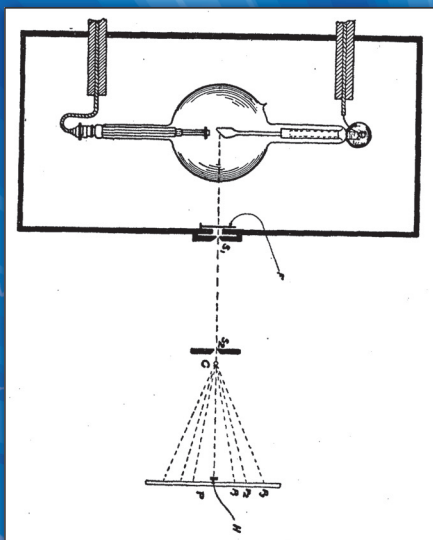
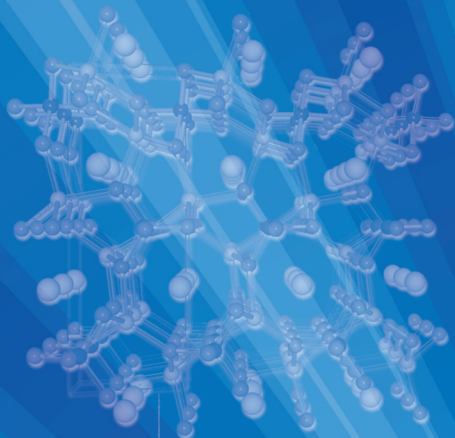


30

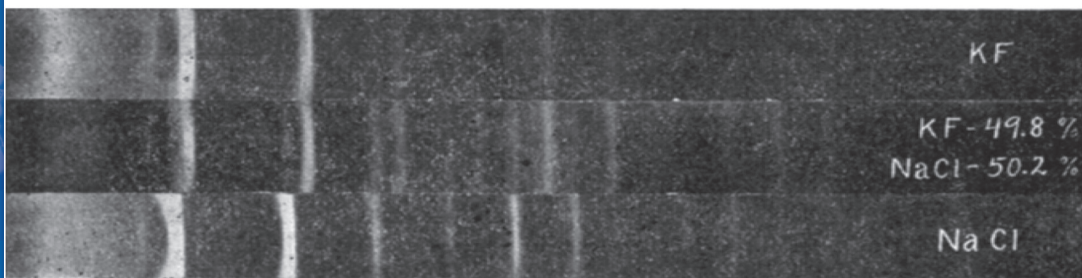
YEARS OF PDJ
1986 - 2016

Powder Diffraction PDJ

Journal of Materials Characterization



100 Year Anniversary of Albert W. Hull's Contributions to X-ray Diffraction



ICDD®
INTERNATIONAL CENTRE FOR DIFFRACTION DATA

CAMBRIDGE
UNIVERSITY PRESS

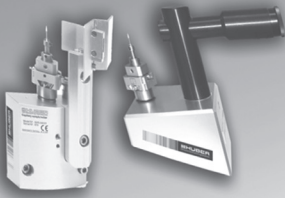
Volume 32 / Number 01 / March 2017

Published online by Cambridge University Press

Improve your Image

G670

Imaging Plate Guinier Camera



Capillary Sample Holder

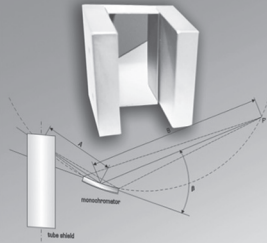


Diamond Anvil Cell Holder



Capillary Heater Device

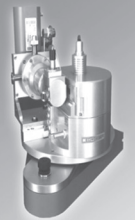
Johansson Monochromator Crystals



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

EDITORIAL

- Camden Hubbard 100 Years Since Albert W. Hull's Contributions to Powder Diffraction 1

REVIEW ARTICLE

- José Miguel Delgado The contributions of Albert W. Hull to X-ray powder diffraction at one hundred years of his landmark publication 2

TECHNICAL ARTICLES

- A. M. G. Carvalho, R. S. Nunes and A. A. Coelho X-ray powder diffraction of high-absorption materials at the XRD1 beamline off the best conditions: Application to (Gd, Nd)₅Si₄ compounds 10
- Weicai Ju, Simin Qiu, Yaqiu Tao, Xiaodong Shen and Zhigang Pan Molecular reorientation in a dehydration process of an organic polar salt of 2,4-diaminotoluene/L(+)-tartaric acid 15
- C. D. Snyders, E. E. Ferg and D. Billing An investigation into the temperature phase transitions of synthesized materials with Al- and Mg-doped lithium manganese oxide spinels by *in situ* powder X-ray diffraction 23
- James A. Kaduk, Amy M. Gindhart and Thomas N. Blanton Crystal structure of hydrocortisone acetate, C₂₃H₃₂O₆ 31

NEW DIFFRACTION DATA

- Jose H. Quintana Mendoza, R. A. Toro, Laura A. Blanco and J. A. Henao Characterization by X-ray powder diffraction of alpha lipoic acid 35
- Degui Li, Kun Luo, Bing He, Ming Qin, Liuqing Liang and Lei Hu Study on the crystal structure of Al₂Cu₃Gd compound with XRPD 40
- Joel W. Reid Powder diffraction data for ferrous gluconate 43

DATA REPORTS

- Qing Wang, Quan Hou, Yong Kui Zhang, Zi Li Suo and Hui Li X-ray powder diffraction data for Ethyl (Z)-2-chloro-2-[2-(4-methoxyphenyl)hydrazin-1-ylidene]acetate, C₁₁H₁₃ClN₂O₃ 46
- Xia Zeng, Qing Wang, Xin Nuo Xiong, Qiao Hong Du and Hui Li X-ray powder diffraction data for alogliptin benzoate, C₁₈H₂₁N₅O₂·C₇H₆O₂ 49

INTERNATIONAL REPORTS

José Miguel Delgado	The Second Meeting of the Latin American Crystallographic Association (LACA) in Mérida, Yucatán, México, 22–27 October 2016	53
Theresa Maguire	14th Pharmaceutical Powder X-ray Diffraction Symposium PPXRD-14 summary	56

CALENDARS

Gang Wang	Calendar of Forthcoming Meetings	58
Gang Wang	Calendar of Short Courses & Workshops	59

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 1, 2 and 10 in "The contributions of Albert W. Hull to X-ray powder diffraction at one hundred years of his landmark publication" written by Professor J. M. Delgado. To left is Hull's experimental set up (© 1917 by the American Physical Society). Top right is photo of Albert Wallace Hull of GE Laboratory (Courtesy of the Museum of Innovation and Science (miSci), Schenectady, New York. Bottom shows the diffraction pattern of a KF-NaCl mixture bracketed by the patterns of pure KF and NaCl from Hull's paper "A new method of chemical analysis", J. Am. Chem. Soc., 41 (8), 1168-1175 (1919) which demonstrates the phase identification of a mixture of phases. (© American Chemical Society).

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 ztokushige@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 2017

	Print & Online	Online
Individual (U.S. & Canada)	\$182	\$133
Individual (outside U.S. & Canada)	£112	£83
Student	N/A	\$35
Institutional or Library	\$449	\$271

Subscription rates to Eastern Hemisphere include air freight service.

Back-Number Prices. 2017 single copies: \$129.

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 © 2017 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
384,613 entries
including
271,449 entries
with atomic coordinates

*Celebrating 75 Years of
Serving the Scientific Community*



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. ©2016 JCPDS—International Centre for Diffraction Data. 07/16