

TOPAS V6

● (Joint) Bragg and PDF Refinements at Lightning Speed

All relevant TOPAS functionalities for Bragg refinements are available for PDF refinements as well, e.g.

Structure refinement and determination

- Simulated annealing
- Constraints, restraints, penalties, e.g.
 - (Semi)Rigid body modeling
 - Distortion mode refinements
- Small and big box modelling
- Shape refinements
- Instrument resolution functions

Multiple datasets

- Joint PDF / Bragg refinements
- Joint X-ray and neutron data refinements
- Joint single crystal and powder data refinements

