

Powder Diffraction

Mark Holomany	EDITORIAL: Internet services for powder diffractionists	155
A. Álvarez-Larena, E. Estop, J. Rodríguez-Romero, E. Tauler, and X. Alcobé	Crystal data and powder diffraction data for p-Iodotoluene at 293 K	156
Zhengmin Fu, Wenxiu Li	Crystal structure of a new compound $\text{Li}_2\text{Mg}_2(\text{WO}_4)_3$	158
M. I. Arriortua, M. Insausti, R. Cortés, and J. I. R. Larramendi	Crystal data for $[\text{Cu}(\text{L}_{\text{III}})\text{XY}] \cdot n\text{H}_2\text{O}$ compounds [L_{III} = pymep, terpy; $X = \text{I}, \text{N}_3$; $Y = \text{I}, \text{NO}_3, \text{PF}_6$; $n = 0, 1$]	161
Brendan J. Kennedy	X-ray powder diffraction study of BiSbO_4	164
P. van der Sluis	Peaks in the background from single-crystal substrates measured with parallel beam optics	168
S. T. Mixture, L. R. Chatfield, and R. L. Snyder	Accurate fully automated powder diffraction data using zero-background sample holders	172
P. Scardi, L. Lutterotti, and P. Maistrelli	Experimental determination of the instrumental broadening in the Bragg-Brentano geometry	180
Hee-Lack Choi, Naoya Enomoto, Nobuo Ishizawa, and Zenbe-e Nakagawa	X-ray diffraction data of $\text{Ti}_2\text{O}_2(\text{C}_2\text{O}_4)(\text{OH})_2 \cdot \text{H}_2\text{O}$	187
A. M. Wims, C. D. Fuerst	X-ray powder data for $\text{Nd}_2\text{Co}_{14}\text{B}$, $\text{Pr}_2\text{Co}_{14}\text{B}$ and $\text{Pr}_2\text{Fe}_{14}\text{B}$	189
Hoong-Kun Fun, Ping Yang, Rusli Othman, Tsong-Jen Lee, Chiou-Chu Lai, and Huan-Chiu Ku	Structure of $\text{TlSr}_2\text{PrCu}_2\text{O}_7$ by Rietveld analysis	194
Michael O. Eatough, Terry L. Aselage	X-ray for the superconducting phase $\text{TlBa}_2\text{Ca}_2\text{Cu}_3\text{O}_9$ diffraction data	200
A. Chrysanthou, N. Hassine	The observation and crystal structure of titanium oxycarbonitride	202
Claudia Weidenthaler, Reinhard X. Fischer, and Robert D. Shannon	Pitfalls in the powder diffraction analysis of zeolites ZSM-5 and ZSM-8	204
J. Valkonen, P. Perkkalainen, I. Pitkänen, and H. Rautiainen	X-ray powder diffraction pattern for lactitol and lactitol monohydrate	213
Sampath S. Iyengar, Simona Percec	Rietveld analysis of high-density polyethylene	
	International Report	221
	Calendar of Meetings	221
	Book Reviews	221
	Computer Comments	222
	Cumulative Author Index	227



