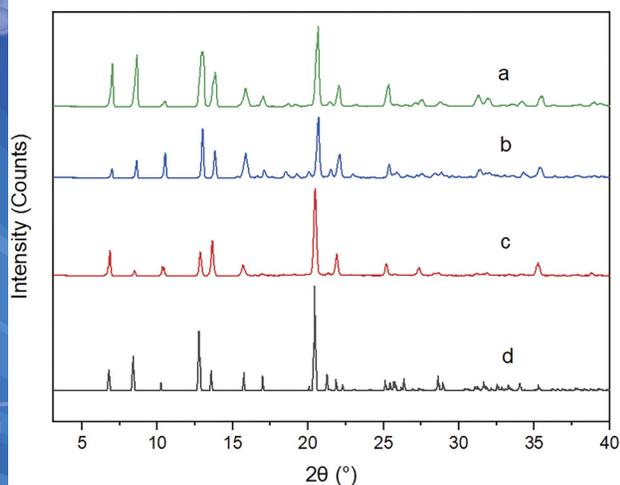


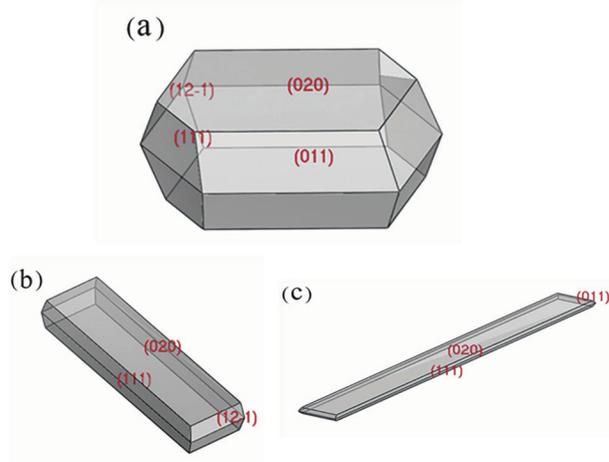
Powder Diffraction PDJ

Journal of Materials Characterization

Predicting Crystal Morphology of Venlafaxine Hydrochloride



PXRD patterns of precipitates from three solvents (a)–(c) and the calculated pattern (d) that is without preferred orientation.



Predicted crystal morphologies for each of the three precipitates

Volume 37 / Number 03 / September 2022

Powder Diffraction

Journal of Materials Characterization

Journal of the International Centre for Diffraction Data

<https://www.cambridge.org/core/journals/powder-diffraction>

Volume 37, Issues 1-4

eISSN: 1945-7413; ISSN: 0885-7156

Editor-in-Chief

Camden Hubbard, Applied Diffraction Services, USA

Managing Editor

Nicole Ernst Boris, International Centre for Diffraction Data, USA

Editors for New Diffraction Data

Stacy Gates-Rector, International Centre for Diffraction Data, USA

Soorya Kabekkodu, International Centre for Diffraction Data, USA

Associate Editor for New Diffraction Data

Frank Rotella, Argonne National Laboratory (Retired), USA

Editors

Xiaolong Chen, Institute of Physics, Chinese Academy of Sciences, China

José Miguel Delgado, Universidad de Los Andes, Venezuela

Norberto Masciocchi, Università dell'Insubria, Italy

Editors for Crystallography Education

James Kaduk, Poly Crystallography Inc., USA

Brian H. Toby, Argonne National Laboratory, USA

International Reports Editor

Winnie Wong-Ng, National Institute of Standards and Technology, USA

Calendar of Meetings and Workshops Editor

Gang Wang, Chinese Academy of Sciences, China

Advisory Board

Evgeny Antipov, Moscow State University, Russian Federation

Xiaolong Chen, Chinese Academy of Sciences, China

Jose Miguel Delgado, University de Los Andes, Venezuela

Steve Hillier, The James Hutton Institute, UK

Takashi Ida, Nagoya Institute of Technology, Japan

Matteo Leoni, University of Trento, Italy

Vanessa Peterson, Australian Nuclear Science and Technology Organisation, Australia

