

# Powder Diffraction

R.L. Kath, M.N. Spilde, B.L. Davis and D.K. Smith	Reference Intensity Ratio and Mass Absorption Measurements of Eleven Biotites	183
W. Wong-Ng and B. Paretzkin	Crystal Chemistry and Phase Equilibria Studies of the BaO-R <sub>2</sub> O <sub>3</sub> -CuO Systems. II: X-Ray Characterization and Standard Patterns of BaR <sub>2</sub> O <sub>4</sub> , R = Lanthanides	187
M. Laügt, M. Teisseire and J. Guion	Crystal Data and Solid-Liquid Transformation Study by DSC of 2 Hydroxymethyl-2 methyl-1,3 propanediol tetrahydrate	190
J.-E. Jørgensen and S.E. Rasmussen	Refinement of the Structure of MnSi by Powder Diffraction	194
G. Bandoli, M. Nicolini and A. Ongaro	Powder Diffraction Data of Three 9-Amino-1,2,3,4- Tetrahydroacridine Alzheimer's Disease Therapeutics	196
D. Rafaja and V. Valvoda	Angular Corrections for the Seemann-Bohlin X-Ray Diffractometer	200
R.L. Snyder, M.C. Nichols and D.R. Boehme	The Crystal Structures and Powder Diffraction Patterns of the Uranium Tellurides: A Critical Review	204
S. Kamoun	Crystal and X-Ray Powder Data for a New Organic Diphosphate [NH <sub>3</sub> (CH <sub>2</sub> ) <sub>2</sub> NH <sub>3</sub> ] <sub>2</sub> ·P <sub>2</sub> O <sub>7</sub>	228
	International Report	231
	Calendar of Meetings	231
	Correspondent's Reports	233
	Computer Comments	235
	Commercial Announcement	236
	Volume 6, 1991    Contents	237
	Author Index	239



Volume 6 Number 4 December 1991

Powder Diffraction    An international journal of materials characterization

# SIEMENS

## Is your diffraction system as flexible as you are?

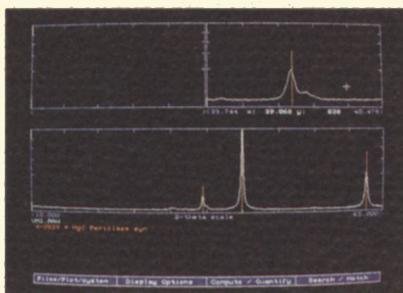
When the only thing you can count on in your lab is change, don't lock yourself in with a system designed to handle only some of your powder diffraction applications. If what you really need is flexibility, your options are open with the Siemens D 5000 X-ray diffractometer.

The modular D 5000 offers superior accuracy and speed with the most flexible and easy-to-learn software available worldwide. Most accessories can be installed or removed in minutes.

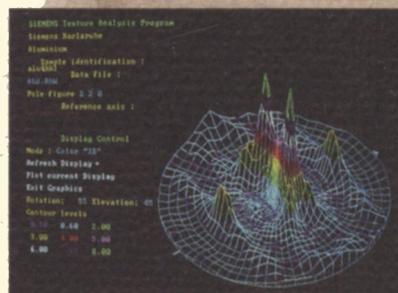
If flexibility is what you need, **Siemens delivers satisfaction.**



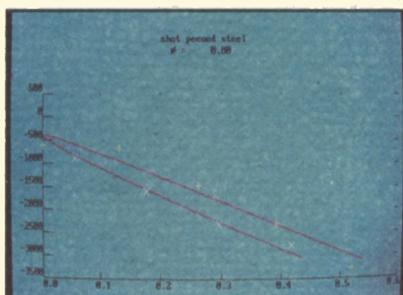
*Raw data, full pattern phase analysis within the EVA2 graphics program.*



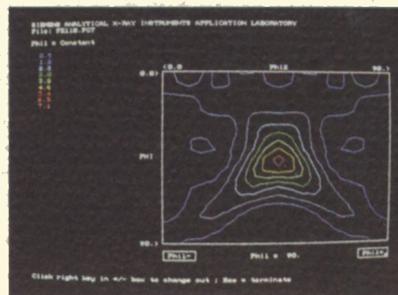
*Flexible 3-D texture analysis software includes polefigure and constant phi displays.*



*Complete calculation of the full residual stress tensor using uniaxial, biaxial or triaxial stress calculations.*



*Orientation distribution function (ODF) evaluation software provides complete analysis of texture effects.*



In USA & Canada contact: Siemens Analytical X-Ray Instruments, Inc. • 6300 Enterprise Lane • Madison, WI 53719 • (608) 276-3000  
Worldwide contact: Siemens AG, Analytical Systems AUT V 371 • P.O. Box 21 1262 • D 7500 Karlsruhe 21 • Germany • (0721) 595-4295



## Look into $\mu$ PDSM . . . It's more than accuracy. It's performance.

Performance makes  $\mu$ PDSM the one search/match software system that approaches universality. It's the result of many years of research into putting all the complexities of qualitative XRD analysis in a single system for your personal computer—and now we've added graphics with a power that matches the unparalleled performance that established  $\mu$ PDSM's reputation.

The utility of function and clarity of content in  $\mu$ PDSM's graphics go beyond merely attractive presentation, to give you a valuable addition to the analytic power  $\mu$ PDSM puts at your finger tips. With options that include fully integrated CD-ROM PDF-2 retrieval, direct instrument control, data acquisition, and diffractogram analysis,  $\mu$ PDSM

gives you a flexibility of application to match the power of its performance.

