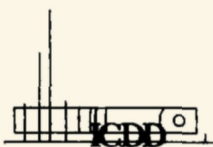


# Powder Diffraction

Ron Jenkins	Guest Editorial	83
J. Ll. Tamarit, N. B. Chanh, P. Négrier, D. O. López, M. Barrio, and Y. Haget	Crystal data of the low-temperature solid form of 2-methyl-2-nitro-propanol (MNP)	84
Ludo K. Frevel	Exhaustive indexing of triclinic powder diffraction patterns with known unit cell parameters	87
David E. McCready, Mikhail S. Alnajjar	Powder data for buckminsterfullerene, C <sub>60</sub>	93
S. Launay, P. Mahé, and M. Quarton	Synthesis and crystal data for K <sub>3</sub> Nb <sub>3</sub> O <sub>6</sub> Si <sub>2</sub> O <sub>7</sub>	96
Jaakko Leppä-aho, Jussi Valkonen	X-ray powder diffraction data for five lanthanoid chromates [Ln <sub>2</sub> (CrO <sub>4</sub> ) <sub>3</sub> (H <sub>2</sub> O) <sub>5</sub> ]·2H <sub>2</sub> O (Ln=La,Pr,Nd,Sm,Eu)	98
X. Cieren, J. Angenault, J-C. Couturier, and M. Quarton	Crystal data of two thiophosphates ATi <sub>2</sub> (PS <sub>4</sub> ) <sub>3</sub> with a new structural type (A=Na, Ag)	105
J. A. Henao, J. M. Delgado, and M. Quintero	X-ray powder diffraction data for CuFeSe <sub>2</sub>	108
Shanmugam Subramaniam, David P. Stinton, O. Burl Cavin, Camden R. Hubbard, Paul F. Becher, and Santosh Y. Limaye	Synthesis and cell refinement of Ba <sub>0.5+x/2</sub> Zr <sub>2</sub> P <sub>3-x</sub> Si <sub>x</sub> O <sub>12</sub> with x=0 and 0.175	111
C. L. Lengauer, G. Giester, and P. Unfried	Sm(OH) <sub>2</sub> NO <sub>3</sub> : Synthesis, characterization, powder diffraction data, and structure refinement by the Rietveld technique	115
J. C. Taylor, C. E. Matulis	A new method for Rietveld clay analysis. Part I. Use of a universal measured standard profile for Rietveld quantification of montmorillonites	119
Stephen L. Lawton, Lawrence S. Bartell	Application of the overlap integral in X-ray diffraction powder pattern recognition	124
W. Paszkowicz, A. Mąkosa	LCBASE: Program and database for phase identification	136
D. E. McCready, J. J. Kingsley	Powder Data for LaCo <sub>0.4</sub> Fe <sub>0.6</sub> O <sub>3</sub>	143
C. Colbeau-Justin, A. Elfakir, and M. Quarton	A monotitanate with a stuffed cristobalite structure type	146
Nabil N. Rammo, Saad B. Farid	Thermal expansion coefficients and Gruneisen parameters of quartz at high temperature by X-ray method	148
	International Report	151
	Calendar of Meetings	151
	Cumulative Author Index	153