Volume 9 Number 3 September 1994

Powder Diffraction An international journal of materials characterization

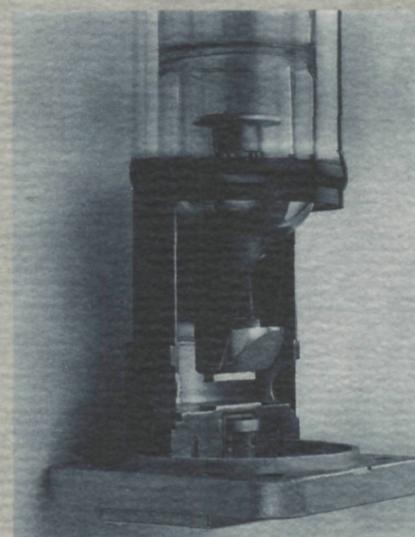
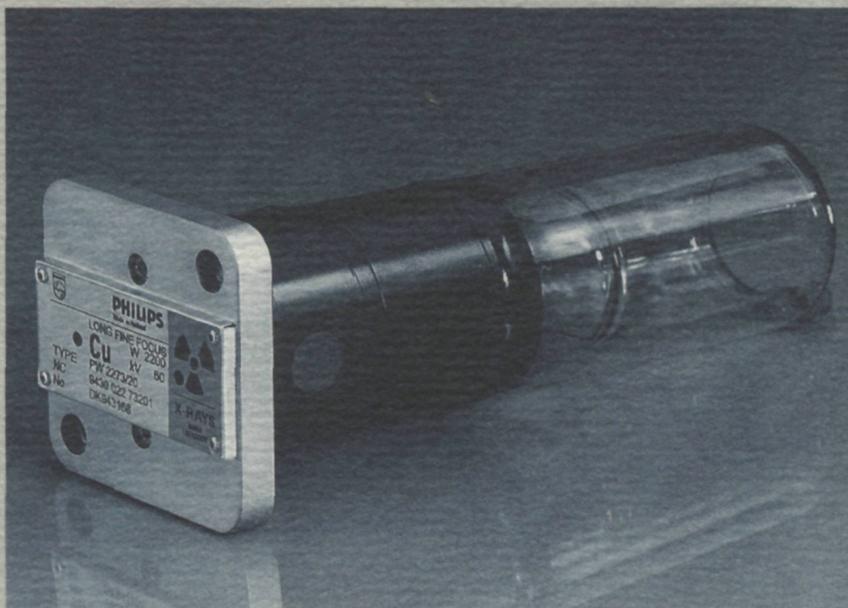
XRD quality and reliability. In a tube.

Even if you don't use our XRD equipment, you can still benefit from Philips' leading-edge diffraction technology. By fitting one of our compatible high-power XRD tubes to your machine.

At Philips we pioneered the tube design now used in all leading X-ray diffractometers on the market.

And we're still ahead. Take, for example, our patented cooling surface applied to the tube's anode. Lower operating temperature means longer tube life. So we guarantee all our XRD tubes for a full 2,500 trouble-free operating hours.

Whatever your XRD application, and wherever in the world you operate, the Philips global supply and service network can deliver the right tube-fast. Our standard range offers seven different types of anode material, covering virtually every aspect of XRD work. And we can advise on and supply less common anode materials too.



Why wait until your current XRD tube comes up for renewal? Talk to us now about a replacement. And we won't even charge you for arranging the safe disposal of your old tube. Whether you want to place an order or discuss a special application, you'll find our people easy to talk to.

Philips Analytical X-Ray BV
Lelyweg 1, 7602 EA Almelo,
The Netherlands.

Tel. +31 546 839430.

Fax +31 546 839598.

**Philips Electronic
Instruments Company**
85 McKee Drive, Mahwah,
NJ 07430, USA.

Tel. +1 201 529 6246.