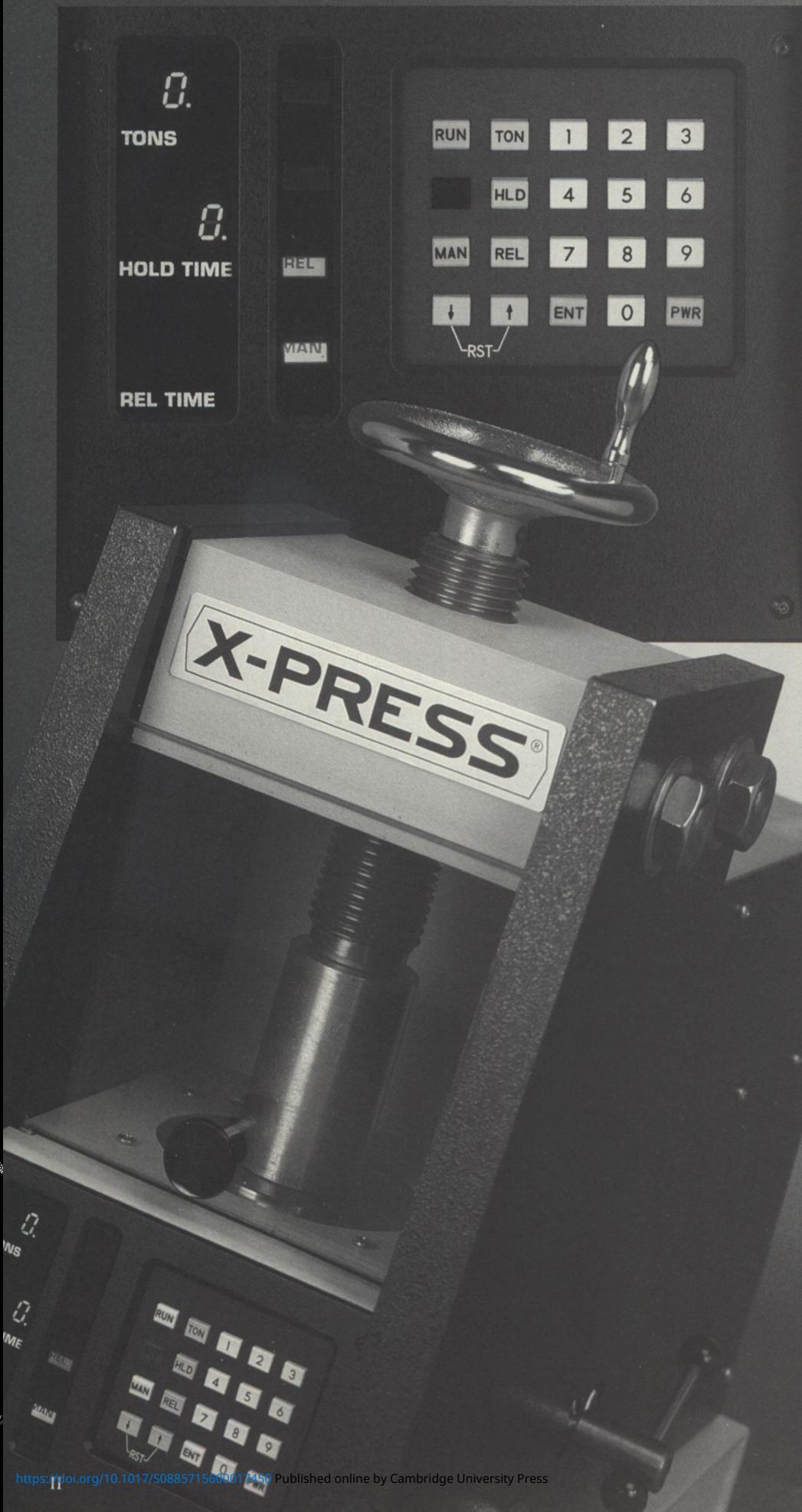
The universal applicability and continuing enhancement of  $\mu$ PDSM reflect the evolving technology of a company dedicated to software innovation. And you realize the results of Fein-Marquart's commitment to progress through a continuing update policy that keeps you at the state of the art.

Look into  $\mu$ PDSM. It takes you beyond accuracy into the next generation of search/match performance.



Fein-Marquart Associates, Inc.  
 7215 York Road · Baltimore, MD 21212  
 (301) 821-5980

# 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

# Powder Diffraction

An International Journal of Materials Characterization

## Deane K. Smith

Editor in Chief  
Dept. of Geosciences  
The Pennsylvania State University  
239 Deike Building  
University Park  
Pennsylvania 16802 USA

## Jan W. Visser

European Editor  
Henry Dunantlaan 81  
2614 GL, Delft  
Netherlands

## Helein D. Hitchcock

International Reports  
Editor  
NASA DM-MSL-1  
Kennedy Space Center  
Florida 32899, USA

## Ron Jenkins

Managing Editor  
JCPDS-International Centre  
for Diffraction Data  
1601 Park Lane  
Swarthmore  
Pennsylvania 19081 USA

## Brian H. O'Connor

Editor for Australia  
and New Zealand  
Curtin University  
Dept. of Applied Physics  
GPO Box U 1987  
Perth 6001 Western Australia  
Australia

## Richard N. Rose

Assistant Editor and  
Manager of Publication

## Gregory J. McCarthy

Editor for New Diffraction Data  
North Dakota State University  
Department of Chemistry  
Fargo, North Dakota 58105-5516 USA

## Hideo Toraya

Editor for Japan  
Ceramics Research Laboratory  
Nagoya Institute of Technology  
Asahigaoka, Tajimi 507 Japan

## Mary M. Rossi

Assistant to the  
Managing Editor

## Editorial Advisory Board

C.S. Barrett, Denver, Colorado  
P. Bayliss, Calgary, Alta., Canada  
C.Z. Bojarski, Katowice, Poland  
A. Brown, Nykoping, Sweden  
L.D. Calvert, Melbourne, Australia  
D. Cox, Upton, New York  
W. Eysel, Heidelberg, West Germany  
J. Fiala, Plzeň, Czechoslovakia  
V.A. Frank-Kamenetsky, Leningrad, U.S.S.R.  
L. Frevel, Midland, Michigan  
P. Gado, Budapest, Hungary  
H. Goebel, Munchen, West Germany  
G.G. Johnson Jr., State College, Pennsylvania  
Q. Johnson, Livermore, California  
J.I. Langford, Birmingham, U.K.

D. Louër, Rennes, France  
H.F. McMurdie, Washington, District of Columbia  
M.E. Mrose, Washington, District of Columbia  
M.H. Mueller, Argonne, Illinois  
M. Nichols, Livermore, California  
B.H. O'Connor, Bentley, Australia  
B. Post, West Roxbury, Massachusetts  
E. Prince, I.U.Cr. Representative  
R.L. Snyder, Alfred, New York  
H. Toraya, Japan  
J.W. Visser, Delft, Netherlands  
S. Weissman, Piscataway, New Jersey  
T. Yamanaka, Tokyo, Japan  
R.A. Young, Atlanta, Georgia  
L. Zevin, Beer-Sheva, Israel

## Publisher

JCPDS-International Centre for Diffraction Data, 1601 Park Lane, Swarthmore, Pennsylvania 19081, U.S.A.

*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.

*Powder Diffraction* is published four times annually by the JCPDS-International Centre for Diffraction Data.

*Manuscript submissions.* The Editors will consider all manuscripts received, but assume no responsibility regarding them. Materials will be returned only when accompanied by appropriate postage.

*Subscriptions.* The annual subscription rate in the United States and Canada is \$55.00; Library; \$95.00; other than U.S.A., Canada and the Far East, the annual subscription is \$75.00. Subscriptions to the Far East, including Japan, China, Taiwan, Malaysia, the Philippines, Indonesia and Korea should be made via Sanyo Information System Corp., Taiyo Bldg. 7-7, Tomizawa-cho Nihonbashi, Chuo-ku, Tokyo 103, Japan. Airmail delivery available for subscribers outside U.S./Canada for an additional cost of \$35.00 per volume (4 issues).

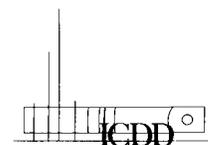
Payment may be made in U.S. dollars by company check, MasterCard, Visa or international money order. Please address communications to the publisher's office.

*Advertising.* For advertising rates and schedules contact the Publisher's Office JCPDS-International Centre for Diffraction Data, 1601 Park Lane, Swarthmore, PA 19082, Telephone (215) 328-9405.

*Reprints and permissions.* Contact the Publisher's office.

*Postal Information.* Powder Diffraction (ISSN 0885-7156) is published quarterly for \$55.00 a year (U.S. and Canada) by JCPDS-International Centre for Diffraction Data, 1601 Park Lane, Swarthmore, Pennsylvania 19081. JCPDS principal office: 1601 Park Lane, Swarthmore, Pa. 19081. Julian Messick, Jr., General Manager. © 1990 JCPDS-International Centre for Diffraction Data. Postmaster: Send address changes to JCPDS-International Centre for Diffraction Data, 1601 Park Lane, Swarthmore, Pennsylvania 19081.

