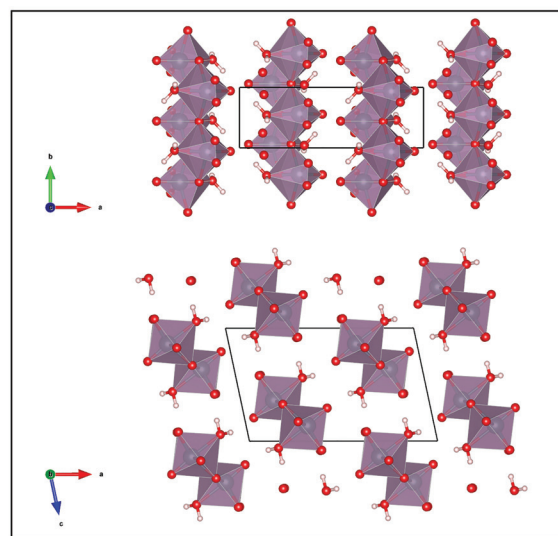
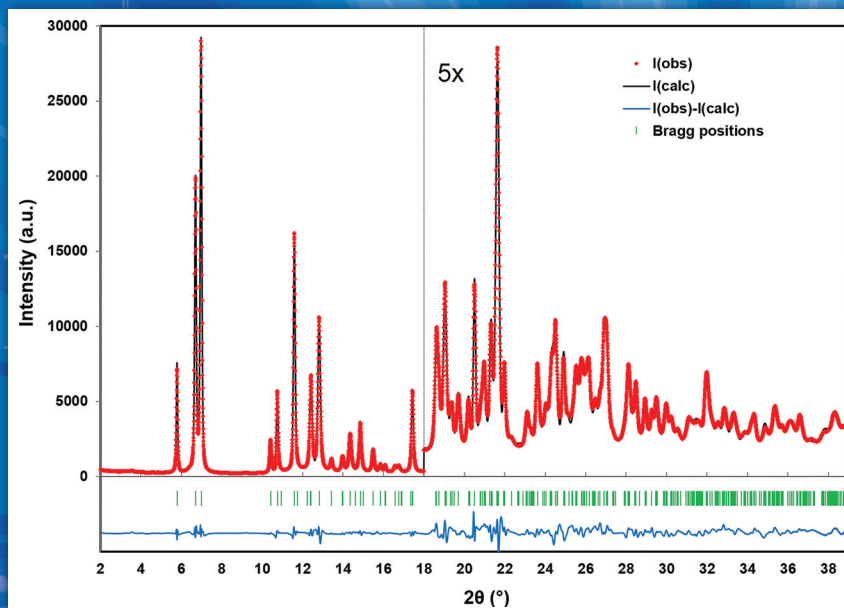
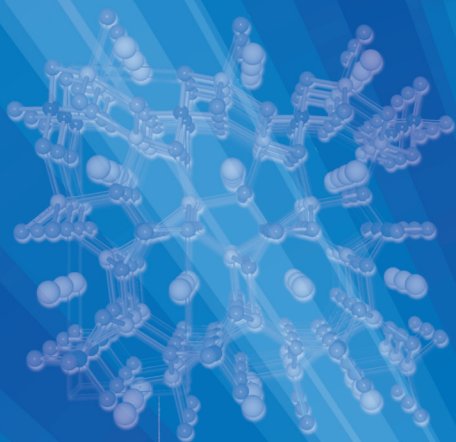


Powder Diffraction PDJ

Journal of Materials Characterization



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! This pricing is effective 1 January to 31 August 2018.