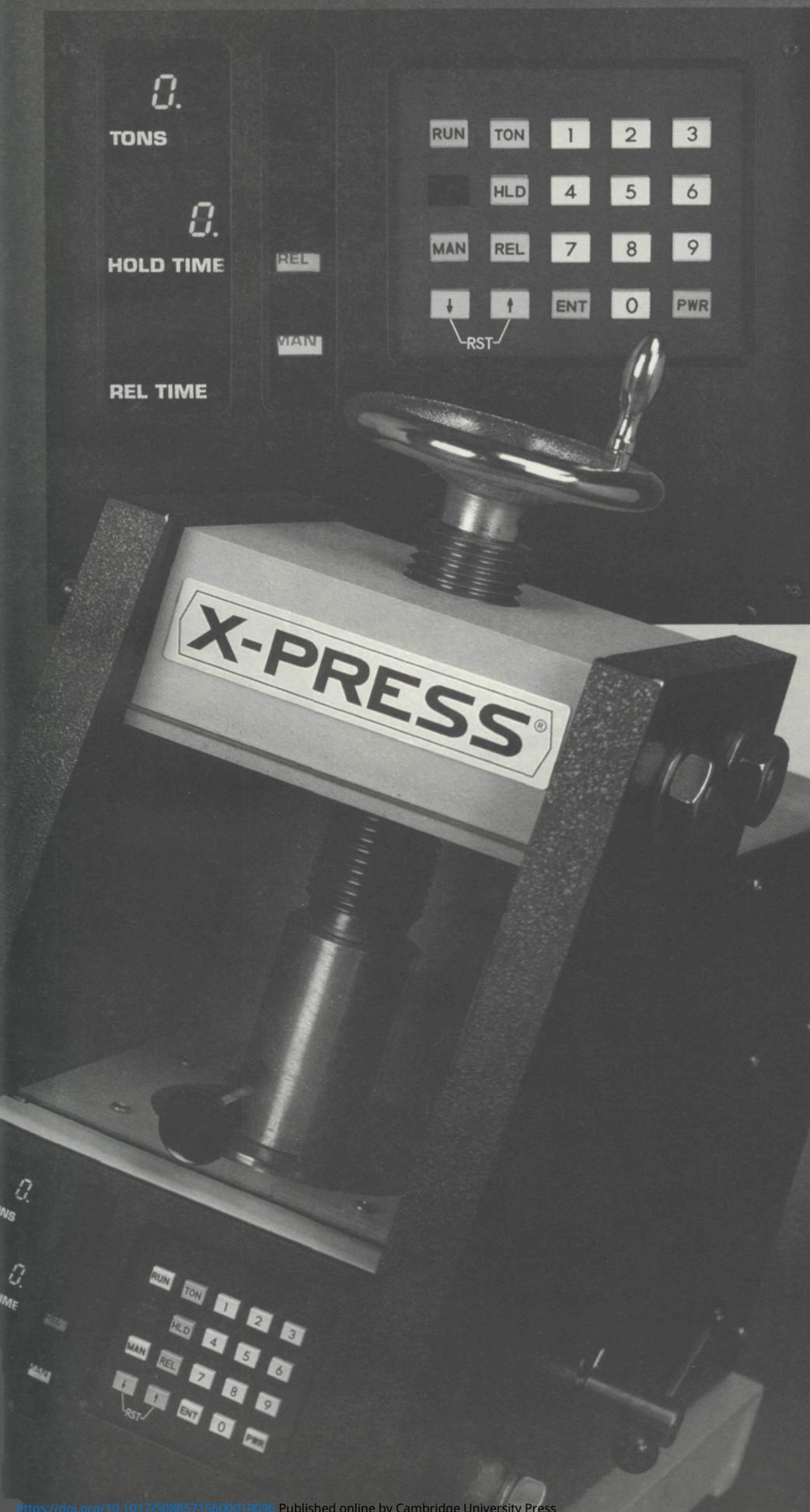
Fax +1 201 529 5084.

**Philips
Analytical
X-Ray**



PHILIPS

Pressed for Time?



Speed up your sample preparation with SPEX's New Automated X-Press

- Microprocessor controlled
- **Complete** pressing cycle performed **automatically**
- 35 ton capacity
- Keypad and LED readout for automatic or manual mode of operation
- All SPEX dies accepted
- System interlock door and pump cutoff for safe unattended operation

For more information about the 3630 automated X-Press and other SPEX products for the analytical laboratory, call (908) 549-7144 or (800) LAB-SPEX

SPEX

INDUSTRIES, INC.
3880 PARK AVENUE
EDISON, NJ 08820 U.S.A.
(908) 549-7144
TELEX: 178341
FAX: (908) 603-9647



DAPPLE[®]
S Y S T E M S

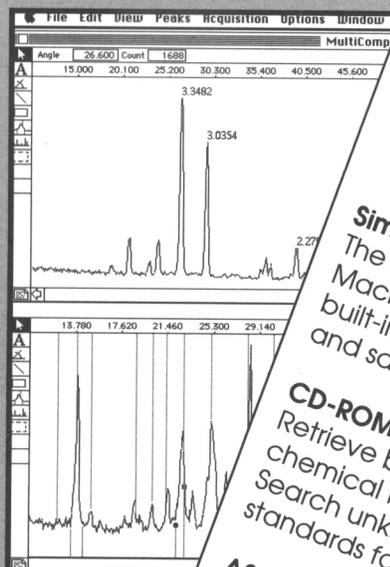
ThetaPlus[®]

Rebuild! Upgrade! Modernize!