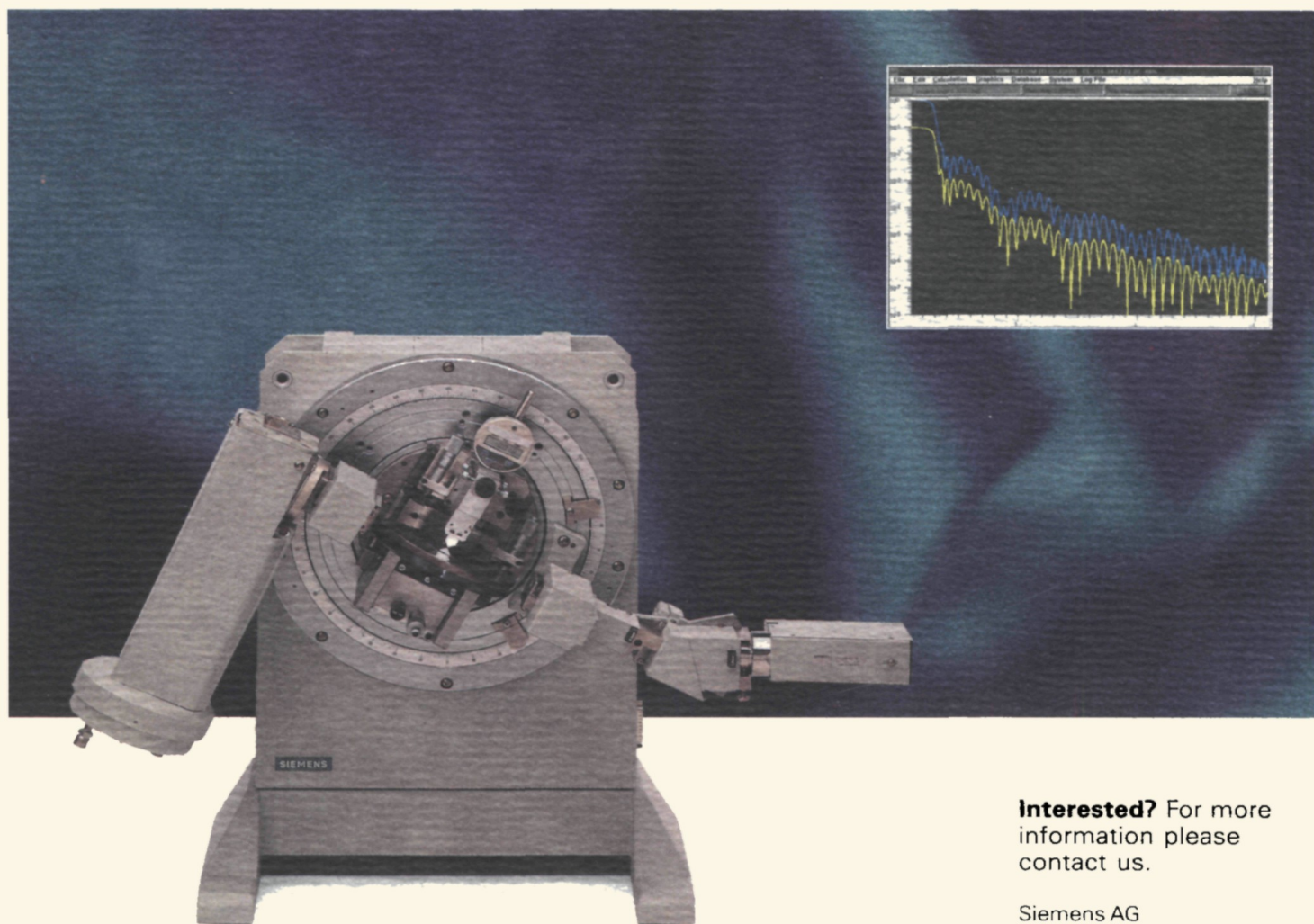


Volume 9 Number 2 June 1994

**Powder Diffraction** An international journal of materials characterization

# SIEMENS

## Enter the real world of thin film characterization – with the D5000 X-ray Reflectometer



- Non-destructive characterization of thin films and layer packages with very high accuracy.
- Determination of **thickness, density, surface and interface roughness** as well as **layer sequence**.
- X-ray diffraction measurements for analysis of **crystallographic phases** and **crystallite size**.
- WIN-REFSIM evaluation software under MS-WINDOWS: simulation of reflectograms and automatic refinement with four different methods.

**Interested?** For more information please contact us.

Siemens AG  
Analytical X-ray Systems  
AUT 37  
D-76181 Karlsruhe  
Germany  
Tel: (+49)-721-595-6213  
Fax: (+49)-721-595-4506

For USA and Canada:

Siemens Industrial  
Automation, Inc.  
6300 Enterprise Lane  
Madison, WI 53719-1173  
Tel: (608) 276-3000  
Fax: (608) 276-3006

The Third Edition of the SPEX Handbook answers questions about **Producing** homogeneous powders **Making** pressed or fused pellets **Controlling** contamination **Eliminating** particle size effects **Handling** liquid samples **Selecting** and ordering products

3rd EDITION

# We'll Help You Get A Handle On Your Sample

The SPEX Handbook includes:

Open-Vessel Microwave Digestion System

Automated 35-ton Hydraulic X-Press

Automated SPEX-Claire Fusion Fluxers

Cryogenic Laboratory Mill

Graphite Crucibles For Fusion

XRF Liquid Cells and Window Films

Boron Carbide Mortars and Pestles

Manual and Motorized Laboratory Presses

Evacuatable Pellet Dies and Spec-Caps

Graphite Crucibles for Fusions  Nylon Sieve Sets

Shatterboxes, Mixer/Mills . . . AND MORE!

