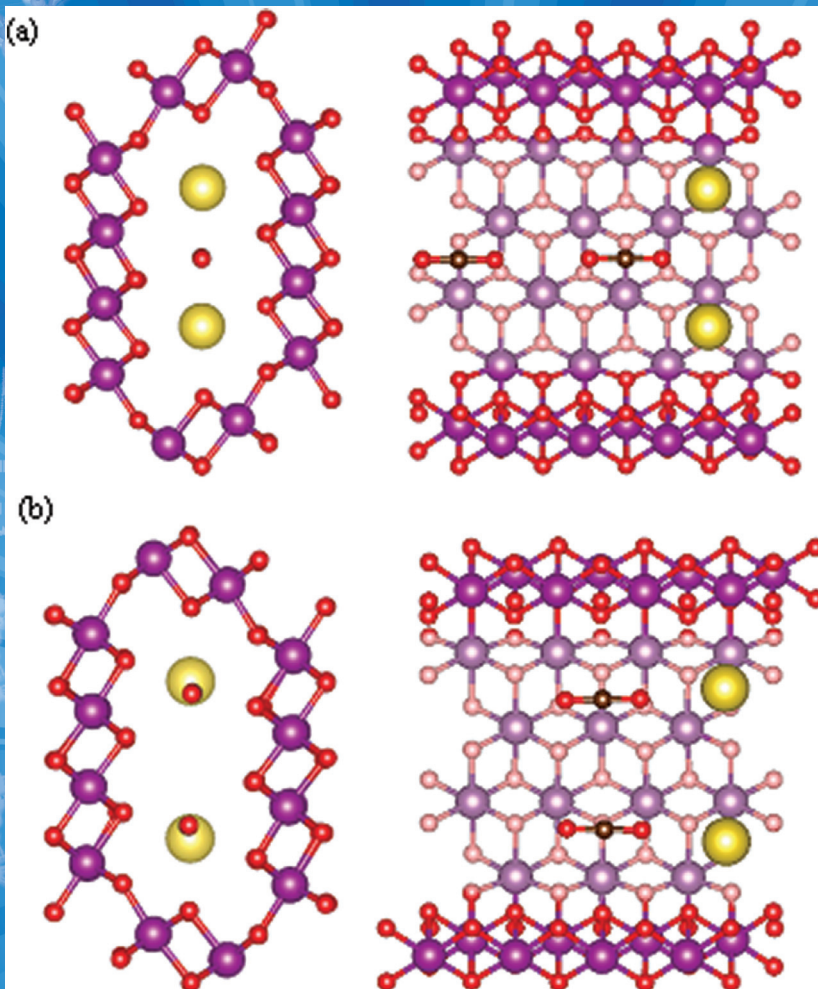
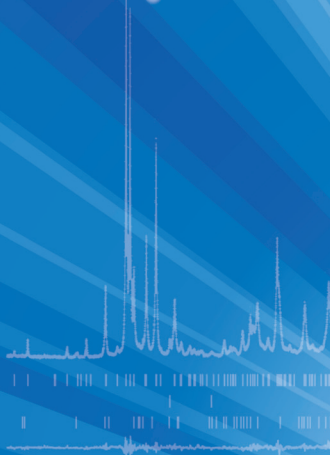
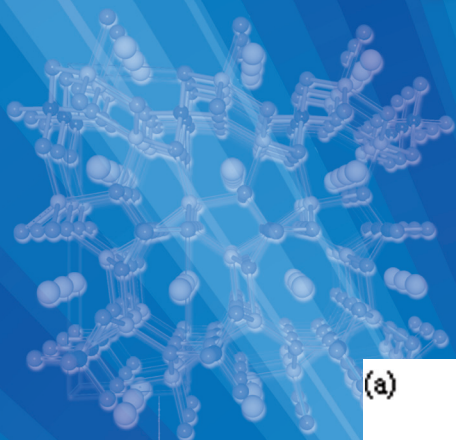


Powder Diffraction PDJ

Journal of Materials Characterization



CAMBRIDGE
UNIVERSITY PRESS

Volume 34 / Number 01 / March 2019

Published online by Cambridge University Press

Diffraction Data You Can Trust

ICDD databases are the only crystallographic databases in the world with quality marks and quality review processes that are ISO certified.