A New Generation in X-ray Diffraction

Precise X-ray diffractometer automation:

- Search/Match incorporates  MultiPDF™ for JCPDS database CD-ROM access.
- X-Mate controller provides t... and acquisi...
- Custom Microstep driver gi...
- Convenient user interface... 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.



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

ThetaPlus can be installed 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, Germany
J. Fiala, Plzeň, Czech Republic
V. A. Frank-Kamenetsky, Leningrad, Russia
L. Frevel, Midland, Michigan
P. Gado, Budapest, Hungary
H. Goebel, Munchen, 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
R. L. Snyder, Alfred, New York
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)*, 222 Rosewood Drive, Danvers, MA 01923.

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

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 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

For 1994/95 from ICDD

**International
Centre
for
Diffraction
Data**



12 Campus Boulevard
Newtown Square, PA
19073-3273, USA
(610) 325-9810
FAX: (610) 325-9823
Internet: info@icdd.com

Set 44 PDF

The Powder Diffraction File for 1994/95

X-ray Powder Diffraction Data on more than 59,800 phases,
including Boolean search retrieval software

EDD

**ELECTRON
DIFFRACTION
DATA BASE (1993)**

(NIST/Sandia/ICDD)

Crystallographic & chemical data
on more than 81,500 materials
with search/match software for
identification by electron diffrac-
tion methods*

CDF

**NIST CRYSTAL
DATA FILE (1994)**

Crystallographic & chemical data
on more than 197,600 materials
with retrieval software**

* Available for IBM-PC compatibles, VAX, Alpha AXP, and Macintosh
** Available for IBM-PC compatibles, VAX, and Alpha AXP

General Manager Position

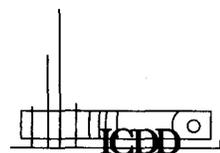
The International Centre for Diffraction Data, a scientific database corporation in the Philadelphia area, is seeking a General Manager. The non-profit corporation operates from a new headquarters facility and serves a world-wide scientific community. Required qualifications include:

- ◆ proven managerial and business experience,
- ◆ a degree (minimum BS) in physical or materials sciences or engineering,
- ◆ experience in XRD work and electronic data handling.

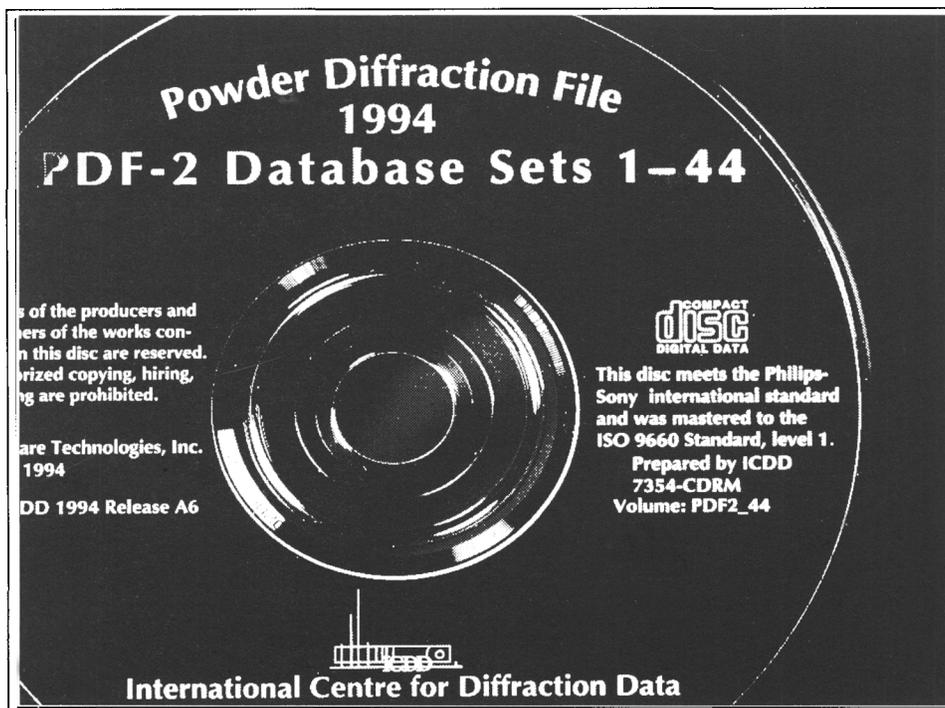
Duties are interesting and diversified and include supervision of 30+ employees and cooperation with about 100 international scientific volunteers.

