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| 1. Record Nr. | UNINA990000450240403321 |
| Autore | Coiffet, Philippe |
| Titolo | Les Robots / Philippe Coiffet |
| Pubbl/distr/stampa | France : Hermes publishing, ©1981 |
| ISBN | 2-86601-001-9 2-86601-002-7 |
| Descrizione fisica | 2 v. : ill. ; 24 cm |
| Disciplina | 629.892 |
| Locazione | DINEL |
| Collocazione | 10 D III 373 10 D III 374 |
| Lingua di pubblicazione | Francese |
| Formato | Materiale a stampa |
| Livello bibliografico | Monografia |
| Nota di contenuto | Tome 1.; Modelisation et commande; Tome 2.: Interaction avec l'environnement; |

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|-------------------------|---|
| 2. Record Nr. | UNINA9910462537503321 |
| Titolo | Extending the reach of powder diffraction modelling by user defined macros : special topic volume with invited peer reviewed papers only // edited by: Paolo Scardi and Robert E. Dinnebier |
| Pubbl/distr/stampa | Stafa-Zurich, Switzerland ; ; Enfield, New Hampshire : , : Trans Tech, , 2010 ©2010 |
| ISBN | 3-03813-333-7 |
| Descrizione fisica | 1 online resource (222 p.) |
| Collana | Materials science forum, , 0255-5476 ; ; volume 651 |
| Altri autori (Persone) | ScardiP (Paolo) DinnebierRobert E |
| Disciplina | 535/.42028551 |
| Soggetti | Diffraction - Mathematics Diffraction - Computer simulation Electronic books. |
| Lingua di pubblicazione | Inglese |
| Formato | Materiale a stampa |
| Livello bibliografico | Monografia |
| Note generali | Description based upon print version of record. |
| Nota di bibliografia | Includes bibliographical references and index. |
| 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