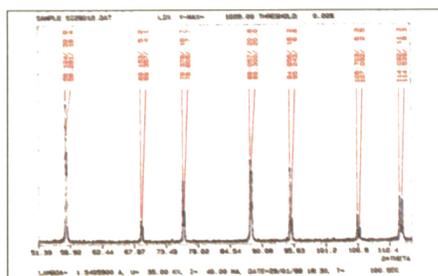
International CODEN Service (Intercode): PODIE2  
ISSN 0885-7156  
Telex 847170  
FAX 215 328 2503



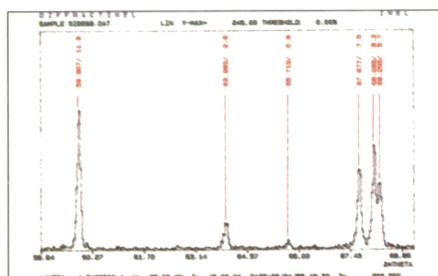
THE CHOICE OF THE FUTURE  
**SIMULTANEOUS XRD**  
**OVER 120° - 2 THETA**  
**- FAST - ACCURATE - RELIABLE -**



CPS 120 MOUNTED ON TGS (TRANSMISSION AND REFLECTION MODE)



SILICON  $\lambda = \text{CuK}\alpha$



QUARTZ  $\text{SiO}_2$   
 MONOCHROMATOR : QUARTZ



FAST DIFFRACTOMETER

**ACCESSORIES :**

**CRYOSTAT - FURNACE - SAMPLE SPINNER -  
 AUTOMATIC SAMPLE CHANGER - and  
 X-RAY GENERATOR etc...**

**APPLICATIONS :**

**POWDER, STRESS, and TEXTURE WITH  
 MATCHING SOFTWARE**

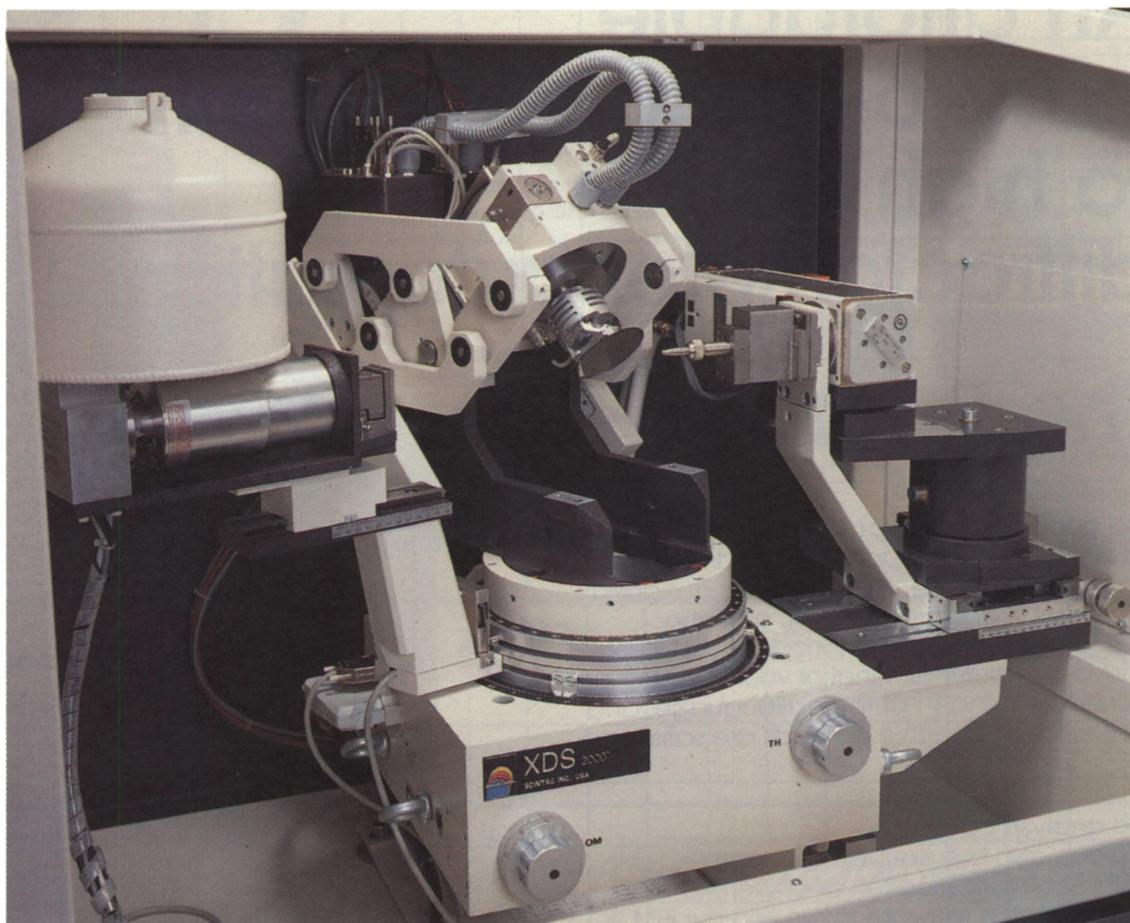
**inel**

12, avenue de Scandinavie  
 91953 LES ULIS CEDEX FRANCE  
 PHONE 33 (1) 69.86.13.30  
 FAX 33 (1) 69.86 14 19  
 TELEX 603965

or: 50 Campus Plaza Drive  
 Edison, NJ 08837  
 PHONE (908) 417-0070  
 FAX (908) 417-0430

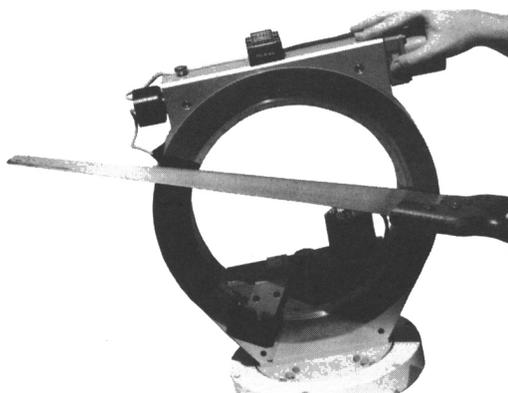
**ASK FOR MORE INFORMATION AND ADDRESS  
 OF OUR REPRESENTATIVE IN YOUR COUNTRY**

**With Scintag's PTS Goniometer there's no longer a reason to modify your circle and limit your range**



- Unrestricted Two-Theta range up to 165°
- Large Psi angle range for stress tensor work
- Versatile sample thickness and weights
- $\pm 90^\circ$  Chi range provides complete stress data

Got an open-ended research project that is "stressing you out?"



Call us today - our Polycrystalline-Texture-Stress goniometer is the 3 in 1 solution to alleviate research stress in the 90's.