Visit **ICDD's website** for our new pricing.
Contact **sales@icdd.com** for a 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 - 2/18

EDITORIAL

Camden Hubbard	2017 was a very special year for powder diffraction	1
Craig M. Brown and Winnie Wong-Ng	Call for papers	2

TECHNICAL ARTICLES

Hui Li, Meng He and Ze Zhang	Evaluating the electron density model by applying an imaginary modification	4
Andrea Bernasconi and Jonathan Wright	Effects of resolution in real and reciprocal spaces from a 2D detector at a high-energy synchrotron beamline	11
Anderson Márcio de Lima Batista, Marcus Aurélio Ribeiro Miranda, Fátima Itana Chaves Custódio Martins, Cássio Morilla Santos and José Marcos Sasaki	Synthesis of cerium oxide (CeO ₂) by co-precipitation for application as a reference material for X-ray powder diffraction peak widths	21
Nicola V. Y. Scarlett and Ian C. Madsen	Effect of microabsorption on the determination of amorphous content via powder X-ray diffraction	26
F.-F. Ma, J.-W. Mao, G.-Q. Shao, S.-H. Fan, C. Zhu, A.-L. Zhang, G.-Z. Xie, J.-N. Gu and J.-L. Yan	Structure of triplite LiFeSO ₄ F powder synthesized through an ambient two-step solid-state route	38

NEW DIFFRACTION DATA

Austin M. Wheatley, James A. Kaduk, Amy M. Gindhart and Thomas N. Blanton	Crystal structure of methylprednisolone acetate form II, C ₂₄ H ₃₂ O ₆	44
Joel W. Reid, James A. Kaduk and Lidia Matei	The crystal structure of MoO ₂ (O ₂)H ₂ O	49
José A. Fernandes, Olufunso Abosedede and Simona Galli	Powder X-ray diffraction structural characterization of the coordination complex <i>cis</i> -[Co(κ^2 N,N'-1,10-phenanthroline-5,6-dione) ₂ Cl ₂]	55
Martin Etter	The crystal structure of trisodium hexachlororhodate (Na ₃ RhCl ₆)	62
H. A. Camargo, C. C. Rosas, J. A. Henao and N. J. Castellanos	Synthesis and X-ray diffraction data of N ¹ ,N ² -di(2-hydroxy)benzylidenbenzene-1,2-di-imine, C ₂₀ H ₁₆ N ₂ O ₂	66

DATA REPORTS

Austin M. Wheatley, James A. Kaduk, Amy M. Gindhart and Thomas N. Blanton Crystal structure of estradiol 17 β valerate (Delestrogen), C₂₃H₃₂O₃ 70

Austin M. Wheatley, James A. Kaduk, Amy M. Gindhart and Thomas N. Blanton Crystal structure of abiraterone acetate (Zytiga), C₂₆H₃₃NO₂ 72

INTERNATIONAL REPORT

Siu-Wai Chan MRS fall 2017 meeting 73

CALENDARS

Gang Wang Calendar of Forthcoming Meetings 75

Gang Wang Calendar of Short Courses & Workshops 77

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

Editor 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

Associate Editor for New Diffraction Data

Stacy Gates-Rector
International Centre for Diffraction Data
12 Campus Boulevard
Newtown Square, Pennsylvania 19073-3273, U.S.A.
gates-rector@icdd.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: As part of a study of new production routes for ^{99}Mo and daughter isotope $^{99\text{m}}\text{Tc}$, in the paper "The Crystal Structure of $\text{MoO}_2(\text{O}_2)\text{H}_2\text{O}$ " by J.W. Reid, J.A. Kaduk and L. Matei the crystal structure was solved and refined with synchrotron powder diffraction data from the Canadian Light Source by Rietveld methods and optimized by density function theory (DFT). The structure is composed of double zigzag molybdate chains running parallel to the b-axis.

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 2018

	Print & Online	Online
Individual (U.S. & Canada)	\$236	\$166
Individual (outside U.S. & Canada)	£182	£128
Student	N/A	\$36
Institutional or Library	\$472	\$285

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, Shaftsbury 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 One Liberty Plaza, 20th floor New York, NY 10006-1435. POSTMASTER: Send address changes to *Powder Diffraction*, One Liberty Plaza, 20th floor New York, NY 10006-1435, USA. Periodicals postage paid in New York, NY and additional mailing offices.

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.