SPEX  
HAND  
BOOK  
OF  
SAMPLE  
PREPARATION  
and HANDLING



INDUSTRIES, INC.  
3880 PARK AVE. • EDISON, N.J. 08820  
TEL: 908-549-7144 • FAX: 908-603-9647



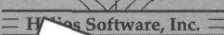
**DAPPLE**<sup>®</sup>  
S Y S T E M S

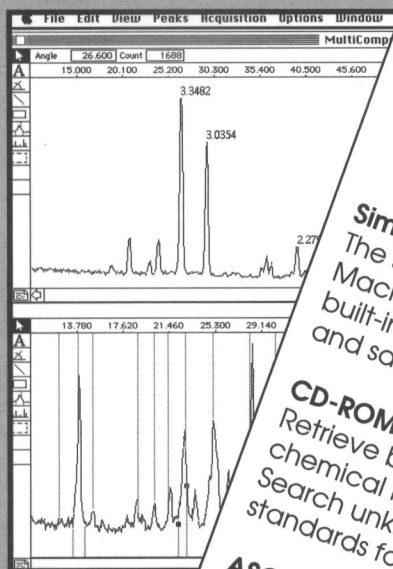
# ThetaPlus<sup>®</sup>

*Rebuild! Upgrade! Modernize!*

## A New Generation in X-ray Diffraction

Precise X-ray diffractometer automation:

- Search/Match incorporates  **Hindustan Software, Inc.** **MatchPDF™** for JCPDS database CD-ROM access.
- X-Mate controller provides the most advanced acquisition and control system available.
- Custom Microstep driver gives you the most precise movement available.
- Convenient user interface available for IBM PC/AT and Macintosh II.



**FLASH**

**"PC" and "MAC" Users!!!**

Tired of obsolete computers controlling your XRD? Do it with a PC or Mac instead.

**Now available** - direct acquisition from the following controllers:

- Philips PW1710
- Philips PW1842
- Siemens D500/Siemac
- Rigaku D/max
- Rigaku Miniflex

**Simple Installation:**

The supplied cable connects the PC/AT or Macintosh II to your controller. Retain all built-in system functions such as set calibration and sample changer.

**CD-ROM PDF-2 Database Access:**

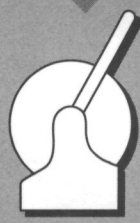
Retrieve by card number, mineral name, chemical name, elements or 3 strongest lines. Search unknown spectra and store selected standards for routine comparison and analysis.

**ASCII Data Files:**

Format compatible with a wide range of third party analytical programs.

Microstep Drive

Stepping Motor Controller



Is your X-ray diffractometer **outdated?**

ThetaPlus can **modernize** your instrument in two ways:

- **Upgrade** to our Microstep drive to increase resolution up to ten-fold without changing the existing stepping motor -OR-
- **Replace** only the outmoded computer and software by communicating directly with the existing motor controller.

**We make your instruments perform!**

Dapple Systems, 355 W. Olive Avenue, Suite 100, Sunnyvale, CA 94086

Tel: (408) 733-3283

Fax: (408) 736-2350

## Editor in Chief

Deane K. Smith  
Department of Geosciences  
The Pennsylvania State University  
239 Deike Building  
University Park, PA 16802-2711 U.S.A.

## Managing Editor

Ron Jenkins  
JCPDS-International Centre for Diffraction Data  
12 Campus Blvd.,  
Newtown Square, PA 19073-3273 U.S.A.

## Editor for New Diffraction Data

Gregory J. McCarthy  
Department of Chemistry  
North Dakota State University  
Fargo, ND 58105-5516 U.S.A.

## European Editor

Jan W. Visser  
Henry Dunantlaan 81, 2614 GL Delft, Netherlands

## Editor for Australia and New Zealand

Brian H. O'Connor  
Curtin University  
GPO Box U 1987, Perth 6001  
Western Australia, Australia

## Editor for Japan

Hideo Toraya  
Ceramics Research Lab  
Nagoya Institute of Technology  
Asahigaoka, Tajima 507 Japan

## International Reports Editor

Helein D. Hitchcock  
NASA DM-MSL-1  
Kennedy Space Center, FL 32899 U.S.A.