**Scintag, Inc.**

707 Kifer Road  
Phone (408) 737-7200

Sunnyvale, CA 94086  
FAX: (408) 737-9841

# Finally. An affordable, easy-to-operate alternative to high cost diffractometer automation.

*Radix Instruments Joins the MDI Team.  
For Complete XRD Solutions  
for your PC, see the MDI Ad in this Issue*

## The Databox.

### The acquisition package:

The Databox is a stepping motor driver and data collection system specifically designed to control your diffractometer, all in the space of a two-wide NIM module. Just talk to it from a computer terminal or your PC using an incredibly friendly command language, and all your data acquisition needs are satisfied.

### The analysis package:

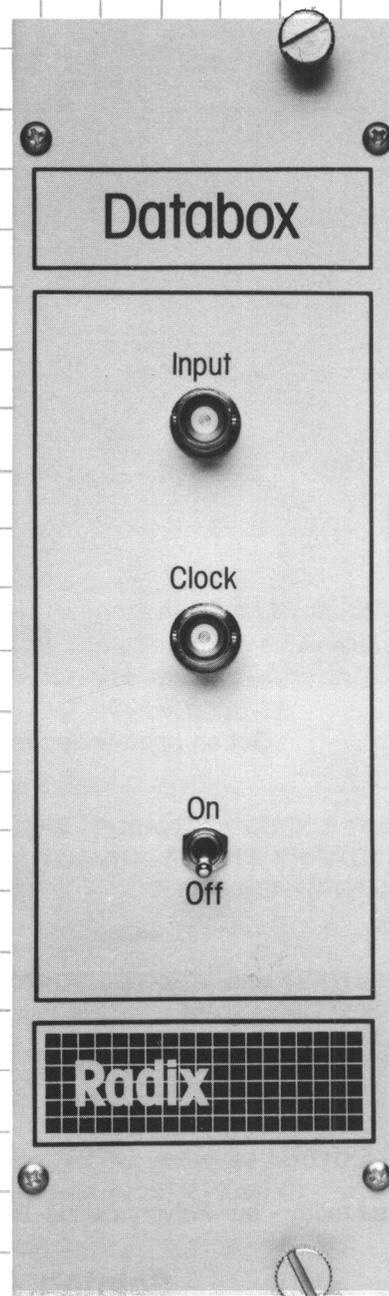
You can also buy the Databox bundled with MDI's Peak Identification and Micro-ID Search/Match software to run on your IBM PC (or compatible), giving you a complete x-ray control, acquisition, and analysis system.

### The bottom line:

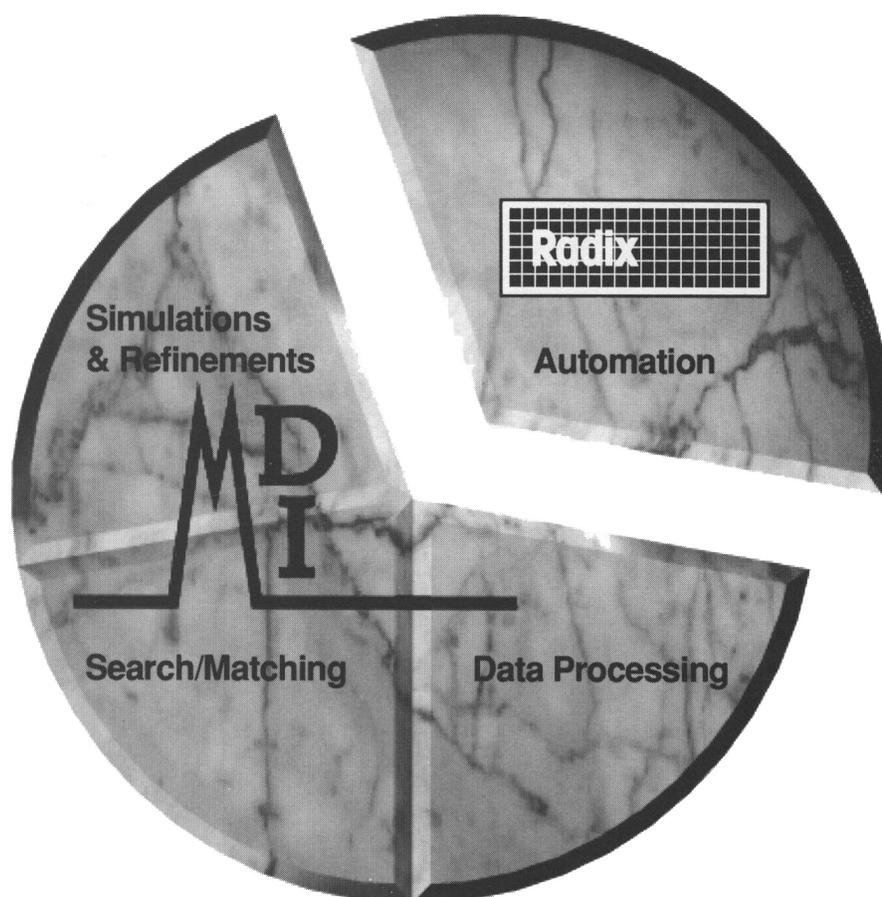
For well under \$5000, the Databox will fully automate your x-ray equipment. Add the analysis software, and the total cost is just over \$10,000.

Finally. A system with proven reliability and performance at a reasonable price. To learn more, contact us at:

Radix Instruments  
3312 Febo Court  
Carlsbad, California 92009  
Phone/FAX: (619) 753-4646



# Complete XRD Solutions for your PC from MDI



## ***Radix Instruments Joins the MDI Team - It's a Perfect Fit!***

Our company creates professional XRD software for the PC - software designed for the specialist, yet easy for the less experienced to use. MDI was founded by Materials Scientists. We speak your language; we have more than a century of materials laboratory experience within our team. At MDI, we develop XRD software for the most effective computer systems; support the newest technologies; and make complex analysis and simulations simple. Now, with the addition of Radix Instruments, MDI can provide you with a single source for PC software and automation for your manual systems. You will find our affordable solutions at National Labs and Fortune 500 companies. If you would like to know more about our complete XRD solutions for your PC, call us.

- **Automation**
- **Data Processing**
- **Search/Matching**
- **Simulations and Refinements**



Radix Instruments is a division of Materials Data, Inc.