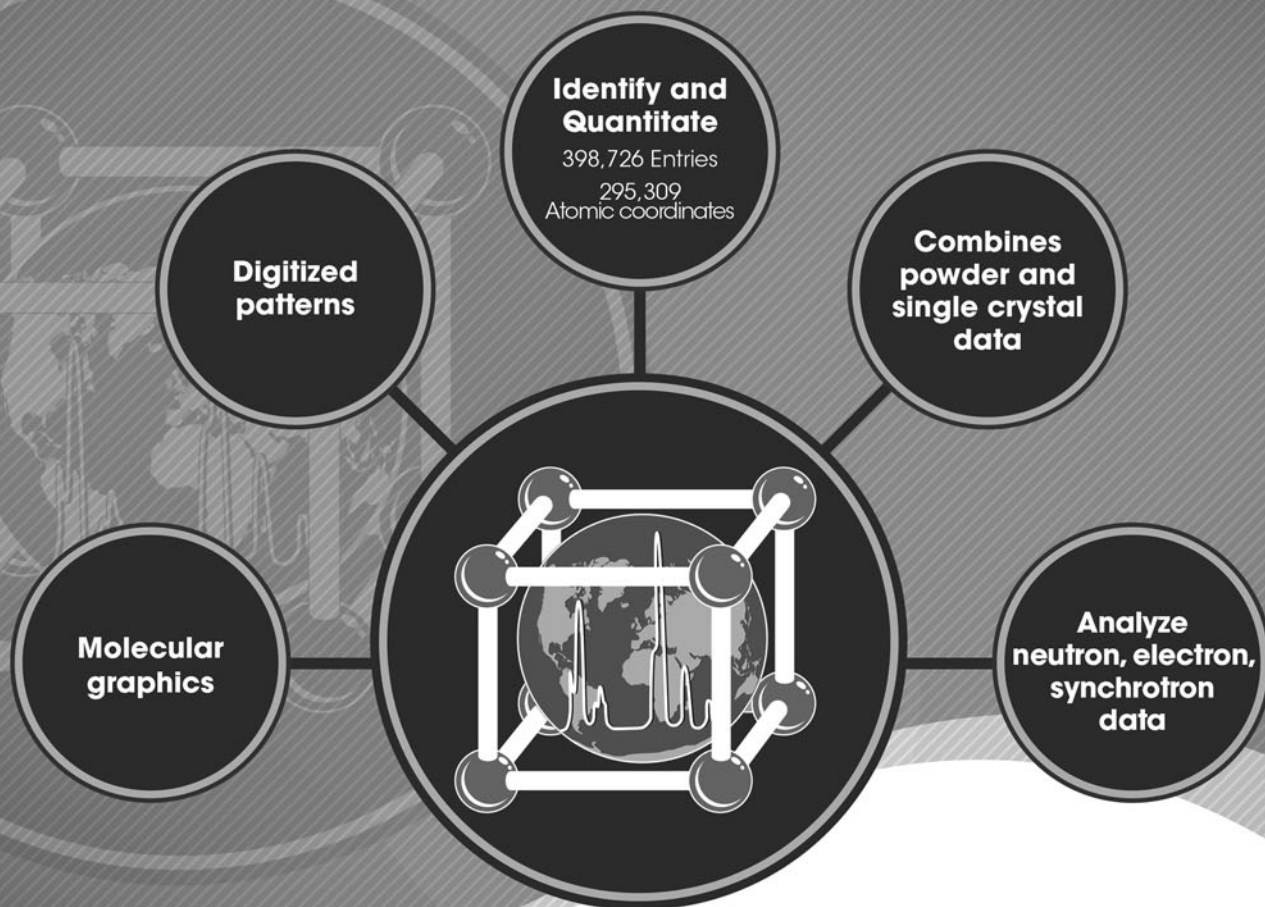
Document Delivery and Online Availability: Abstracts of journal articles published by Cambridge University Press are available from Cambridge Core (<https://www.cambridge.org/pdj>).

Copyright © 2018 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

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+



Standardized Data

More Coverage

All Data Sets Evaluated For Quality

Reviewed, Edited and Corrected Prior To Publication

Targeted For Material Identification and Characterization

www.icdd.com/products/pdf4.htm



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 ©2017 JCPDS-International Centre for Diffraction Data - 6/17