The deadline for applications is 1 October 1994. Send resumés to:

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



Your Source for X-ray Diffraction Data



The Powder Diffraction File

Approximately 60,000 unique phases.

PC-PDF

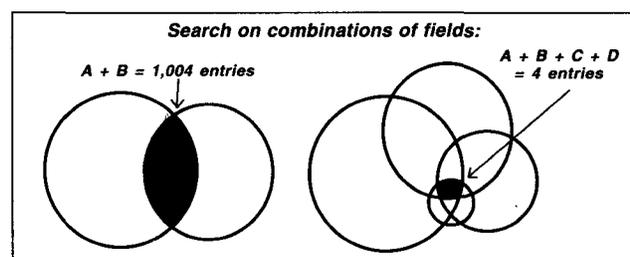
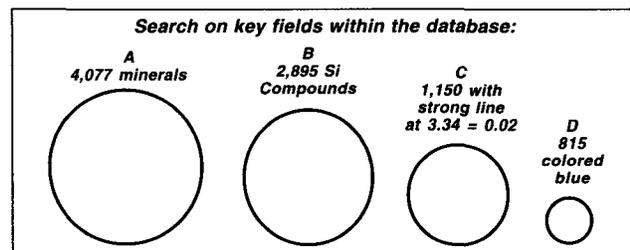
A unique scientific database

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.

DOS or Windows® retrieval programs available

Speed and Flexibility

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

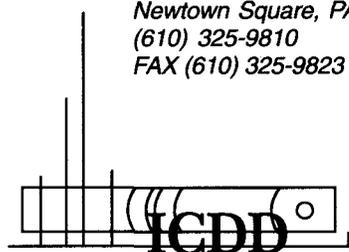


Other Files, Publications & Services

- PC Search Index, a "computer-readable" search manual for the Powder Diffraction File
- 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...
 - The Dow Polymer Pattern Collection
- Regularly scheduled clinics and workshops.

For information, contact:

M. M. Fornoff
Sales/Marketing Manager
12 Campus Boulevard
Newtown Square, PA 19073-3273, USA
(610) 325-9810
FAX (610) 325-9823



Expand your x-ray diffraction capabilities — not your overhead.

Whether you just need services or your XRD lab is on "overload," IC Laboratories provides every testing service and advanced capability you need in qualitative or quantitative x-ray diffraction analysis — from austenite to zeolites, from air filters to thin films. You are assured of rapid turn-around of results — as little as 48 hours — because IC Labs is one of the most highly automated commercial labs in the U.S., with knowledgeable personnel ready to address all your applications. For a copy of our technical prospectus, contact IC Laboratories.

IC Laboratories

Post Office Box 721
Amawalk, New York 10501
(914) 962-2477

We're the Specialists in XRD

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

INDEX TO ADVERTISERS

Dapple Systems	A2
Gem Dugout	A6
IC Laboratories	A6
ICDD	A4, A5
Philips Analytical X-Ray	Cover 2
Scintag	Cover 4
Seifert X-Ray Corp.	Cover 3
Spex Industries	A1

Advertising Sales Office

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

Advertising Manager:	Richard T. Kobel
Asst. Advertising Manager:	Arnie W. Schweitzer
Advertising Representative:	Robert G. Finnegan
Production:	Marcia Schlissel