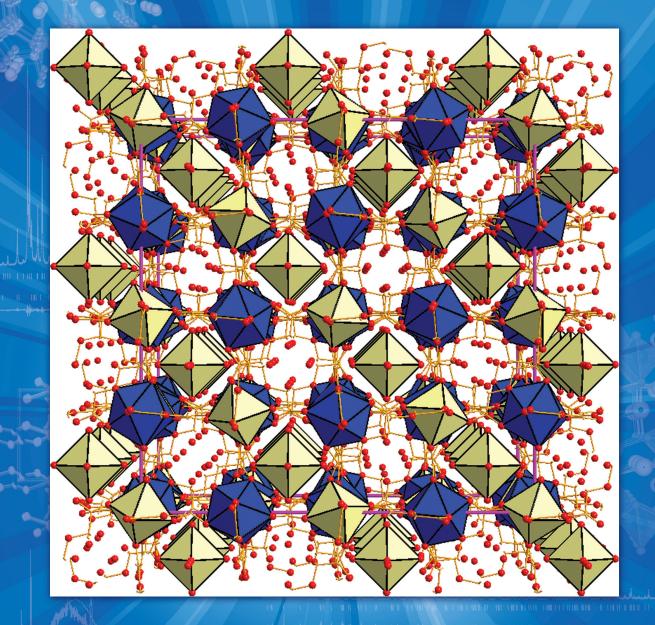
Powder Diffraction An International Journal of Materials Characterization



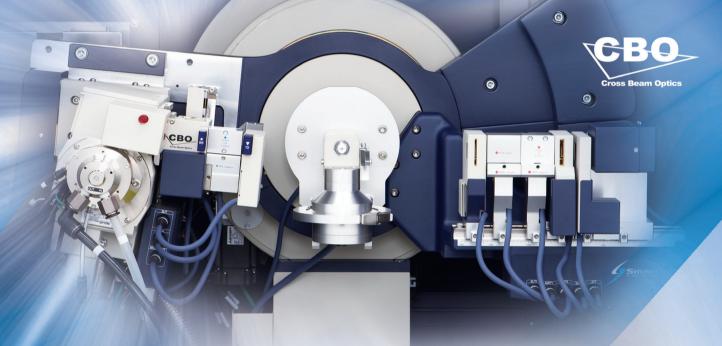
UNI

e by Cambridge University Pre

AMBRIDGE NIVERSITY PRESS Volume 27 / Number 04 / December 2012



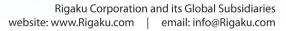
The world's only intelligent X-ray diffraction system



Powder diffraction • Thin film diffraction • SAXS • In-plane scattering

The **SmartLab Guidance** software provides you with an intelligent interface that guides you through the intricacies of each experiment. It is like having an expert standing by your side.







Powder Diffraction

CODEN: PODIE2 ISSN: 0885-7156

EDITORIAL

Nicole Ernst Boris	Editorial	231

TECHNICAL ARTICLES

Leopoldo Suescun, Jun Wang, Ricardo Faccio, Guzmán Peinado, Julia Torres, Carlos Kremer, and Robert A. Burrow	The structure of cubic MOF [{Ca(H ₂ O) ₆ }{CaGd(oxydiacetate) ₃ } ₂].4H ₂ O. A comparison between structural models obtained from Rietveld refinement of conventional and synchrotron X-ray powder diffraction data and standard refinement of single-crystal X-ray diffraction data	
M.L. Ettorche, M. Sebais, and Z. Hammoudi	A novel powder diagrams indexing, using classical geometry	243
Salwa Hamdi, Samia Ouni, Hanen Chaker, and Rached Ben Hassen	Synthesis, structural and electrical characterizations of $Er_{0.33}Sr_{1.67}Ni_{0.8}Cu_{0.2}O_{4-\delta}$	252
W. Wong-Ng, J. A. Kaduk, H. Wu, and M. Suchomel	Synchrotron X-ray studies of metal-organic framework $M_2(2,5-dihydroxyterephtha-late), M = (Mn, Co, Ni, Zn) (MOF74)$	256

