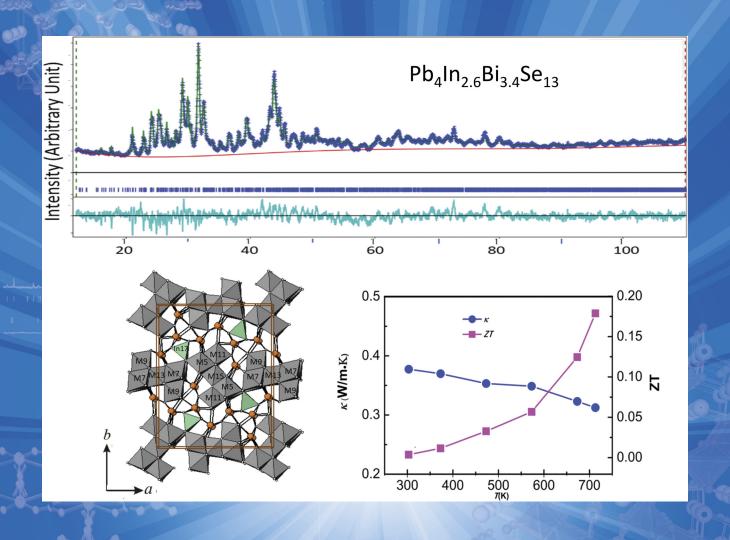
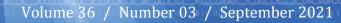
# Powder Diffraction PDJ Journal of Materials Characterization

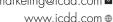
















# **WORKING TOGETHER**

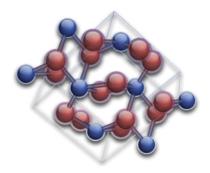
# **FOR YOU**

With over 1,000,000 patterns available at your fingertips, ICDD's PDF® databases and MDI's JADE® software work together to make your life easier. Let the software work for the science and take your results further.



### **ABOUT US**

For over 30 years, The ICDD and MDI have worked together in a complementary manner since MDI began in 1987. The XRD community has trusted MDI to provide unbiased results and help interpret both the everyday and the difficult XRD data. We are proud of our products and the daily effort we put forth towards advancing the science of XRD. Materials Data creates XRD software applications to collect, analyze, and simulate XRD data. These products are here to help solve issues in an enormous array of materials science projects, and may be found in labs around the world with data collected on virtually every brand of XRD equipment.



## **OUR PRODUCTS**



#### PDF-4

#### **Phase Identification and Quantitation**

The world's largest sources of inorganic diffraction data from crystals and powders in a single database featuring 460,900+ entries, including 353,300+ entries with atomic coordinates.



#### PDF-4+/Web

#### Data on the Go

Provides portability to the PDF-4+ database via the internet.



#### PDF-4/Axiom

#### **Quality Plus Value**

Phase identification and quantitation that requires diffraction equipment manufacturer or vendor software.



#### PDF-2

#### **Phase Identification + Value**

Quality and subfile filters combined with 71 different searches and 57 display fields enable you to target your results for more accurate identification.



#### PDF-4/Organics

#### **Solve Difficult Problems, Get Better Results**

Designed to solve difficult problems that are analyzed by powder diffraction analysis for a multitude of applications in the pharmaceutical, regulatory, specialty chemical, biomaterial, and forensic fields.



#### **PDF-4/Minerals**

#### Comprehensive Mineral Collection

Ninety-seven percent of all known mineral types, as defined by the International Mineralogical Association (IMA), are represented in the database, as well as many unclassified minerals.



#### **JADE Pro**

#### **JADE Works The Way You Do**

Automate your analysis with JADE. In so many cases, it's just one click and you're done. Often these results are better than those an experienced analyst could report and in a more timely manner.

