigma(I)$:

$$R(F) = \frac{\sum |F_o - F_c|}{\sum F_o}, \quad wR(F) = \sqrt{\frac{\sum w_F (F_o - F_c)^2}{\sum w_F F_o^2}}$$

$$w_F = \frac{1}{\sigma_F^2 + (0.01 F_o)^2}, \quad \sigma_F = \frac{\sigma_I}{2\sqrt{\max(I_o, \sigma_I)}}$$

$$\text{GoF} = \sqrt{\frac{\sum w_F (F_o - F_c)^2}{N - N_p}}$$

where N is the number of reflections and N_p the number of refined parameters. With several crystals GoF is given only for all crystals together, because N_p is counted over the whole refinement, not for one crystal. For qtz-dyn-0.inp:

```
ED, on F = sqrt(I), observed I > 3 sigma(I), w = 1/(sigma(F)^2 + (0.01 F)^2)
crystal 1 ../quartz_dyn/200603-02-iEDT-1.00_dyn_s1m2.cif_pets: 99 frames, t 477.5, N
obs/all 1093/2476, R obs 7.625 all 16.155, wR obs 8.675 all 9.478, GoF obs 3.432 all 2.432
hand: 1332 of 2476 reflections nearer Iobs than with the other hand at the same
parameters (scale fitted again): z 3.78, adjusted 4.81, P 1.0000
```

1.17The absolute structure

For an acentric structure, the absolute structure is tested at the end of refinement for inversion by replacing F with F^* , with the **scale** of each frame again fitted. Following Klar et al. (2023), and with N the total number of reflections, N_+ is the number of reflections whose calculated intensity is closer to the observed intensity for the refined structure than for the inverted structure:

$$z = \frac{2N_+ - N}{\sqrt{N}}, \quad z_{adj} = \frac{2N_+ - N}{\sqrt{N - W}}$$

$$W = \sum \left[1 - \Phi \left(\frac{|I_c - I_{c,inv}|}{2\sigma_I} \right) \right]$$

Φ is the normal distribution function. A reflection whose two calculated intensities differ by much less than $\sigma(I)$ gives no information on the absolute structure. W is a weighted count of such reflections, and is subtracted from N . The report gives $P = \Phi(z_{adj})$. A positive z favours the hand refined. This test favours the hand refined. Klar et al. refines each hand separately and compares the two refinements; **ed_hand_out** and **ed_hand_compare** makes that comparison, passing the intensities of one refinement to the other in a file:

```

' refinement 1: the hand of the model
ed_hand_out "hand-1.txt"
' refinement 2: the same INP file, with ed_invert_hand 1 in every ed_crystal
ed_hand_out "hand-2.txt"
ed_hand_compare "hand-1.txt"

```

`ed_hand_out` writes the crystal, frame, hkl, observed and calculated intensity, σ and the hand of every reflection. `ed_hand_compare` reads such a file and matches its reflections to this refinement by crystal, frame and hkl. z is then reported as above, with N_+ counting the reflections whose calculated intensity is nearer the observed one in this refinement than in the other. A warning is given for reflections not found in the file, and of a file refined with the same hand. `ed_invert_hand` 1 fits the inverted structure by using F^* in place of F , and leaves the coordinates unchanged. The coordinates written by that refinement must therefore be inverted to give the structure fitted, and the report of the agreement factors notes this.

`ed_hand_out` writes the crystal, frame, hkl, observed and calculated intensity, σ , and the hand of every reflection. `ed_hand_compare` reads such a file and matches its reflections to the current refinement by crystal, frame, and hkl. z is then reported as above, with N_+ counting the reflections whose calculated intensity is closer to the observed one in this refinement than in the other. A warning is issued for reflections not found in the file, and for a file refined with the same hand. A `ed_invert_hand` of 1 fits the inverted structure by using F^* in place of F and leaves the coordinates unchanged. The coordinates written by that refinement must therefore be inverted to give the structure actually fitted, and the report of the agreement factors notes this.

