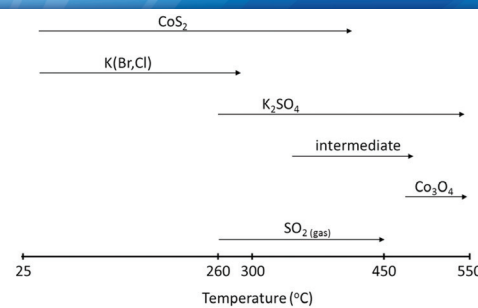
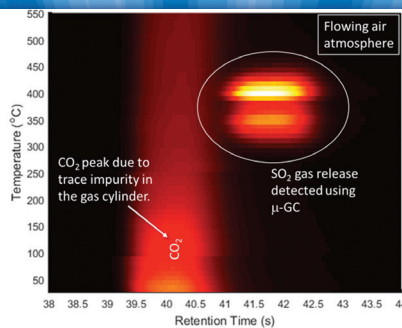
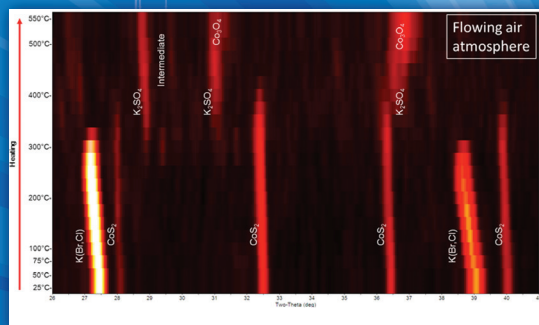
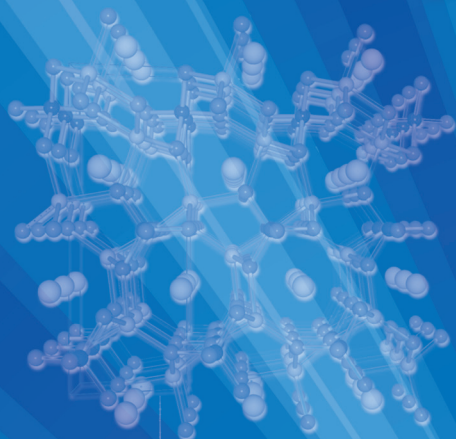


30

YEARS OF PDJ
1986 - 2016

Powder Diffraction PDJ

Journal of Materials Characterization



ICDD®
INTERNATIONAL CENTRE FOR DIFFRACTION DATA

CAMBRIDGE
UNIVERSITY PRESS

Volume 31 / Number 02 / June 2016

Published online by Cambridge University Press



MYTHEN2 R



Microstrip Hybrid Photon Counting X-ray Detector Series

*Top performance in all high-throughput
applications*

- *Noise-free single-photon counting
from Ti to Ag radiation*
- *Compact design fits in any
diffractometer*
- *640- and 1280-strip modules*
- *Multi-modular systems for the
laboratory*

laboratory and industry

EDITORIAL

- Tom Blanton The Denver X-ray Conference – celebrating 65 years of bringing together the high-energy scattering community 89

TECHNICAL ARTICLES

- Mark A. Rodriguez, Eric N. Coker, James J. M. Griego, Curtis D. Mowry, Adam S. Pimentel and Travis M. Anderson Monitoring of CoS₂ reactions using high-temperature XRD coupled with gas chromatography (GC) 90
- James A. Kaduk, Kai Zhong, Amy M. Gindhart and Thomas N. Blanton Crystal structure of rivastigmine hydrogen tartrate Form I (Exelon[®]), C₁₄H₂₃N₂O₂(C₄H₅O₆) 97
- Baozhuo Zhang and Marcus L. Young High-energy synchrotron X-ray diffraction measurements of simple bending of pseudoelastic NiTi shape memory alloy wires 104
- Zhixun Wang, Hangkong Li, Gemei Cai and Zhanpeng Jin Synthesis, crystal structure, and thermal stability of new borates Na₃REB₂O₆ (RE = Pr, Sm, Eu) 110
- James A. Kaduk, Kai Zhong, Amy M. Gindhart and Thomas N. Blanton Crystal structure of mupirocin form I, C₂₆H₄₄O₉ 118
- Peter Metz, Robert Koch, Bernadette Cladek, Katharine Page, Joerg Neufeind and Scott Misture X-ray and neutron total scattering analysis of H_y · (Bi_{0.2}Ca_{0.55}Sr_{0.25})(Ag_{0.25}Na_{0.75})Nb₃O₁₀ · xH₂O perovskite nanosheet booklets with stacking disorder 126
- James A. Kaduk, Kai Zhong, Amy M. Gindhart and Thomas N. Blanton Crystal structure of paliperidone, C₂₃H₂₇FN₄O₃ 135
- James A. Kaduk, Kai Zhong, Amy M. Gindhart and Thomas N. Blanton Crystal structure of choline fenofibrate (Trilipix[®]), (C₅H₁₄NO) (C₁₇H₁₄ClO₄) 142

