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Nota di contenuto   Extending the Reach of Powder Diffraction Modelling; Preface; Table of Contents; Advanced Input Files & Parametric Quantitative Analysis Using Topas; Problem Solving with the TOPAS Macro Language: Corrections and Constraints in Simulated Annealing and Rietveld Refinement; Robust Refinement as Implemented in TOPAS; In Situ Diffraction Studies: Thermal Decomposition of a Natural Plumbojarosite and the Development of Rietveld-Based Data Analysis Techniques Molecular Motion by Refinement of TLS Matrices from High Resolution Laboratory Powder Diffraction Data: Implementation in the Program TOPAS and Application to Crystalline NaphthaleneSimulated Annealing Approach for Global Minimum Verification in Modeling of Pressure-Volume Dependence by Equations of State Obtained by High-Pressure Diffraction; Direct Access to the Order Parameter: Parameterized Symmetry Modes and Rigid Body Movements as a Function of Temperature; "Powder 3D Parametric"- A program for Automated Sequential and Parametric Rietveld Refinement Using Topas
MEM Calculations on Apatites Containing Peroxide Using BAYMEM and TOPASProtein Powder Diffraction Analysis with TOPAS; Composition-Induced Microstrain Broadening: From Pattern Decomposition to whole

Powder Pattern Modelling Procedures; WPPM: Microstructural Analysis beyond the Rietveld Method; WPPM: Advances in the Modeling of Dislocation Line Broadening; Domain Size Analysis in the Rietveld Method; The Application of the Fundamental Parameters Approach as Implemented in TOPAS to Divergent Beam Powder Diffraction Data; Keywords Index; Authors Index

Sommario/riassunto

The main focus of this special topic volume is the development and possibilities of the MACRO language within TOPAS, with a specific session dedicated to WPPM. The collection is presented here in the form of a ""macro tutorial"" for the benefit of the entire powder diffraction community. More than a collection of standard scientific papers, the contributions to this special issue provide methods, tutorials and practical suggestions and solutions for the proper use of TOPAS and WPPM in a number of applications; ranging from the most common to the most refined and specific cases. Readers will fi