NEW DIFFRACTION DATA

D. F. Rendle, and E. J. Glazier	Powder diffraction data for methylenedioxymethylamphetamine hydrochloride monohydrate (MDMA.HCl.H ₂ O, Ecstasy hydrate)	263
J. Maixner, R. Pažout, M. Hrdá, and P. Kačer	X-ray powder diffraction data for a PicoPtBr ₂ , <i>cis</i> -amminedibromo(2-methylpyridine)platinum complex $[Pt(NH_3)(2-pic)Br_2]$	266
J. A. Pinilla, J. A. Henao, M. A. Macías, Arnold R. Romero Bohórquez, and Vladimir V. Kouznetsov	Synthesis and X-ray powder diffraction data of <i>N</i> -benzyl-6-chloro-4-(4-methoxy-phenyl)-3-methyl-1,2,3,4-tetrahydroquinoline	269
R. Pažout, J. Maixner, J. Přech, and P. Kačer	X-ray powder diffraction data for (<i>1R</i> , <i>5S</i> , <i>7R</i>)-7-[(<i>S</i>)-4-benzyl-4,5-dihydrooxazole-2-yl]-1,5,7-trimethyl-3-azabicyclo-[3.3.1]-nonane-2,4-dione, another new chiral Kemp's acid diamide	273

INTERNATIONAL REPORTS

Denise Flaherty	2012 Denver X-ray Conference (DXC) Summary	276
Claudia Rawn	American Crystallographic Association Annual Meeting 2012	280

CALENDARS

Gang Wang	Calendar of Forthcoming Meetings	282
Gang Wang	Short Courses and Workshops	284

Powder Diffraction

An International Journal of Materials Characterization

Editor-in-Chief

Ting C. Huang Emeritus, IBM Almaden 9 Fl., #61 Sec. 1, Ao-Ho Road Taipei, Taiwan tinghuang@tinghuang.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

W. Frank McClune International Centre for Diffraction Data 12 Campus Boulevard Newtown Square, Pennsylvania 19073-3273, U.S.A. mcclune@icdd.com

Editors

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

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

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

Ian Madsen CSIRO Minerals P.O. Box 312 Clayton South, Victoria 3169 Australia ian.madsen@csiro.au

Editors for Crystallography Education

James Kaduk Analytical Science Research Services 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. 433/D003, Argonne, Illinois 60439-4856, U.S.A. brian.toby@anl.gov

International Reports Editor

Winnie Wong-Ng National Institute of Standards and Technology 100 Bureau Drive, Mail Stop 8520 Gaithersburg, Maryland 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 Nansanjie, Zhongguancun, Haidian District, Beijing 100190, China gangwang@aphy.iphy.ac.cn

On the cover: Figure 5(b) Packing of $[\{Ca(H_2O)_6\}\{CaGd(oda)_3\}_2]$ 4H₂O showing alternation of Gd and Ca polyhedral in the cubic network with Ca(H₂O)₆ octahedra occupying half of the cubic holes and crystallization water molecule the other half but in an

off-centre position. (Courtesy of Leopoldo Suescun¹, Jun Wang, Ricardo Faccio, Guzmán Peinado, Julia Torres, Carlos Kremer, and Robert A. Burrow).

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 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 kdaly@cambridge.org. Proofs and all correspondence concerning papers in the process of publication can also be addressed to: Production Editor, *Powder Diffraction*, Cambridge University Press, 32 Avenue of the Americas, New York, NY 10013-2473, U.S.A. Please include the job number in all correspondence.

For advertising rates and schedules contact Cambridge University Press Advertising Sales. Orders, advertising copy, and offset negatives should be sent to: Advertising Sales, Cambridge University Press, 32 Avenue of the Americas, New York, NY, 10013-2473, U.S.A.; Phone: 212-924-3900; Fax: 212-924-3900. Email: USAdSales@cambridge.org.

Subscription Prices 2012

	Print & Online	Print	Online
Individual (U.S. & Canada)	\$130	\$110	\$110
Individual (outside U.S. & Canada)	\$160	\$135	\$110
Student	N/A	N/A	\$35
Institutional or Library	\$225	\$215	\$160

Subscription rates to Eastern Hemisphere include air freight service.

Back-Number Prices. 2012 single copies: \$62.

Subscription, renewals, and address changes should be addressed to Subscription Fulfillment, *Powder Diffraction*, Cambridge University Press, 100 Brook Hill Drive, West Nyack, NY 10013-2113 (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*, Cambridge University Press, 100 Brook Hill Drive, West Nyack, NY 10013-2113. 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, 32 Avenue of the Americas, New York, NY 10013-2473. POSTMASTER: Send address changes to *Powder Diffraction*, Cambridge University Press, 100 Brock Hill Drive West Nyack, NY 10994-2113, 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://journals.cambridge.org/action/rightsAndPermissions. 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 Journals Online (http://journals.cambridge.org/action/displayJournal?jid=PDJ).

Copyright © 2012 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