NEW DIFFRACTION DATA

- Jose H. Quintana Mendoza, J. A. Henao, Aurora L. Carreño Otero and Vladimir V. Kouznetsov Synthesis and X-ray diffraction data of 2-morpholino-2-(3,4,5-trimethoxyphenyl) acetonitrile, (C₁₅H₂₀N₂O₄) 149
- Liu Qi Guo, Shou Jun Zheng, Xiao Li Ma and Hui Li X-ray powder diffraction data for trelagliptin succinate, C₁₈H₂₀FN₅O₂ · C₄H₆O₄ 153

Shoujun Zheng, Kailin Xu, Qing Wang, XiaoLin Tang, Yanmei Huang, Pei Xiao Tang, Lijuan Chen and Hui Li	X-ray powder diffraction data for 2-[[[(3R)-5-oxo-4-phenyltetrahydrofuran-3-yl)methyl]isoindoline-1,3-dione, C ₁₉ H ₁₅ NO ₄	155
--	--	-----

DATA REPORT

Qing Wang, Dan Guo, Bin Tang and Hui Li	X-ray powder diffraction data for 5-chloro- <i>N</i> -(4-(5,6-dihydro-3-(4-morpholinyl)-2-oxo-1(2H)-pyridinyl)phenyl)-pentanamide, C ₂₀ H ₂₆ ClN ₃ O ₃	159
--	--	-----

INTERNATIONAL REPORT

Winnie Wong-Ng	The 2015 Materials Science & Technology (MS&T15) Conference & Exhibition	162
----------------	--	-----

CALENDARS

Gang Wang	Calendar of Short Courses & Workshops	164
Gang Wang	Calendar of Forthcoming Meetings	165

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

Editors

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

On the Cover: From Figures 4, 5 and 8 in Technical Article "Monitoring of CoS₂ Reactions Using High Temperature XRD Coupled with Gas Chromatography (GC)": Concurrent Gas Chromatography was coupled with High Temperature X-Ray Diffraction to successfully revealed the reaction sequences of cobalt disulfide cathode materials in air as a function of temperature. Left – HTXRD patterns showing decomposition of the CoS₂ and formation of new phases. Middle – gas chromatography results revealing SO₂ off-gas species between ~260° C and 450° C. Right – the derived reaction sequences. The vertical axis in each plot shows the temperature. (Courtesy: Rodriguez, M. A.; Coker, E. N.; Griego, J. J. M.; Mowry, C. D.; Pimentel, A. S. and Anderson, T. M. of Sandia National Laboratory).

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 nbansen@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 2016

	Print & Online	Online
Individual (U.S. & Canada)	\$173	\$127
Individual (outside U.S. & Canada)	£107	£79
Student	N/A	\$32
Institutional or Library	\$345	\$217

Subscription rates to Eastern Hemisphere include air freight service.

Back-Number Prices. 2016 single copies: \$99.

Subscription, renewals, and address changes should be addressed to Subscription Fulfillment, *Powder Diffraction*, Cambridge University Press, 32 Avenue of the Americas, New York, NY 10013-2473 (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, 32 Avenue of the Americas, New York, NY 10013-2473. Phone: 845-353-7500; Toll free: 800-872-7423; Fax: 845-353-4141. Email: subscriptions_newyork@cambridge.org.