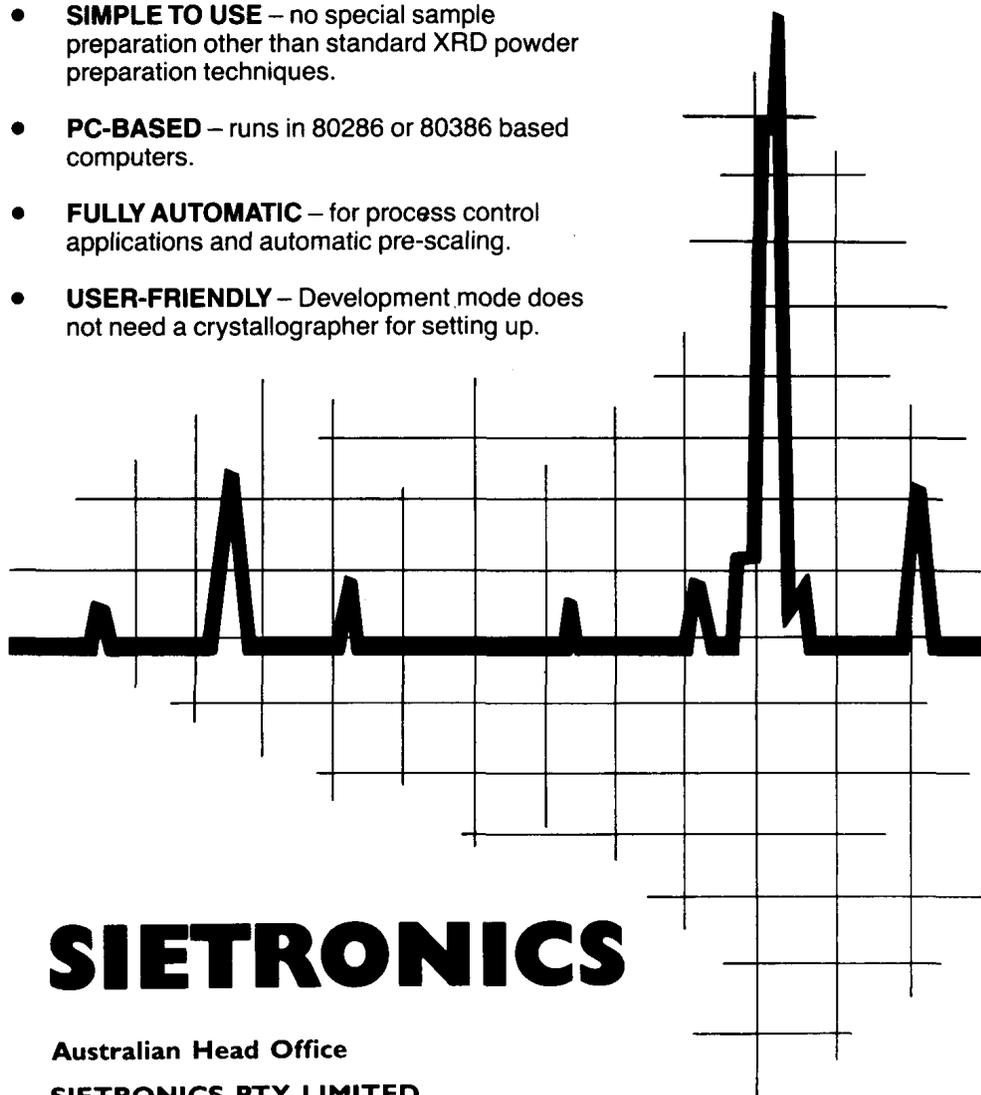


Materials Data, Inc.  
Post Office Box 791  
Livermore, California 94551  
Tel. 415/449/1084  
FAX 415/373/1659

# STANDARDLESS QUANTITATIVE XRD PHASE ANALYSIS SOFTWARE

## SIROQUANT<sup>(c)</sup> IS:

- **ACCURATE** – overcomes preferred orientation and absorption contrast errors to give 5% absolute accuracy.
- **SENSITIVE** – due to full-profile fitting, concentrations down to 1% can be determined.
- **STANDARDLESS** – no requirements for artificial mixtures except to check amorphous contents.
- **SIMPLE TO USE** – no special sample preparation other than standard XRD powder preparation techniques.
- **PC-BASED** – runs in 80286 or 80386 based computers.
- **FULLY AUTOMATIC** – for process control applications and automatic pre-scaling.
- **USER-FRIENDLY** – Development mode does not need a crystallographer for setting up.



## **SIETRONICS**

Australian Head Office

**SIETRONICS PTY LIMITED**  
P.O. Box 3066  
Belconnen ACT 2617 Australia

Phone: (06) 251 6611

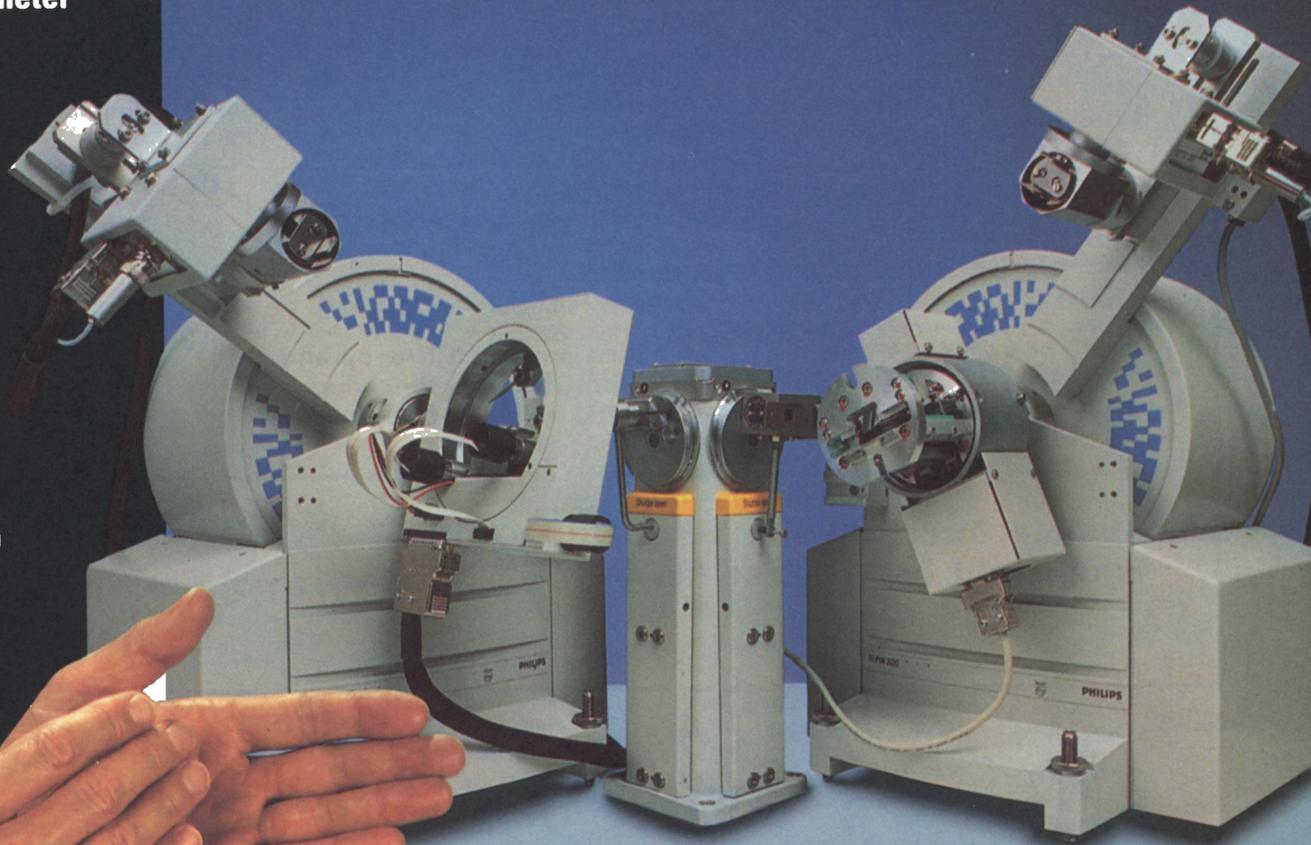
Telex: AA 62754

Fax: (06) 251 6659

# A twinstar is born. The brilliant Philips X'Pert.

A brand-new  
X-ray diffractometer  
for analytical  
versatility!