Mark Rodriguez, Sandia National Labs, USA

T.N. Guru Row, Indian Institute of Science, India

Allison Keene, Cambridge University Press, USA

Information about editors and editorial board members correct as of 1st January 2022. For the latest information please see <https://www.cambridge.org/core/journals/powder-diffraction/information/editorial-board>

Aims & Scope

ICDD's quarterly, and special topical issue, international journal, *Powder Diffraction*, focuses on materials characterization employing X-ray powder diffraction and related techniques. With feature articles covering a wide range of applications, from mineral analysis to epitaxial growth of thin films to advances in application software and hardware, this journal offers a wide range of practical applications. ICDD, in collaboration with the Denver X-ray Conference Organizing Committee, has increased services for the subscribers of Powder Diffraction and authors of Advances in X-ray Analysis. Beginning in 2006, ICDD offered a copy of the previous year's edition of AXA to Powder Diffraction institutional subscribers who receive both print and on-line versions. This effectively doubles the number of articles annually available to Powder Diffraction subscribers and significantly increases the circulation for the authors in Advances in X-ray Analysis.

Subject coverage includes:

- Techniques and procedures in X-ray powder diffractometry
- Advances in instrumentation
- Study of materials including organic materials, minerals, metals and thin film superconductors
- Publication of powder data on new materials

International Centre for Diffraction Data

The International Centre for Diffraction Data (ICDD®) is a non-profit scientific organization dedicated to collecting, editing, publishing, and distributing powder diffraction data for the identification of materials. The membership of the ICDD consists of worldwide representation from academe, government, and industry.

© International Centre for Diffraction Data

Published by Cambridge University Press.



EDITORIAL

- Camden R. Hubbard Recent readership and impact metrics for the Journal *Powder Diffraction* (PDJ) 121
doi:10.1017/S0885715622000306

TECHNICAL ARTICLES

- Winnie Wong-Ng, Yuqi Yang, YuCheng Lan, Guangyao Liu, Amrit Kafle, Weifang Liu, Jie Hou, Donald Windover, Qing Huang, Sergiy Krylyuk and James A. Kaduk Powder X-ray structural analysis and bandgap measurements for $(\text{Ca}_x\text{Sr}_{2-x})\text{MnWO}_6$ ($x = 0.25, 0.5, 0.75, 1.5, 1.75$) 122
doi:10.1017/S0885715622000185
- Chenjing Liang, Jianghai Zhuang, Chenghan Zhuang, Zhaoxia Zhang, Guanglie Lv and Guoqing Zhang Crystal morphology prediction and experimental verification of venlafaxine hydrochloride 133
doi:10.1017/S0885715622000264

NEW DIFFRACTION DATA

- James A. Kaduk, Stacy Gates-Rector, Amy M. Gindhart and Thomas N. Blanton Crystal structure of merimepodib, $\text{C}_{23}\text{H}_{24}\text{N}_4\text{O}_6$ 143
doi:10.1017/S0885715622000148
- Yewon Lee, Yulong Wang, Peter G. Khalifah, Peter W. Stephens, James A. Kaduk, Stacy Gates-Rector, Amy M. Gindhart and Thomas N. Blanton Crystal structure of baricitinib, $\text{C}_{16}\text{H}_{17}\text{N}_7\text{O}_2\text{S}$ 150
doi:10.1017/S088571562200015X
- James A. Kaduk, Nicholas C. Boaz, Stacy D. Gates-Rector, Amy M. Gindhart and Thomas N. Blanton Crystal structure of fulvestrant hydrate (ethyl acetate), $\text{C}_{32}\text{H}_{47}\text{F}_5\text{O}_3\text{S}(\text{H}_2\text{O})_{0.16}(\text{C}_4\text{H}_8\text{O}_2)_{0.025}$ 157
doi:10.1017/S0885715622000239
- Dier Shi, Jiyong Liu and Xiurong Hu Crystal structure and X-ray powder diffraction data for two solid-state forms of topiroxostat 166
doi:10.1017/S088571562200029X
- James A. Kaduk Crystal structure of alfuzosin hydrochloride, $\text{C}_{19}\text{H}_{28}\text{N}_5\text{O}_4\text{Cl}$ 171
doi:10.1017/S0885715622000288