## Assistant to the Managing Editor

Mary M. Rossi

## Editorial Advisory Board

C. S. Barrett, Denver, Colorado  
P. Bayliss, Sydney, Australia  
C. Z. Bojarski, Katowice, Poland  
A. Brown, England  
D. Cox, Upton, New York  
W. Eysel, Heidelberg, West Germany  
J. Fiala, Plzeň, Czech Republic  
V. A. Frank-Kamenetsky, Leningrad, U.S.S.R.  
L. Frevel, Midland, Michigan  
P. Gado, Budapest, Hungary  
H. Goebel, Munchen, West Germany  
T. Huang, San Jose, CA (IUCr Representative)  
G. G. Johnson Jr., State College, Pennsylvania  
Q. Johnson, Livermore, California  
J. I. Langford, Birmingham, U.K.  
D. Louër, Rennes, France  
H. F. McMurdie, Gaithersburg, Maryland  
M. E. Mrose, Gaithersburg, Maryland  
M. H. Mueller, Argonne, Illinois  
M. Nichols, Livermore, California  
B. Post, Brookline, Massachusetts  
R. L. Snyder, Alfred, New York  
S. Weissmann, Metuchen, New Jersey  
T. Yamanaka, Tokyo, Japan  
R. A. Young, Atlanta, Georgia

**AIP Production:** Lin Miller, *Editorial Supervisor*;  
Andrea Witt, *Journal Coordinator*;  
Connie Nedohon, *Senior Production Editor*

*Powder Diffraction* is a quarterly journal published for the JCPDS-International Centre for Diffraction Data by the American Institute of Physics (AIP). *Powder Diffraction* is a journal of practical technique, publishing articles relating to the widest range of application—from mineral 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** (3 copies) to the most appropriate *Powder Diffraction* Editor listed on this page. The Editors will consider all manuscripts received, but assume no responsibility regarding them. Materials will be returned only when accompanied by appropriate postage. There is no publication charge. See *Powder Diffraction Notes for Authors* for additional information.

**Proofs and all correspondence** concerning papers in the process of publication should be addressed to: Editorial Supervisor, Powder Diffraction, AIP, 500 Sunnyside Blvd., Woodbury, NY 11797-2999.

**For advertising rates** and schedules contact AIP Advertising Department. Orders, advertising copy, and offset negatives should be sent to: Advertising Department, American Institute of Physics, 500 Sunnyside Blvd., Woodbury, NY 11797-2999; phone: (516) 576-2440; fax: (516) 576-2481.

## Subscription Prices (1994)

	U.S.A & Canada	Mexico, Central & South America	Europe, Mid-East & Africa*	Asia & Oceania*
Individual	\$55	\$75	\$75	\$75
Institutional or Library	\$95	\$95	\$95	\$95

\*Subscription rates to Eastern Hemisphere include air freight service.

**Back-Number Prices.** 1994 single copies: \$30. Prior to 1993 single copies: \$30.

**Subscription, renewals, and address changes** should be addressed to *AIP Circulation and Fulfillment Division (CFD)*, 500 Sunnyside Blvd., Woodbury, NY 11797-2999. 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 and Back Volumes:** 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 AIP Circulation and Fulfillment Division (CFD) at (516) 576-2288; (800) 344-6901. Institutional or library subscribers please contact AIP Subscriber Services at (516) 576-2270; (800) 344-6902.

**Reprint Billing:** Contact: AIP Circulation and Fulfillment Division, Woodbury, NY 11797-2999; (516) 576-2234; (800) 576-6909.

**Copyright Notice:** Authorization to photocopy items for internal or personal use, or the internal or personal use of specific clients, is granted by AIP, provided that the appropriate fee per page is paid directly to the *Copyright Clearance Center (CCC)*, 27 Congress Street, Salem, MA 01970.

The item-fee code for this publication is 0885-7156/94 \$6.00.

**Permission For Other Use:** Individual teachers, students, researchers, and libraries acting for them are permitted to make copies of articles in this journal for their own use in research or teaching, including multiple copies for classroom or library reserve use, provided such copies are not sold. Copying for sale is subject to payment of copying fees. Permission is granted to quote from the journal with the customary acknowledgment of the source. To reprint a figure, table, or other excerpt requires in addition the consent of one of the original authors and notification to AIP. Reproduction for advertising or promotional purposes, or republication in any form, is permitted only under license from AIP, which will normally require that the permission of one of the authors also be obtained. Direct inquiries to: AIP Office of Rights and Permissions, 500 Sunnyside Blvd., Woodbury, NY 11797-2999.