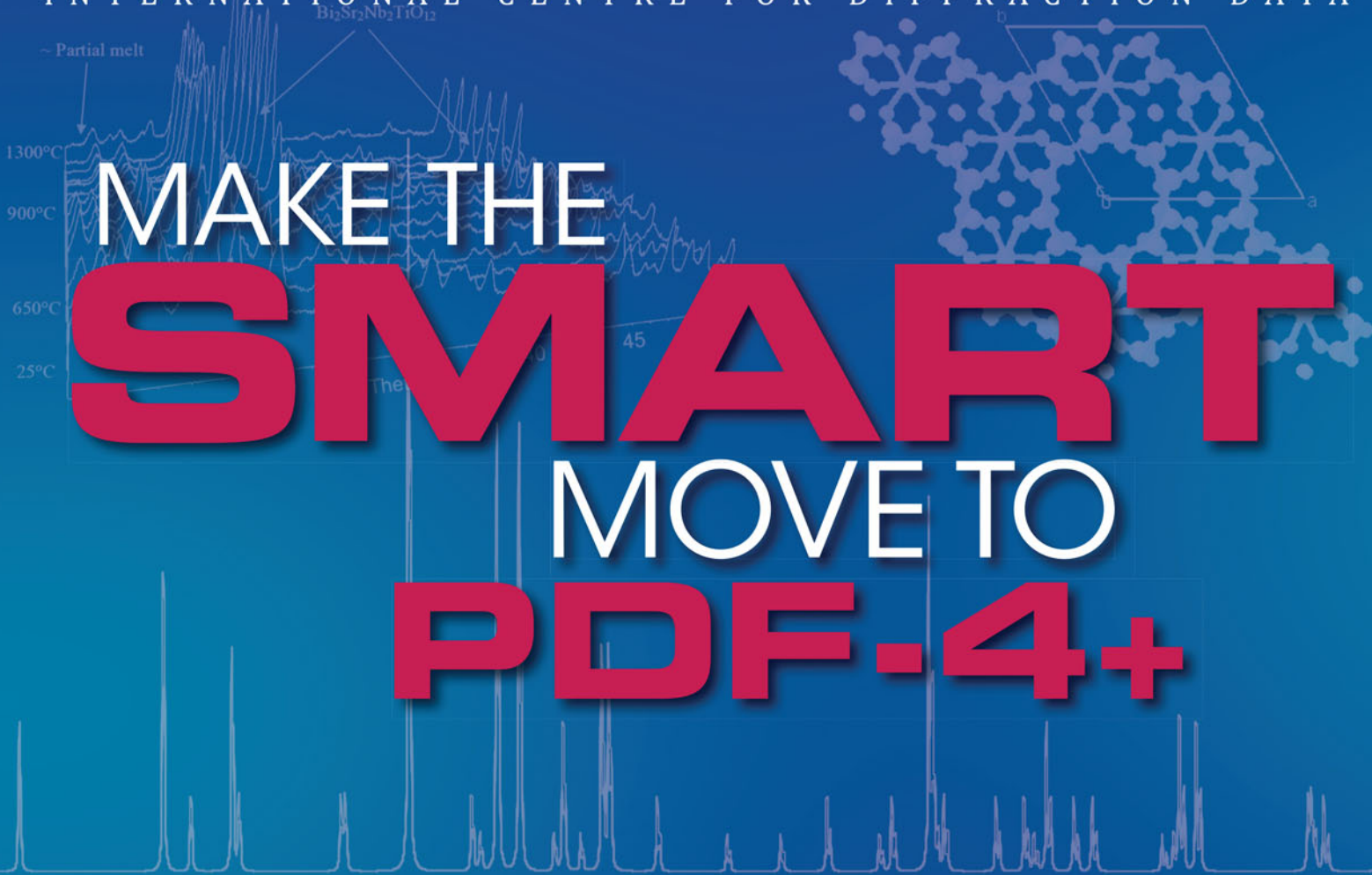
Powder Diffraction (ISSN: 0885-7156) is published quarterly (4X annually) by the JCPDS-International Centre for Diffraction Data through Cambridge University Press, 32 Avenue of the Americas, New York, NY 10013-2473. POSTMASTER: Send address changes to *Powder Diffraction*, Cambridge University Press, 32 Avenue of the Americas, New York, NY 10013-2473, 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 © 2016 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



MAKE THE SMART MOVE TO PDF-4+

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

S	Standardized data
M	More coverage
A	All data sets are evaluated for quality
R	Reviewed, edited, and corrected prior to publication
T	Targeted for material identification and characterization

Featuring
365,877 entries
including
251,640 entries
with atomic coordinates

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 ©2015 JCPDS—International Centre for Diffraction Data – 8/15

LET OUR TEAM OF EXPERTS HELP YOU TAKE YOUR SKILLS TO THE NEXT LEVEL!