(Yet this is one of  
216 possibilities...)



Well, we have brought it off. We developed a new generation of Multi-Purpose Diffractometer systems. No need any longer for instrument reconfiguration. Now you can perform multiple experiments in a twinkle, without component interchange. And: in a highly accurate way thanks to advanced optical technology. Philips X'Pert is really made to measure, and designed for twin configuration. And if your requirements alter in the long term? The X'Pert is easily expanded to fit new applications. Of course there is a lot more to say about the brilliant X'Pert.

If you want to know all about its analytical versatility and your specific applications: just write, phone or fax for it. Or contact your local Philips office.

#### **Philips Analytical**

Lelyweg 1, 7602 EA Almelo  
The Netherlands  
Tel: 0 (31) 5490 - 39911  
Telex: 36591 PPIT NL  
Telefax: 0 (31) 5490 - 39598

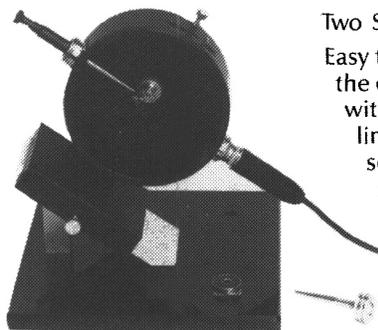


PD9

# PHILIPS

# Supper

## Complete Debye-Scherrer Powder Camera Systems Accessories, and Film



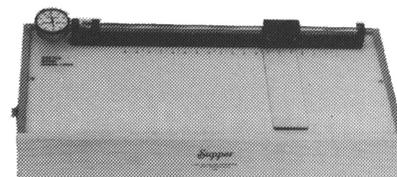
114.6mm Powder Camera with optional viewing stand, illuminator, and Gandolfi "Single Crystal Randomizer" which is interchangeable with standard powder sample holders

Two Sizes: 114.6mm camera, 57.3 camera  
Easy to load and unload in the darkroom, the cameras are precision manufactured with no screw-on components. The collimator and beamtrap are accurately secured in position magnetically and a removable sample holder permits insertion of the specimen sample outside the body of the camera.

Guinier Camera for transmission and reflection photographs is also available.

**Simplified Specimen Line-up and Darkroom Handling Procedures Offer the Ultimate in Convenience**

- Gandolfi "Single Crystal Randomizer"
- Sturdy Viewing Stand and Illuminator
- Precision Film Punch and Trimmer
- Universal Track and Tripod Mount
- Large Inventory of Capillary Tubes
- Large Inventory of Kodak 35mm Film
- Film Measuring Device and Illuminator



Reads accurately to 0.01mm and eliminates eyestrain

**Manufacturers of Fine X-Ray Diffraction Equipment For Over 45 Years**

*Charles Supper Company*  
INCORPORATED

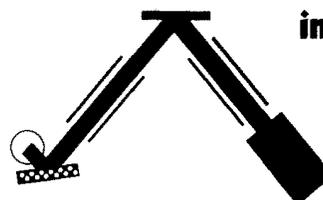
15 TECH CIRCLE, NATICK, MA 01760, U.S.A.  
TELEPHONE: (508) 655-4610  
1-800-323-9645

PD10

## Advance Your Skills Attend an ICDD Short Course or Clinic



in XRD



in XRF

### In our Three Day Short Course you will ...

- Learn to identify/characterize crystalline substances using powder diffraction data.
- Build proficiency in interpretation of powder patterns of unknown materials, using the *Powder Diffraction File*.
- Have hands-on work sessions in manual and computer search methods ... Comprehensive work book provided.

### Our Clinics consist of two one-week courses each, in either XRD or XRF...

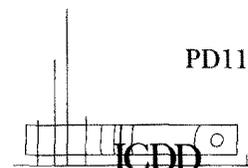
- 1st week ... Fundamentals of discipline, emphasis on instrumentation, specimen preparation & data acquisition ... Qualitative & simple quantitative analysis methods.
- 2nd week ... Advanced methods in XRD and XRF, respectively, with emphasis on computer-based methods of data collection & interpretation.

**Short courses:** Florida, March, 1992 ... West Coast, November, 1992

**XRD & XRF Clinics:** June/July 1992. Swarthmore College, Swarthmore, PA, USA

For information contact ... Ms. Josephine Felizzi ... Dr. Ron Jenkins  
(Short Courses) (Clinics)

International Centre for Diffraction Data  
1601 Park Lane, Swarthmore, PA 19081 USA  
Tel: (215) 328-9400 FAX: (215) 328-2503  
Telex: 847170



PD11

# Requiem for a heavyweight

The fact is, our new Psi Peltier cooled silicon detector obsoletes monochromators and proportional detectors and their "blind" PHA electronics.

Psi is small and lightweight, mobile and worry free—the first to deliver solid state detector performance without the clumsiness of liquid nitrogen.

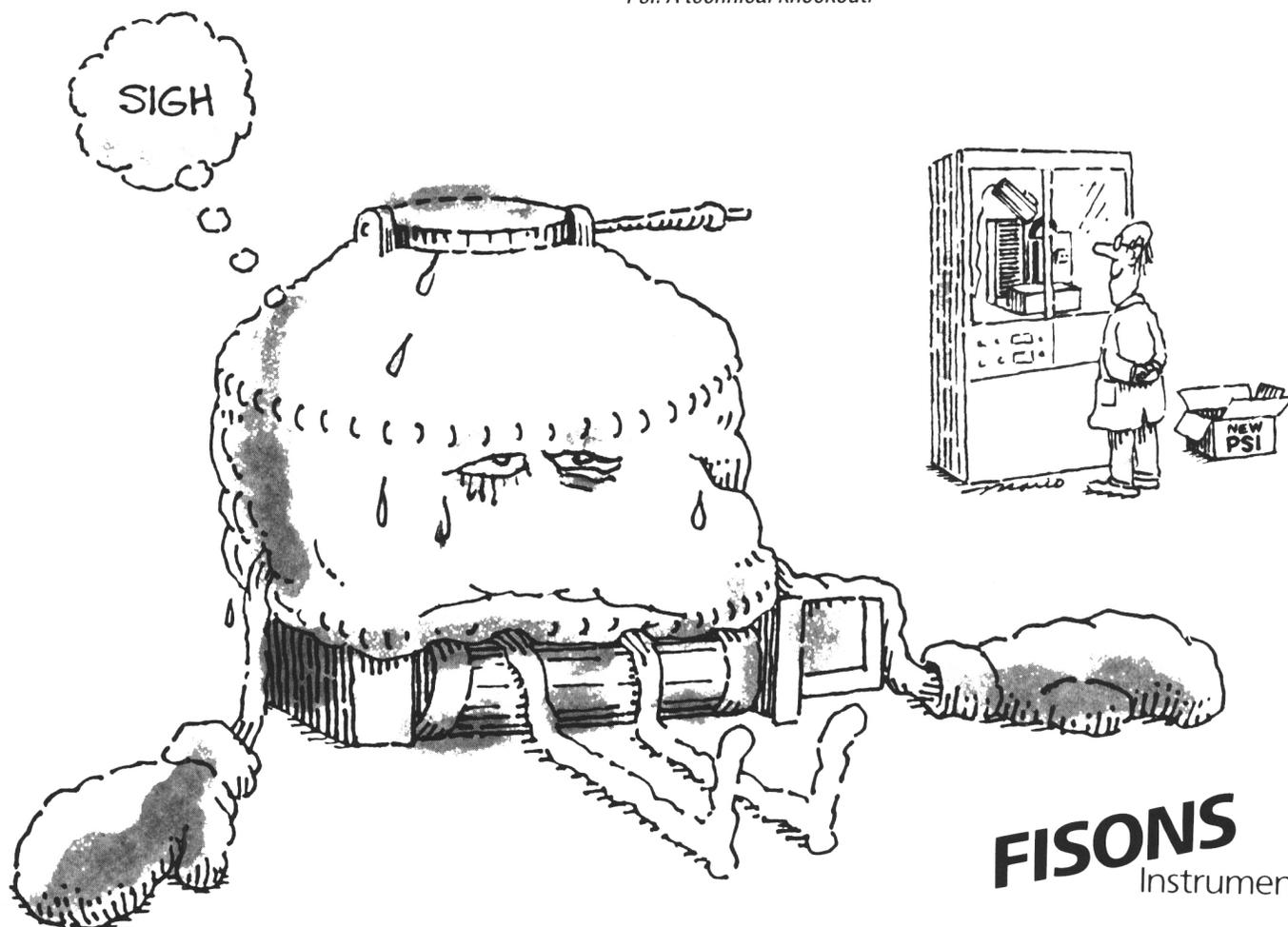
With Psi, you get 3 to 5 times faster throughput, 10 times better energy resolution. And the best diffraction patterns you've ever seen. Psi is like having an electronic monochromator. You get clear  $K\alpha$  or  $K\beta$  patterns from any tube anode.