PDF-4/Axiom

NEW!

Focused Identification and Quantitation

87,988 Entries
59,683 Atomic coordinates

Cost Effective
3 Year License

Combines
Powder and
Single Crystal
Data

Two Additional
Seats - Low Cost

Requires
Vendor
Software

Standardized Data

All Data Sets Evaluated For Quality

Reviewed, Edited and Corrected Prior To Publication

Targeted For Material Identification and Characterization

www.icdd.com



www.icdd.com | marketing@icdd.com

ICDD, the ICDD logo and PDF are registered in the U.S. Patent and Trademark Office. Powder Diffraction File is a trademark of JCPDS - International Centre for Diffraction Data ©2019 JCPDS-International Centre for Diffraction Data - 01/19

EDITORIAL

Camden Hubbard	Metal Organic Framework papers are a select set of papers in this issue	1
Craig Brown and Winnie Wong-Ng	Special section: crystallography and properties of metal organic framework (MOF) compounds	2

REVIEW ARTICLE

John B Parise, Xianyin Chen, Anna M. Plonka, William R. Woerner, Debasis Banerjee, David Connors and Nancy Goroff	XRD-DSC: a screening tool for identifying effective MOFs for selective gas sorption from humid gas streams	3
---	--	---

TECHNICAL ARTICLES

Matthew Lawson, Jarod Horn, Winnie Wong-Ng, Laura Espinal, Saul H. Lapidus, Huong Giang Nguyen, Yongtao Meng, Steven L. Suib, James A. Kaduk and Lan Li	First-principles study of carbon capture and storage properties of porous MnO ₂ octahedral molecular sieve OMS-5	13
B. H. O'Connor, R. M. Clarke and J. A. Kimpton	Synchrotron radiation diffraction study of the mineral moolooite, and synthetic copper oxalates	21
Austin M. Wheatley and James A. Kaduk	Crystal structures of ammonium citrates	35
Joel W. Reid, James A. Kaduk and Lidia Matei	The crystal structure of MoO ₂ (O ₂)(H ₂ O)·H ₂ O	44

NEW DIFFRACTION DATA

James A. Kaduk, Nicholas C. Boaz, Amy M. Gindhart and Thomas N. Blanton	Crystal structure of oxybutynin hydrochloride hemihydrate, C ₂₂ H ₃₂ NO ₃ Cl(H ₂ O) _{0.5}	50
Austin M. Wheatley, James A. Kaduk, Amy M. Gindhart and Thomas N. Blanton	Crystal structure of minocycline hydrochloride dihydrate form A, C ₂₃ H ₂₈ N ₃ O ₇ Cl(H ₂ O) ₂	59
Jordan A. Krueger, James A. Kaduk, Amy M. Gindhart and Thomas N. Blanton	Crystal structure of hydroxyzine dihydrochloride, C ₂₁ H ₂₉ ClN ₂ O ₂ Cl ₂	66

RAPID COMMUNICATION

J. A. Kaduk, K. Zhong, T. N. Blanton, S. Gates-Rector and T. G. Fawcett	Powder X-ray diffraction of bendamustine hydrochloride monohydrate, $C_{16}H_{22}Cl_2N_3O_2Cl \cdot H_2O$	74
---	--	----

INTERNATIONAL REPORTS

Denise Zulli	67th Annual Denver X-ray Conference Report	76
Cindy Bolme, Gilliss Dyer and Siegfried Glenzer	Sixth user workshop on high-power lasers at the linac coherent light source	79

CALENDARS

Gang Wang	Calendar of short courses and workshops	85
Gang Wang	Calendar of forthcoming meetings	87

Powder Diffraction

An International Journal of Materials Characterization

Editor-in-Chief

Camden Hubbard
Applied Diffraction Services
110 Crestview Lane
Oak Ridge, Tennessee 37830, U.S.A.
camden.hubbard@me.com

Managing Editor

Nicole M. Ernst Boris
International Centre for Diffraction Data
12 Campus Boulevard
Newtown Square, Pennsylvania 19073-3273, U.S.A.
boris@icdd.com