Rietveld Refinement & Indexing Workshop

Basic Workshop: 26 – 28 September 2016

*Advanced Workshop: 28 – 30 September 2016

Powder Pattern Indexing and Rietveld structural refinement techniques are complementary and are often used to completely describe the structure of a material. Successful indexing of a powder pattern is considered strong evidence for phase purity. Indexing is considered a prelude to determining the crystal structure, and permits phase identification by lattice matching techniques. This workshop introduces the theory and formalisms of various indexing methods and structural refinement techniques. One unique aspect of this workshop is the extensive use of computer laboratory problem solving and exercises that teach method development in a hands-on environment.

Take the three-day basic workshop, the three-day advanced workshop or both together for a full week of hands-on training.

Practical X-ray Fluorescence: Spring 2017

From theory to hands-on exercises, this course offers techniques and skills to improve lab performance. Discover the latest in cutting-edge instruments such as TXRF, hand-held devices, energy dispersive and wavelength dispersive spectrometers through live demonstrations.

The XRF course covers the basics of X-ray spectra; instrumentation design; methods of qualitative and quantitative analysis; specimen preparation and applications for both wavelength and energy dispersive spectrometry. Emphasizing quantitative methods; use of automated X-ray spectrometers; review of mathematical matrix correction procedures and new developments in XRF.

Fundamentals of X-ray Powder Diffraction: Spring 2017

For the novice with some XRD knowledge or for the experienced with an interest in the theory behind XRD, this clinic offers a strong base for increased lab performance.

The clinic covers instrumentation, specimen preparation, data acquisition and qualitative phase analysis. Hands-on use of personal computers for demonstration of the latest software; data mining with the PDF. The powder diffractometer: optical arrangement, factors affecting instrumental profile width, choice and function of divergence slit, calibration and alignment, detectors, X-ray optics.

*Advanced Methods in X-ray Powder Diffraction: Spring 2017

For the experienced XRD scientist, this session offers enhanced analysis skills through intense problem solving, as well as an introduction to the Rietveld Method. Emphasizing computer-based methods of data collection and interpretation, both for qualitative and quantitative phase analysis.

The advanced clinic covers factors affecting d-spacings of crystals: unit cell, crystal structure, and solid solutions, as well as factors affecting diffraction-line intensities: relative and absolute intensities; structure-sensitive properties (atomic scattering and structure factors), polarization effects, and multiplicity; specimen-sensitive effects (orientation, particle size), measurement-sensitive effects (use of peak heights and peak areas), and choice of scanning conditions.

* See the ICDD web site for prerequisites for advanced courses.



Register Today at WWW.ICDD.COM/EDUCATION

LOCATION

ICDD Headquarters, 12 Campus Boulevard
Newtown Square, Pennsylvania 19073-3273 U.S.A.



**Celebrating 75 Years Serving
the Scientific Community**



FOR MORE INFORMATION CONTACT

Eileen Jennings, Education Coordinator

Tel: **610.325.9814** Fax: **610.325.9823**

Email: clinics@icdd.com

©2016a JCPDS-International Centre for Diffraction Data

Improve your Image

G670

Imaging Plate Guinier Camera



Capillary Sample Holder

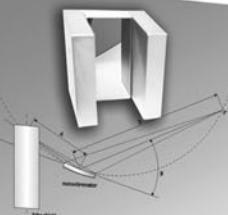


Diamond Anvil Cell Holder



Capillary Heater Device

Johansson Monochromator Crystals



Diode Laser Furnace



Low Temperature Device



Vertical Base for Liquids/Thin Films



Sample Changer

Capillary Boy



Plane Sample Holder

Your Decision for Precision



HUBER
Diffraction and Positioning Equipment

www.xhuber.com
info@xhuber.com