Teamed with spectrum analyzer electronics, Psi gives you the complete sample spectrum. Fully resolved. This means you choose your peaks, then optimize the patterns to fit your application—Compton-Rayleigh for instance. Or XRF/XRD studies.

Better still, Psi comes with mechanical and electronic interfaces that make it 100-percent compatible with existing diffractometers. Not just new ones.

For a list of leading companies now using Psi with their systems—plus complete technical and upgrade information—write or call toll-free today. 800-227-0277.

*Psi. A technical knockout.*



KeveX Instruments 355 Shoreway Road, San Carlos, CA 94070-1308 415-591-3600 800-227-0277  
KeveX Affiliate (Getac GmbH) Tel 49-6131-40091 KeveX France (Fondis, S.A.) Tel 33-1-34810024 KeveX Japan (Kawasho) Tel 03-578-5187

**FISONS**  
Instruments

**keveX**

# The Controller for Powder Diffractometers

that you can control

**UDS 2** is a self contained controller which can count up to 500000 events per second, store countrates internally, drive a stepper motor, can communicate with every computer via the standard serial line and is programmable in BASIC (in case you want to write your own application). It comes with a built in program in EPROM to run a powder diffractometer, which starts as soon as you switch it on. It accepts measuring parameters via the RS 232 line and then carries out the measurements on it's own, i.e. any computer can be disconnected. It stores over



12000 countrates internally, all of which can be read out via the serial line within a couple of minutes. There are 16 I/O lines to control various other things, if you wish to. **UDS 2** is not designed as a PC card, so as not to restrict it's use to a particular type of computer. Thus practically any computer can run a powder diffractometer and still be used in the normal way while the measurement is going on. You can connect **UDS 2** to an ATARI, VAX or whatever is available. There is no need to wholly devote a computer to a diffractometer.

When writing your own applications with **UDS 2**, all resources are accessible without the knowledge of any assembly language - just through BASIC statements. To store your own programs permanently in an EPROM doesn't take any separate device, but only one simple command - the necessary hardware is already built in. **UDS 2** is a controller you can tailor to your needs - or use as is. It is available as either a table top or as a NIM module.

And should you happen to have a Philips PW 1050/70 diffractometer which you would like to run with **UDS 2**, there is a conversion kit available, complete with stepper motor, mounting adapter, limit switch and connecting cables.

Another attractive item is it's - especially for universities - low price tag.

Steuerungstechnik Skowronek Antoniusstr.3 P.O. Box 1346 5170 Jülich Germany PD13

**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

PD14

For 1991/92 from ICDD...



## Set 41 PDF

In all current media

CD-ROM & Mag Tape... Microfiche ... Book

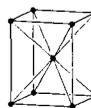
Over 2000 new &/or updated entries in PDF-1 and PDF-2†



## EDD Electron Diffraction Data Base

(NIST/Sandia/ICDD)

Crystallographic & chemical data on over 71,000 crystalline materials.\*

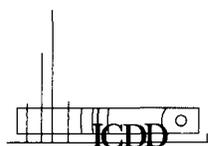


## NIST Crystal Data File

Crystallographic & chemical data on over 149,000 crystalline materials\*

†Available for IBM-PC compatibles, VAX & Macintosh

\*Available for IBM-PC compatibles & VAX



International Centre for Diffraction Data  
1601 Park Lane, Swarthmore, PA 19081  
USA (215) 328-9400 Telex: 847170

