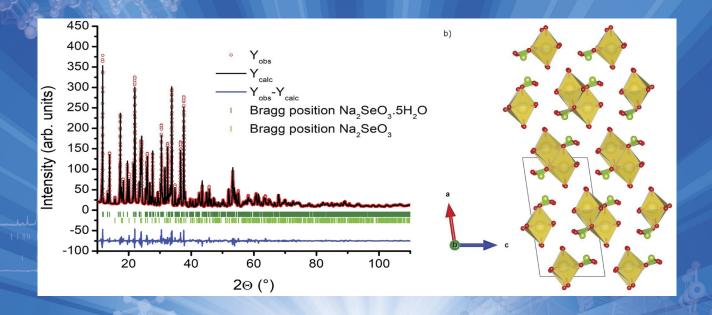
# Powder Diffraction PDJ Journal of Materials Characterization



Volume 38 / Number 03 / September 2023





#### **Powder Diffraction**

Journal of Materials Characterization

Journal of the International Centre for Diffraction Data https://www.cambridge.org/core/journals/powder-diffraction Volume 38, 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

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 epitactic 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**

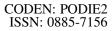
The International Centre for Diffraction Data (ICDD®) is a non-profit scientific organization dedicated to collecting, editing, publishing, and distributing powder diffraction data for the identification of materials. The membership of the ICDD consists of worldwide representation from academe, government,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

© International Centre for Diffraction Data

Published by Cambridge University Press.







168

180

185

194

201

207

215

220

224

231



# **EDITORIAL**

Camden Richards Hubbard Powder Diffraction journal editors Miguel Delgado and Xiaolong Chen awarded the 167

2023 ICDD Distinguished Fellow award

doi:10.1017/S0885715623000325

# **TECHNICAL ARTICLES**

Fabio F. Ferreira, Aline P. C. Pereira, Ianny B. Reis, Bianca R. S. Sasaki, Wagner J. Fávaro and Nelson Durán Quantitative phase analysis of commercial ammonium phosphates by PXRD for

application in biological systems doi:10.1017/S0885715623000167

Gwilherm Nénert A new polymorphic form of Na<sub>2</sub>SeO<sub>3</sub>·5H<sub>2</sub>O: structure determination from X-ray

laboratory powder diffraction doi:10.1017/S0885715623000301

# **NEW DIFFRACTION DATA**

Tawnee M. Ens, James A. Kaduk, Anya Vieira Dosen and Thomas N. Blanton Crystal structure of meglumine diatrizoate, (C<sub>7</sub>H<sub>18</sub>NO<sub>5</sub>)(C<sub>11</sub>H<sub>8</sub>I<sub>3</sub>N<sub>2</sub>O<sub>4</sub>)

doi:10.1017/S0885715623000180

Tawnee M. Ens, James A. Kaduk, Anja Dosen and Thomas N. Blanton Crystal structure of danofloxacin mesylate (C<sub>19</sub>H<sub>21</sub>FN<sub>3</sub>O<sub>3</sub>)(CH<sub>3</sub>O<sub>3</sub>S)

doi:10.1017/S0885715623000271

Anastasia Gorodnova, Vladimir N. Ivanov, Alexander V. Kurkin and Crystal structure of 5-(3-methoxyphenyl)indoline-2,3-dione

doi:10.1017/S0885715623000192

Artem Dmitrienko

James A. Kaduk,

Crystal structure of calcium L-5-methyltetrahydrofolate trihydrate type I,

Nilan V. Patel and  $C_{20}H_{23}N_7O_6Ca(H_2O)_3$ 

Joseph T. Golab doi:10.1017/S0885715623000246

Liuqing Liang, Weijun Li, Meiwen Lu, Sheng Li, Degui Li and Bin Gu Experimental synthesis and crystal structure refinement of a new ternary intermetallic

compound Al<sub>3</sub>GaCu<sub>9</sub>

doi:10.1017/S0885715623000155

Xiang Xu, Chongxin Liu,

Kang Wu and Hongxiang Chen Crystal structure and X-ray powder diffraction data of barium copper iodate

 $Ba_2Cu(IO_3)_6$ 

doi:10.1017/S0885715623000258

Joel W. Reid Synchrotron powder diffraction data for some smectite clay mineral standards

doi:10.1017/S0885715623000283

# CALENDARS OF MEETINGS, SHORT COURSES AND WORKSHOPS

Gang Wang Calendar of Forthcoming Meetings

doi:10.1017/S088571562300026X

On the Cover: The cover figure was prepared using figures from the manuscript "A New Polymorphic Form of  $Na_2SeO_3 \cdot 5H_2O$ : Structure Determination From X-ray Laboratory Powder Diffraction" by Gwilherm Nénert of Malvern Panalytical B. V. The  $\Box$ -sodium selenate pentahydrate is a new polymorph differing from the alpha sodium selenate pentahydrate and related structures. This pentahydrate polymorph was found to readily loses its water of crystallization and thus the powder pattern is that of a mixture of the pentahydrate and that of  $Na_2SeO_3$ .