**Document Delivery:** For information on obtaining copies of individual articles, contact AIP Circulation and Fulfillment Division, 500 Sunnyside Blvd., Woodbury, NY 11797-2999; phone: (516) 576-2277; (800) 344-6908; fax: (516) 394-9704; E-mail: elecprod@pinet.aip.org.

*Powder Diffraction* (ISSN: 0885-7156) is published quarterly (4X annually) by the American Institute of Physics for the JCPDS-International Centre for Diffraction Data, 500 Sunnyside Blvd., Woodbury, NY 11797-2999. JCPDS-ICDD principal office: 12 Campus Blvd., Newtown Square, PA 19073-3273. POSTMASTER: Send address changes to *Powder Diffraction*, American Institute of Physics, 500 Sunnyside Blvd., Woodbury, NY 11797-2999. Second class postage rates paid at Woodbury, NY and additional mailing offices.

Copyright 1994 by JCPDS-International Centre for Diffraction Data

## **INTERNATIONAL CENTRE FOR DIFFRACTION DATA ANNOUNCES OFFICERS AND DIRECTORS FOR 1994**

Chairman - Gerald G. Johnson, Jr.  
Vice Chairman - Helein D. Hitchcock  
Treasurer - Gerhard R. Fischer  
Chairman, Technical Committee - Ting C. Huang  
Members-at-Large, Board of Directors  
Thomas N. Blanton  
Cyrus E. Crowder  
Walter Eysel  
Charlotte Lowe-Ma  
Melvin H. Mueller  
Past Chairman - Ludo K. Frevel

### **GENERAL MANAGER POSITION**

The International Centre for Diffraction Data, a scientific database corporation in the Philadelphia area, is seeking a General Manager. The non-profit corporation operates from a new headquarters facility and serves a world-wide scientific community. Required qualifications include proven managerial and business experience, a degree (minimum BS) in physical or materials sciences or engineering, and experience in XRD work and electronic data handling. Duties are interesting and diversified and include supervision of 30+ employees and cooperation with about 100 international scientific volunteers.

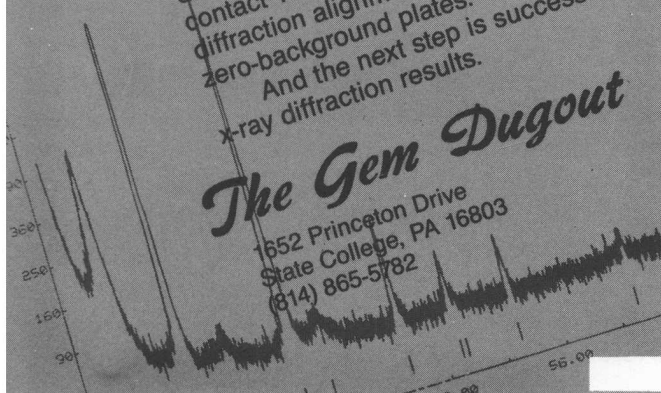
The deadline for applications is 1 September 1994. Send resumes to:

**ICDD  
2200 Kings Highway  
Bldg. L-3, Suite No. 54  
Port Charlotte, FL 33980**

**X-ray  
Diffraction  
Reference Standards  
and Zero-background  
Sample Plates  
Custom Designed  
and Built for any  
Application**

Your first step to improved x-ray diffraction results should be to contact The Gem Dugout for quality diffraction alignment standards and zero-background plates. And the next step is successful x-ray diffraction results.

**The Gem Dugout**  
1652 Princeton Drive  
State College, PA 16803  
(814) 865-5782



## ICDD Elects Distinguished Fellow

The International Centre for Diffraction Data is pleased to announce that Professor Doctor Pieter deWolff has been elected to join the ICDD list of Distinguished Fellows. Professor deWolff has been recognized by the ICDD Board of Directors for his sustained, outstanding work in the field of powder diffraction.