Editors for New Diffraction Data

Soorya Kabekkodu
International Centre for Diffraction Data
12 Campus Boulevard
Newtown Square, Pennsylvania 19073-3273, U.S.A.
kabekkodu@icdd.com

Stacy Gates-Rector
International Centre for Diffraction Data
12 Campus Boulevard
Newtown Square, Pennsylvania 19073-3273, U.S.A.
gates-rector@icdd.com

Associate Editor for New Diffraction Data

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

Editors

Xiaolong Chen
Institute of Physics
Chinese Academy of Sciences
No. 8 Nanshanjie, Zhongguancun, Haidian District,
Beijing 100190,
China
xlchen@iphy.ac.cn

José Miguel Delgado
Universidad de Los Andes
Facultad de Ciencias
Departamento de Química
Lab. de Cristalografía
Mérida 5101
Venezuela
miguel@ula.ve

Norberto Masciocchi
Università dell'Insubria
Dipartimento di Scienza e Alta Tecnologia
via Valleggio 11
Como 22100
Italy
norberto.masciocchi@uninsubria.it

Editors for Crystallography Education

James Kaduk
Poly Crystallography Inc.
423 East Chicago Avenue
Naperville, Illinois 60540-5407, U.S.A.
Kaduk@polycrystallography.com

Brian H. Toby
Argonne National Laboratory
Advanced Photon Source
9700 S. Cass Ave., Bldg. 401/B4192,
Argonne, Illinois 60439-4856, U.S.A.
brian.toby@anl.gov

International Reports Editor

Winnie Wong-Ng
Materials Measurement Science Division
National Institute of Standards and Technology
100 Bureau Drive, Mail Stop 8520
Gaithersburg, MD 20899-8520, U.S.A.
winnie.wong-ng@nist.gov

Calendar of Meetings and Workshops Editor

Gang Wang
Institute of Physics
Chinese Academy of Sciences
No. 8 Nanshanjie, Zhongguancun, Haidian District,
Beijing 100190,
China
gangwang@iphy.ac.cn

On the Cover: This Issue's cover shows three Figures from the manuscript "Evolution in the structure of akaganeite and hematite during hydrothermal growth: An *in situ* synchrotron X-ray diffraction analysis" by Kristina M. Peterson, Peter J. Heaney and Jeffrey E. Post. Their paper reports the temperature-time resolved studies of hydrothermal precipitation of akaganeite (b-FeOOH) as it is precipitated and then transformed to hematite (Fe₂O₃) using time resolved synchrotron X-Ray diffraction as a function of temperature.

Powder Diffraction is a quarterly journal published by the JCPDS-International Centre for Diffraction Data through Cambridge University Press.

Powder Diffraction is a journal of practical technique, publishing articles relating to the widest range of application—from materials analysis to epitaxial 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 2019

	Print & Online	Online
Individual (U.S. & Canada)	\$248	\$175
Individual (outside U.S. & Canada)	£192	£135
Student	N/A	\$38
Institutional or Library	\$496	\$300

Subscription rates to Eastern Hemisphere include air freight service.

Back-Number Prices. 2018 single copies: \$136.

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, Shaftesbury Road, Cambridge, CB2 8RU, Cambridge, England (for UK and elsewhere). Allow at least 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 © 2019 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

NEW LOWER PRICING!

Take Advantage of ICDD's New Combo Site License
for PDF-4+ and PDF-4/Organics



Improve Your Analyses with the Most Comprehensive
Inorganic and Organic Databases for Powder Diffraction!

The combo site license allows you to purchase a PDF-4+, WebPDF-4+,
or PDF-4/Organics database in one site.

We lowered our prices for Site/Multi-year licenses!

Now is the best time to purchase your Site or Combo Site License/
Multi-year License at discounted pricing!

Visit ICDD's website for our new pricing.
Contact sales@icdd.com for sales quote.



www.icdd.com | sales@icdd.com

ICDD, the ICDD logo and PDF are registered in the U.S. Patent and Trademark Office.
Powder Diffraction File is a trademark of JCPDS - International Centre for Diffraction Data
©2018 JCPDS-International Centre for Diffraction Data - 7/18