INTERNATIONAL REPORT

- Susan A. Bourne ePCCr: an online conference organized jointly with the African Light Source and the African Physical Society 183
doi:10.1017/S0885715622000276

CALENDARS OF MEETINGS, SHORT COURSES AND WORKSHOPS

Gang Wang	Calendar of forthcoming meetings doi:10.1017/S0885715622000318	187
Gang Wang	Calendar of short courses and workshops doi:10.1017/S088571562200032X	188

On the Cover: In the manuscript "Crystal Morphology Prediction and Experimental Verification of Venlafaxine Hydrochloride" by C. Liang, *et al*, it was shown that modeling can be successfully used to predict the influence of solvent effects on crystal habit of venlafaxine hydrochloride. Modeling of habit of the precipitates was based on the modified attachment energy model using molecular dynamics simulation and was supported by showing the differences in the X-ray powder diffraction patterns of the three precipitates compared with the calculated pattern. Further, physical properties of the precipitates from the three solvents were shown to be related with the morphologies of the crystals.

LET OUR TEAM OF EXPERTS HELP YOU TAKE YOUR SKILLS TO THE NEXT LEVEL!



Fundamentals of X-ray Powder Diffraction Clinic:

For the novice with some XRD knowledge or for the experienced with an interest in the theory behind XRD, this clinic offers a strong base for increased lab performance.

The clinic covers instrumentation, specimen preparation, data acquisition and qualitative phase analysis through live demonstrations. It also covers hands-on use of personal computers for demonstration of the latest software including data mining with the Powder Diffraction File (PDF) and use of the powder diffractometer: optical arrangement, factors affecting instrumentation profile width, choice and function of divergence slit, calibration and alignment, detectors, and X-ray optics.

www.icdd.com/xrd



Advanced Methods in X-ray Powder Diffraction Clinic:

For the experienced XRD scientist, this session offers enhanced analysis skills through intense problem solving, as well as an introduction to the Rietveld Method. The course emphasizes computer-based methods of data interpretation, both for qualitative and quantitative phase analysis.

The advanced course covers a wide range of topics including systematic errors, factors affecting intensities of diffraction peaks; data reduction algorithms; phase identification; advanced data mining with the PDF and its application in search/match; powder pattern indexing methods; structure solution methods; quantitative phase analysis using both reference intensity ratio (RIR) and Rietveld Method.

www.icdd.com/xrd



Rietveld Refinement & Indexing Clinic:

Powder pattern indexing and Rietveld structural refinement techniques are complementary and are often combined to determine the structure of a material. Successful indexing of a powder pattern is considered strong evidence for phase purity. Indexing is considered a prelude to determining the crystal structure, and permits phase identification by lattice matching techniques. This clinic introduces the theory and formalisms of various indexing methods and structural refinement techniques along with quantitative analysis. One unique aspect of this clinic is the extensive use of computer laboratory problem solving and exercises that teach method development in a hands-on environment.

www.icdd.com/rietveld



Practical X-ray Fluorescence Clinic:

From theory to hands-on exercises, this course offers techniques and skills to improve lab performance. Discover the latest in cutting-edge instruments such as TXRF, hand-held devices, energy dispersive and wavelength dispersive spectrometers through live demonstrations.

The XRF course covers the basics of X-ray spectra; instrumentation design; methods of qualitative and quantitative analysis; specimen preparation and applications for both wavelength and energy dispersive spectrometry. The course emphasizes quantitative methods, use of automated X-ray spectrometers, review of mathematical matrix correction procedures, and new developments in XRF.

www.icdd.com/xrf

More information at www.icdd.com/icdd-education

Please note: A minimum of 10 registrants per course is required, otherwise the course will be cancelled and your registration fee will be refunded. You will be notified of a course cancellation no later than two weeks prior to the start of the course.

For More Information Contact:

Eileen Jennings, Education Coordinator
Tel: 610.325.9814 Fax: 610.325.9823
Email: clinics@icdd.com

Location

ICDD Headquarters
12 Campus Boulevard
Newtown Square, Pennsylvania 19073-3273 USA