## INDEX TO ADVERTISERS

Dapple Systems .....	A2
Gem Dugout.....	A5
ICDD.....	A4, A5, A6, A7
Philips Analytical X-Ray.....	A8
Scintag, Inc.....	Cover 4
Seifert X-Ray Corp.....	Cover 3
Siemens Analytical.....	Cover 2
SPEX.....	A1

### Advertising Sales Office

American Institute of Physics  
500 Sunnyside Boulevard  
Woodbury, N.Y. 11797-2999  
Telephone: (516) 576-2440  
Advertising Fax: (516) 576-2481

**Advertising Director**  
Edward P. Greeley

**Advertising Manager**  
Richard T. Kobel

**Asst. Advertising Manager** Arnie W. Schweitzer  
**Advertising Representative** Robert G. Finnegan

**Production**  
Wendy Cona

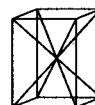
For 1993/94 from ICDD...



**EDD** Electron Diffraction  
Data Base

(NIST/Sandia/ICDD)

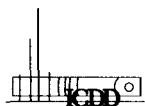
Crystallographic & chemical data on  
over 81,000 crystalline materials.†



**NIST** Crystal Data  
File

Crystallographic & chemical data on  
over 182,500 crystalline materials.\*

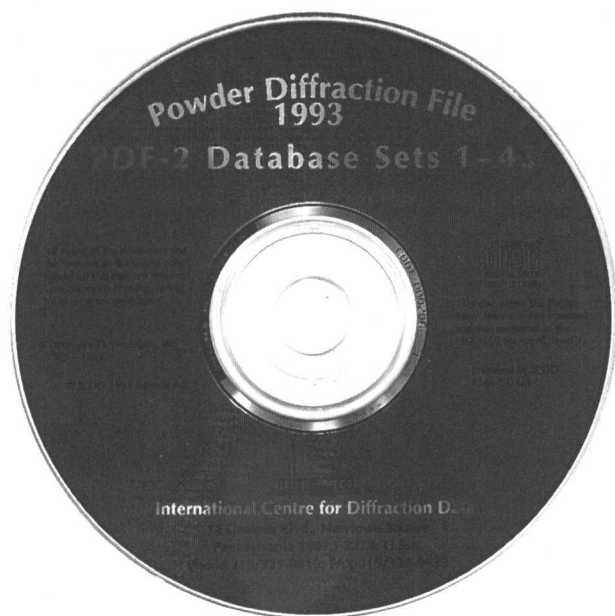
†Available for IBM-PC compatibles, VAX & Macintosh  
\*Available for IBM-PC compatibles & VAX



International Centre for Diffraction Data  
12 Campus Blvd., Newtown Square, PA 19073-3273, U.S.A.  
Phone: 215/325-9810; FAX: 215/325-9823

# ICDD

International Centre for Diffraction Data



## Your source for X-ray Diffraction Data

**The Powder Diffraction File—  
Over 58,000 patterns**

**PC-PDF —**

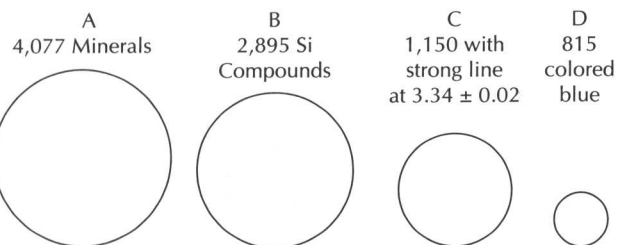
**A unique scientific database**

PC-PDF, a high density, data storage/retrieval system, uses a personal computer equipped with a CD-ROM drive and disk which contains the entire PDF-2 database and index files.

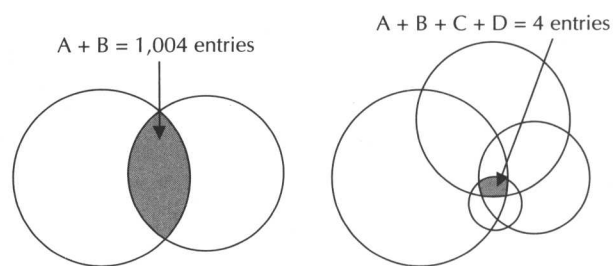
**Speed and flexibility**

PC-PDF, through use of optimum packing and access algorithms, displays results within seconds. You can, for example:

**Search on key fields within the database:**



**Search on combinations of fields:**

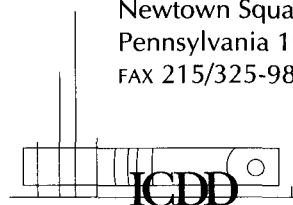


## Other Files, Publications & Services

- ◆ On CD-ROM: NIST Crystal Data File
- ◆ On magnetic tape or floppy disks: Electron Diffraction Database
- ◆ In print:
  - Metals and Alloys Indexes** – a 680-page book containing
    - Alphabetical Index
    - Pearson Symbol Code Index
    - Common Names Index
    - Strukturbericht Symbol Index
  - Minerals Databooks... Search Manuals... Educational Materials...
  - Powder Diffraction**, a quarterly journal
- ◆ Regularly scheduled clinics, workshops and short courses.

## For information contact —

M. M. Fornoff  
Sales/Marketing Manager  
International Centre for  
Diffraction Data  
12 Campus Boulevard  
Newtown Square  
Pennsylvania 19073-3273, U.S.A.  
FAX 215/325-9823





# INTERNATIONAL CENTRE FOR DIFFRACTION DATA CRYSTALLOGRAPHY SCHOLARSHIP AWARDS

The science of crystallography has played a key role in the development of X-ray diffraction, electron diffraction and neutron diffraction for the elucidation of the atomic structure of matter. Crystallography is an interdisciplinary branch of science taught in departments of physics, chemistry, geology, molecular biology, metallurgy and material science. To encourage promising graduate students to pursue crystallographically-oriented research, the International Centre has established a Crystallography Scholarship Fund. While the Ewald Prize is awarded every three years to an internationally recognized crystallographer, little effort has been made by science departments to cultivate aspiring crystallographers. Convinced of the beneficial, scientific impact of the proposed scholarships for crystallographically-oriented research, the ICDD has solicited funds from private and industrial sectors to support this program. The ICDD awarded two scholarships in 1992, two in 1993 and three in 1994. Applications for the 1995 awards must be received by ICDD no later than 31 October 1994.

**Qualifications** for the applicants: The applicant should be a graduate student seeking a degree with major interest in crystallography (crystal structure analysis, crystal morphology, modulated structures, correlation of atomic structure with physical properties, systematic classification of crystal structures, phase identification and materials characterization). There are no restrictions on country, race, age or sex. The term of the scholarship is one year. Application for one renewal may be made by the recipient at the end of the first year. Because a limited number of scholarships are awarded, renewal applications will be considered on a competitive basis in conjunction with all applications that have been submitted up to the closing date.

## Submit:

- a. Curriculum Vita.
- b. A one-page proposal by the graduate student describing the type of crystallographic research to be partially supported by scholarship.
- c. A supportive letter from the sponsoring professor of an accredited university or an institute of technology.

## Restrictions on the scholarship fund:

- a. The scholarship stipend of \$2,000 is to be used by the graduate student to help defray tuition and laboratory fees. A portion of the stipend may be applied to registration fees to accredited scientific meetings related to crystallography.
- b. No more than one scholarship will be awarded to any one accredited institution per year.
- c. The funds of the scholarship are not to be used for travel.

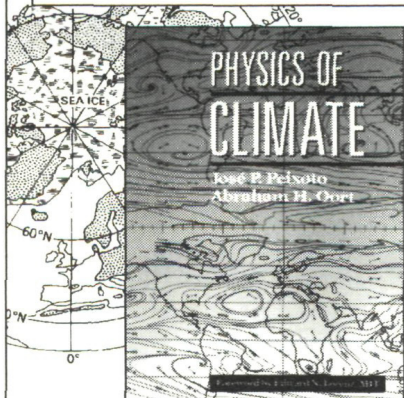
The awarding of the scholarships shall be administered by a committee consisting of the ICDD Chairman, the Chairman of the ICDD Technical Committee, and the Chairman of the ICDD Education Subcommittee. One or more accredited professors (with no conflicts of interest) may be invited to assist in the selection of successful candidates.

Applications must be received by 31 October 1994. Please mail to:

Secretary, International Centre for Diffraction Data  
Newtown Square Corporate Campus  
12 Campus Boulevard  
Newtown Square, PA 19073-3273 U.S.A.