For more information contact ICDD at marketing@icdd.com















#### **EDITORIAL** Camden Hubbard Editorial 147 TECHNICAL ARTICLE 148 Carina Schlesinger, Crystal structure of the anticancer drug carmustine determined by X-ray powder Edith Alig and diffraction Martin U. Schmidt W. Wong-Ng, J. Guo, Structural and thermoelectric properties of Pb<sub>4</sub>In<sub>2.6</sub>Bi<sub>3.4</sub>Se<sub>13</sub> 151 Y. Yan and J. A. Kaduk REVIEW ARTICLE Hideo Toraya Review of the direct derivation method: quantitative phase analysis with observed 159 intensities and chemical composition data PROCEEDINGS PAPER Takashi Ida 169 Equatorial aberration for powder diffraction data collected by continuous-scan integration of a silicon strip X-ray detector **NEW DIFFRACTION DATA** A. O. Dmitrienko, Crystal structure of 3-[(3,4-dinitro-1*H*-pyrazol-1-yl)-*NNO*-azoxy]-4-nitro-1,2,5-176 oxadiazole A. A. Konnov and M. S. Klenov Crystal structure of levocetirizine dihydrochloride Form I, C21H27ClN2O3Cl2 James A. Kaduk, 181 Amy M. Gindhart and Thomas N. Blanton Joel W. Reid Powder X-ray diffraction data for dimethylarsinic acid, (CH<sub>3</sub>)<sub>2</sub>AsO(OH) 190 James A. Kaduk, Crystal structure of palbociclib isethionate Form B, (C<sub>24</sub>H<sub>30</sub>N<sub>7</sub>O<sub>2</sub>)(C<sub>2</sub>H<sub>5</sub>O<sub>4</sub>S) 196 Amy M. Gindhart and Thomas N. Blanton DATA REPORT Powder X-ray diffraction of varenicline hydrogen tartrate Form B (Chantix®), James A. Kaduk, 202 Amy M. Gindhart and $(C_{13}H_{14}N_3)(HC_4H_4O_6)$ Thomas N. Blanton James A. Kaduk, Powder X-ray diffraction of pazopanib hydrochloride Form 1, C<sub>21</sub>H<sub>24</sub>N<sub>7</sub>O<sub>2</sub>SCl 205 Amy M. Gindhart and

Thomas N. Blanton

Ryan L. Hodge, James A. Kaduk, Amy M. Gindhart and Thomas N. Blanton	Powder X-ray diffraction of daclatasvir dihydrochloride Form N-2 (Daklinza®), $C_{40}H_{52}N_8O_6Cl_2$	208	
CRYSTALLOGRAPHY EDUCATION NOTE			
Stephanie Jennings	ICDD® InSession: Mastering the PDF® Database and JADE® Software	212	
CALENDARS OF MEETINGS, SHORT COURSES AND WORKSHOPS			
Gang Wang	Calendar of Forthcoming Meetings	213	
Gang Wang	Calendar of Short Courses and Workshops	214	
ADDENDUM			
Yali Su, Dayong Lu and Shan Wang	Characterization and Rietveld refinements of new dense ceramics $Ba_{3-x}Sr_xTb_{3-x}Ce_xO_9$ ( $x = 1$ and 1.5) perovskites – ADDENDUM	215	
G. Murugesan, R. Nithya and S. Kalainathan	Rietveld refinement of $Sm_{0.55}Sr_{0.45}Mn_{0.4}Fe_{0.6}O_3$ – ADDENDUM	216	
CORRIGENDUM  W. Wong-Ng, G. Y. Liu, D. D. Shi, Y. Q. Yang, R. Derbeshi, D. Windover and J. A. Kaduk	Crystal chemistry, X-ray diffraction reference patterns, and bandgap studies for $(Ba_xSr_{1-x})_2CoWO_6$ ( $x = 0.1, 0.2, 0.3, 0.5, 0.7, and 0.9$ ) – CORRIGENDUM	217	
ERRATUM			
Gerald Falkenberg, Frank Seiboth, Frieder Koch, Ken Vidar Falch, Andreas Schropp, Dennis Brückner and Jan Garrevoet	CRL optics and silicon drift detector for P06 Microprobe experiments at 35 keV — ERRATUM	218	
Analio J. Dugarte-Dugarte, Jacco van de Streek, Graciela Díaz de Delgado, Alicja Rafalska-Lasocha and José Miguel Delgado	Crystal structure from laboratory X-ray powder diffraction data, DFT-D calculations, Hirshfeld surface analysis, and energy frameworks of a new polymorph of 1-benzothiophene-2-carboxylic acid — ERRATUM	219	