For quartz, QTZ-DYN-0.INP gives an Rwp of 13.18 when the coordinates of O1 are refined with the published hand, and 15.57 when the hand is inverted. The test at the end of the refinement, against the other hand at the same parameters, gives $z = 4.02$ for the published hand. Comparing the two refinements with `ed_hand_compare` gives $z = 5.02$ in the refinement of the published hand and -5.02 in the inverted one.

1.18Refinement strategy

- > Start with `iters` 0 to check the frames, the beams and the first Rwp.
- > When the starting Rwp is poor, refine the frame `scale` parameters at a series of fixed `ed_thickness` values, for example every 100 Å, and then refine `ed_thickness` starting with a value that gave the lowest Rwp.
- > Raise `ed_num_integration_steps` (42 for glycine, 53 for albite) and correct the frame orientations with `ed_orient_search` 0.4 to 0.5. Refine on `ed_frame_rotate_x` and `ed_frame_rotate_y` afterwards.
- > Then refine the structure.
- > For an acentric crystal, refine each hand, the second with `ed_invert_hand` 1, and compare them with `ed_hand_out` and `ed_hand_compare`.

1.19Examples

Glycine: GLY-DYN-0.INP gives an Rwp of 16.4 on 75 frames (frame 76 is removed), using the model of the Jana2020 refinement and a starting thickness of 500 Å. GLY-DYN-1.INP keeps the 74 frames used in Jana2020 and gives an Rwp of 16.2 at the Jana2020 thickness of 402 Å. On those seventy-four frames, without Bethe potentials (`ed_sg_bethe` = 0), refining `ed_thickness` and the `scale` parameters gives a thickness of 397 Å. The frame orientations were then refined with 42 steps. The coordinates and ADPs of the non-hydrogen atoms were refined next and converged in three cycles. Rwp converged to 13.0 and the thickness to 429 Å; the largest shift of an atom from the Jana2020 positions is 0.013 Å for C1.

Quartz is acentric. With the reflections and frame orientations of the Jana2020 refinement, the published absolute structure gives an Rwp of 14.26 at 438 Å (Jana2020: 437.8 Å), and the inverted structure gives 16.91. QTZ-DYN-0.INP uses every frame and reaches an Rwp of 13.3 at 477 Å. Because the reflections of QTZ-DYN-0.INP differ from those of the Jana2020 refinement, the Rwp of 13.3 cannot be compared with 14.26 and 16.91.

Albite: three crystals, blocks 1, 2, and 5 of the Jana2020 refinement, were refined together, with one `ed_crystal` for each. The refined parameters were the `x`, `y`, `z` coordinates and `beq` of the thirteen sites, a `scale` for each of the 152 frames, and an `ed_thickness` for each crystal. The refinement used `ed_orient_search` 0.5, fifty-three integration steps, and Bethe potentials (`ed_sg_max` 0.02, `ed_sg_bethe` 0.005). R(F) obs was 9.16 and wR(F) obs 8.46, compared with 9.31 and 8.58 from Jana2020; for the three crystals individually, R(F) obs was 9.62, 7.89, and 9.54, compared with 9.68, 7.85, and 10.03.

1.20.....Limitations

- > An f' calculated from the displacement parameters of each atom is not implemented. In electron diffraction the absorptive form factor f' is the imaginary part of the atomic scattering factor, $f_e + if'$, and describes the absorption caused by thermal diffuse scattering; it is not the anomalous dispersion f' of X-ray diffraction. `ed_absorption` is the same as setting $f' = \kappa f_e$ for every atom, and the `f11` of `f0_f1_f11_atom` sets $f' = \kappa_i f_e$ for each atom type.
- > `Flack` cannot be used with `xdd_ed`. Instead, the absolute structure is found by comparing the two hands.

1.21.....Acknowledgement

Claude Opus 5.5, the AI model from Anthropic, played an important part in the mathematics. Working with the author, it contributed to the implementation of the Bloch wave calculation and its analytical derivatives, Bethe potentials, absorption and the tests of the absolute structure, the reader for CIF_PETS files and `#inp_from_cif_pets`, and the tests against the published Jana2020 refinements and against finite differences.

1.22.....References

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