# PHYSICS OF CLIMATE

A REVOLUTIONARY VIEW OF CLIMATE AS AN INTEGRATED PHYSICAL SYSTEM



## PHYSICS OF CLIMATE

J. P. Peixoto, University of Lisbon, and  
A. H. Oort, National Oceanic and  
Atmospheric Administration

*"A modern treatment of the nature  
and theory of climate."*

From the foreword by Edward N. Lorenz, MIT

Cloth \$95.00 Members \$76.00  
Paper \$45.00 Members \$36.00



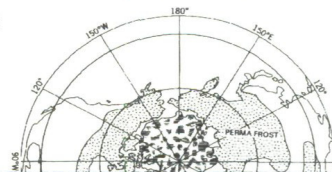
Books of the American Institute of Physics  
500 Sunnyside Boulevard  
Woodbury, NY 11797

The global upper air network... satellite data... nonlinear mathematical models... Using the tools that have breathed new life into the study of climate, this ground breaking work demonstrates how environmental phenomena worldwide interact in a single unified system.

With more than 220 drawings, charts, and graphs, PHYSICS OF CLIMATE offers you the best current understanding of the Earth's climate :

*"A superb reference.... Belongs on the shelf of anyone  
seriously interested in meteorology and climatology."*

—Curt Covey and Karl Taylor, *Physics Today*



For faster service call toll free 1-800-488-BOOK

To order, mail to: American Institute of Physics c/o AIDC • P.O. Box 20 • Williston, VT 05495

Check enclosed (U.S. dollars only)     Mastercard     Visa     American Express

Card No. \_\_\_\_\_ Exp. Date \_\_\_\_\_

Signature (Required on all credit card orders) \_\_\_\_\_

Name \_\_\_\_\_

Institution (if applicable) \_\_\_\_\_

Street Address \_\_\_\_\_

City / State / Zip \_\_\_\_\_

Qty	Edition	ISBN	Price*	Total
	Cloth	0-88318-711-6		
	Paper	0-88318-712-4		

Subtotal \_\_\_\_\_

Shipping: \$2.75 for 1st book (\$7.50  
foreign), \$.75 for each additional book \_\_\_\_\_

TOTAL \_\_\_\_\_

\*Member prices apply to members of AIP Member Societies. To qualify, please circle your affiliation. APS/OSA/ASA/SoR/AAFT/ACA/AAS/AAPM/AVS/AGU/SPS

9241

## X'Pert-MPD

### The last word in XRD precision

The X'Pert-MPD is the most accurate diffractometer ever. Simple as that. And no surprise that it comes from Philips.

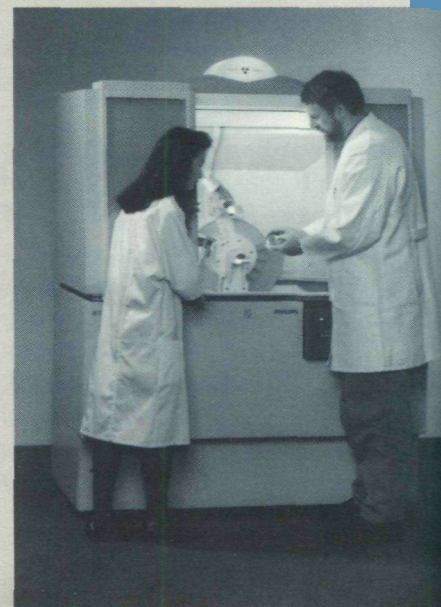
This multi-purpose diffractometer is capable of high-precision XRD investigation in every polycrystalline X-ray diffraction application - from routine phase to advanced stress and texture analysis, from process control to leading-edge research.

If you're in the business of XRD, check out the X'Pert-MPD for its theta/theta and theta/2-theta versatility - with simultaneous operation. Note its innovative ceramic X-ray tube and twin, optically-encoded goniometers. And see how easy it is to use, with windows-based phase and texture analysis software.

Above all, the X'Pert-MPD is unrivalled for accuracy. So if you're looking for the last word in XRD precision for your laboratory, first have a word with us.

Philips Analytical X-Ray, Lelyweg 1, 7602 EA Almelo,  
The Netherlands. Telephone +31 546 839911. Fax +31 546 839598.

Philips Electronic Instruments Inc., 85 McKee Drive, Mahwah,  
NJ 07430, USA. Telephone +1 201 529 6107. Fax +1 201 529 5084.



Philips  
Analytical  
X-Ray



# PHILIPS