#### An International Journal of Materials Characterization

Editor-in-Chief

Camden Hubbard Applied Diffraction Services, U.S.A. camden.hubbard@me.com

**Managing Editor** 

Nicole M. Ernst Boris International Centre for Diffraction Data, U.S.A. boris@icdd.com

**Content Editor** 

Kayla Riddleberger Cambridge University Press, U.S.A. kriddleberger@cambridge.org

#### **Editors for New Diffraction Data**

Soorya Kabekkodu International Centre for Diffraction Data, U.S.A. kabekkodu@icdd.com

Stacy Gates-Rector International Centre for Diffraction Data, U.S.A. gates-rector@icdd.com

#### Associate Editor for New Diffraction Data

Frank J. Rotella Argonne National Laboratory (Retired), U.S.A. fjrotella1949@gmail.com

#### **Editors**

Xiaolong Chen Institute of Physics, Chinese Academy of Sciences, China xlchen@iphy.ac.cn

José Miguel Delgado Universidad de Los Andes, Venezuela migueld@ula.ve

Norberto Masciocchi Universitá dell'Insubria, Italy norberto.masciocchi@uninsubria.it

#### **Editors for Crystallography Education**

James Kaduk Poly Crystallography Inc., U.S.A. Kaduk@polycrystallography.com

Brian H. Toby Argonne National Laboratory, U.S.A. brian.toby@anl.gov

#### International Reports Editor

Winnie Wong-Ng National Institute of Standards and Technology, U.S.A. winnie.wong-ng@nist.gov

#### Calendar of Meetings and Workshops Editor

Gang Wang Institute of Physics, Chinese Academy of Sciences, China gangwang@iphy.ac.cn

The Advisory Board is served by the International Centre for Diffraction Data's Regional Co-Chairs and representatives from Cambridge University Press.

Advisory Board Mark Rodriguez Takashi Ida Matteo Leoni T.N. Guru Row Vanessa Peterson

**Evgeny Antipov** 

Sandia National Labs, U.S.A Nagoya Institute of Technology, Japan University of Trento, Italy Indian Institute of Science, India Australian Nuclear Science and Technology

Organisation, Australia Moscow State University, Russa Chinese Academy of Sciences, People's

Xiaolong Chen Republic of China

Jose Miguel Delgado Steve Hillier University de Los Andes, Venezuela The James Hutton Institute, Scotland, UK Cambridge University Press, U.S.A. Sara Yanny-Tillar

On the Cover: The cover figures come from the article "Structural and Thermoelectric Properties of  $Pb_4ln_{2.6}Bi_{3.4}Se_{13}$ " by W. Wong-Ng, Y. Yan, J. Guo, and J. Kaduk. The compound was prepared by solid-state techniques, and the structure was determined using powder X-ray diffraction methods. The low figure of merit (ZT) of about 0.175 at 700 K is low compared to that of commercial thermal electric Bi<sub>2</sub>Ti<sub>3</sub>.

Powder Diffraction is a journal of practical technique, publishing articles relating to the widest range of application—from materials analysis to epitactic growth of thin films and to the latest advances in software. Although practice will be emphasized, theory will not be neglected, especially as its discussion will relate to better understanding of technique.

Submit manuscripts online at http://mc.manuscriptcentral.com/pdj. See the instructions on submitting your manuscript linked on that page. The editors will consider all manuscripts received, but assume no responsibility regarding them. There is no publication charge.

Most proofs are handled via email at kriddleberger@cambridge.org. Please include the job number in all correspondence.

For advertising rates and schedules contact M.J. Mrvica Associates, 2 West Taunton Avenue, Berlin, NJ 08009; Phone: 856-768-9360; Fax: 856-753-0064; Email: mjmrvica@mrvica.com

Subscription Prices 2021			
	Print & Online	Online	
Individual (U.S. & Canada)	\$269	\$190	
Individual (outside U.S. & Canada)	£208	£146	
Student	N/A	\$42	
Institutional or Library	\$536	\$324	

Subscription rates to Eastern Hemisphere include air freight service.

Back-Number Prices. 2020 single copies: \$158.

**Subscription, renewals, and address changes** should be addressed to Subscription Fulfillment, *Powder Diffraction*, Cambridge University Press, One Liberty Plaza, 20th floor New York, NY 10006-1435 (for U.S.A., Canada, and Mexico); or Cambridge University Press, The Edinburgh Building, Shaftsbury Road, Cambridge, CB2 8RU, Cambridge, England (for UK and elsewhere). Allow at least its works advance police. For address changes places could both old and now six weeks advance notice. For address changes please send both old and new addresses and, if possible, include a mailing label from the wrapper of a recent issue.

Claims, Single Copy Replacement, Back Volumes, and Reprints: Missing issue requests will be honored only if received within six months of publication date (nine months for Australia and Asia). Single copies of a journal may be ordered and back volumes are available in print or microform. Individual subscribers please contact Subscription Fulfillment, *Powder Diffraction*, One Liberty Plaza, 20th floor New York, NY 10006-1435. Phone: 845-353-7500; Toll free: 800-872-7423; Fax: 845-353-4141. Email: subscriptions\_newyork@cambridge.org.

Powder Diffraction (ISSN: 0885-7156) is published quarterly (4X annually) by the JCPDS-International Centre for Diffraction Data through Cambridge University Press, One Liberty Plaza, 20th floor, New York, NY 10006. Periodicals postage rate paid at New York, NY, and at additional mailing offices. POSTMASTER: Send address changes in the USA, Canada, and Mexico to: Powder Diffraction, Cambridge University Press, Journals Fulfillment Department, One Liberty Plaza, 20th floor, New York, NY 10006. Send address changes elsewhere to Powder Diffraction, Cambridge University Press, Journals Fulfillment Department, UPH, Shaftesbury Road, Cambridge CB2 8BS, England.

Permission for Other Use: Permission is granted to quote from the journal with the customary acknowledgment of the source. To reprint a figure, table, or other excerpt requires the consent of one of the authors and notification to Cambridge University Press.

Requests for Permission: No part of this publication may be reproduced in any forms or by any means, electronic, photocopying, or otherwise, without permission in writing from Cambridge University Press. Policies, request forms, and contacts are available at: http://www.cambridge.org/about-us/rights-permissions/. Permission to copy (for users in the U.S.A.) is available from Copyright Clearance Center: http://www.copyright.com. Email: info@copyright.com.

**Document Delivery and Online Availability:** Abstracts of journal articles published by Cambridge University Press are available from Cambridge Core (https://www.cambridge.org/pdj).

Copyright © 2021 JCPDS- International Centre for Diffraction Data, 12 Campus Blvd., Newtown Square, PA 19073-3273, U.S.A. All rights reserved. www.icdd. com/products/journals.htm

# GRANT-IN-AID FUNDS ARE AVAILABLE DO NOT DELAY!

Proposal Submission Deadlines 31 January and 31 July

Does your research project involve the preparation and characterization of new materials using powder diffraction techniques?

If the answer is YES, then ICDD's Grant Program is the perfect fit for you!

https://www.icdd.com/grant-in-aid

Please email sample patterns to:

Denise DelCasale ICDD Grant-in-Aid Coordinator Delcasale@icdd.com

ICDD for over *80 years* has been dedicated to collecting, editing, publishing, and distributing powder diffraction data for the identification of crystalline materials. To assist us in this growth, ICDD has called on researchers from around the world to contribute their experimental data. In return, ICDD supports their efforts by funds provided through our Grant-in-Aid Program.



#### ICDD's approved grantees receive these additional benefits:

- A 50% price reduction on a PDF-4+ or PDF-4/Organics product
- · Financial support to aid current research projects
- Publication of pattern(s) in the Powder Diffraction File™ (PDF®)
   once approved by the Editorial Department
- Acknowledgement of your publication in the PDF with a certificate
- First-time grantees receive a complimentary one-year subscription to Powder Diffraction Journal