PD15

# APD 2000 Diffractometric System

## GD 2000 Goniometer

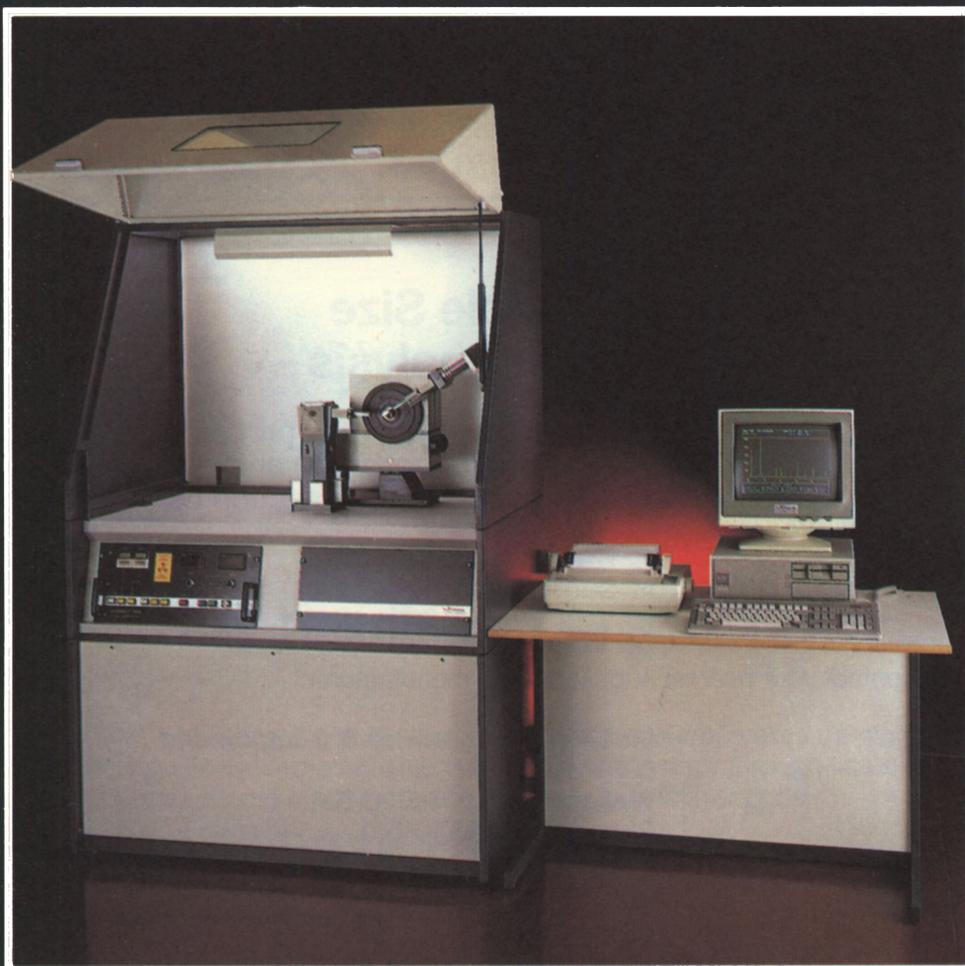
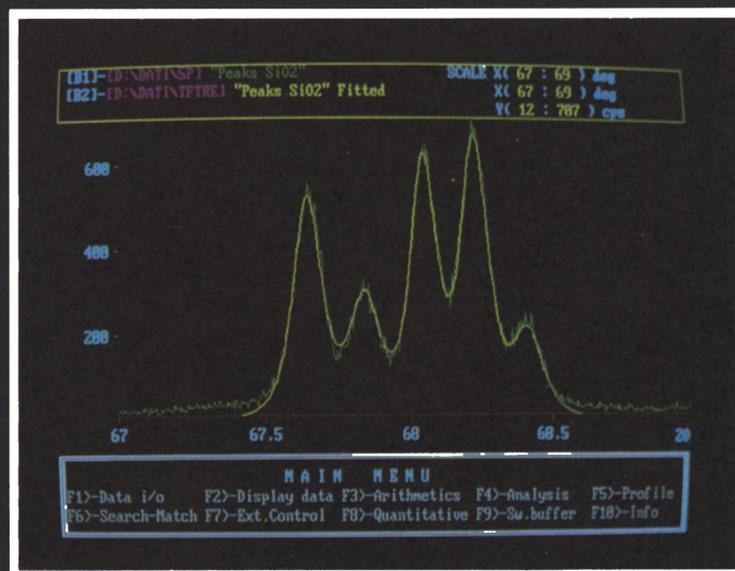
- High resolution
- 2 step motors
- Horizontal and vertical configuration

### SPECIAL VERSION:

*Seeman-Bohlin geometry*

## Compact 3K5 Generator

- Advanced technology design
- High stability
- Less than 40 kg



## PDAP 45 Powders Software Package

- Profile Analysis
- Search-Match
- Crystallinity
- Quantitative Analysis
- Stress

## Accessories

- Position Sensitive Detector
- Focusing Monochromator
- Eulerian Cradle
- High- and Low-Temperature Chamber



38066 RIVA DEL GARDA - Zona Industriale Baltera (ITALY) - Tel. 0464/553426 - Fax 0464/555270

<https://doi.org/10.1017/S0885715600017450> Published online by Cambridge University Press

PD16

XIII

# Theta.XRD<sup>TM</sup> ThetaPlus<sup>TM</sup>

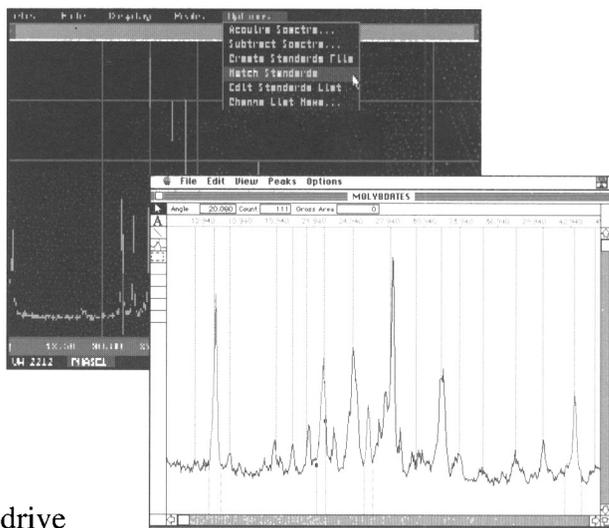
X-ray Diffractometer Automation  
from Dapple Systems

Enhance the analytical performance of your x-ray diffractometer. Choose **Theta.XRD** for IBM PC compatibles or **ThetaPlus** for the Macintosh II series computers.

Both provide:

- Precise stepping motor control of the two-theta drive
- Automatic peak height and d-spacing calculation
- Time-saving search/match operation
- Clear and efficient operator interface

Assure continued reliable operation from your existing system, at a fraction of the cost of replacement. To learn more about the best way to automate your x-ray diffractometer, call or write today.



355 W. Olive Avenue, Suite 100  
Sunnyvale, CA 94086  
Tel: (408) 733-3283  
Fax: (408) 736-2350

PD17

## Rapid Reduction of Sample Particle Size for Quantitative X-Ray Diffraction Analysis

The **McCrone Micronising Mill** has been designed to overcome problems associated with preparation of solid samples for qualitative and quantitative analysis. Quick size reduction of troublesome samples by linear and planar grinding action using agate or corundum grinding elements.

Wet grinding in polypropylene containers promotes sample homogeneity. Sample capacity: up to 5 ml.

For further details and technical brochure, contact your nearest supplier or the manufacturer:

**McCrone Research Associates Ltd.**  
(Manufacturer)  
2 McCrone Mews, Belsize Lane  
London NW3 5BG U.K.  
Phone: 071 435 2282  
FAX: 071 435 5270

**Tintometer GmbH**  
Schleefstrasse 84  
D-4600 Dortmund 41  
West Germany  
Phone: (0231) 435051  
FAX: 0231 44 80 20

**McCrone Accessories & Components**  
850 Pasquinelli Drive  
Westmont, IL 60559 U.S.A.  
Phone: (708) 887-7100  
FAX: (708) 887-7417

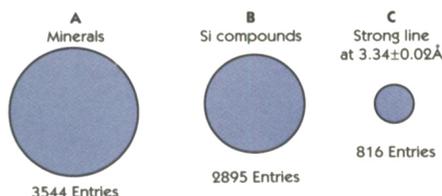
**Selby Anax**  
2 Kilroe Street  
Milton  
Queensland 4064  
Australia  
Phone: (07) 371 1566  
FAX: 0787 03769

PD18

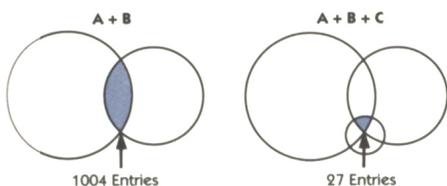
# PC-PDF

## The Powder Diffraction File on CD-ROM

**Search** on key fields within the data base.



**Search** on combinations of fields.



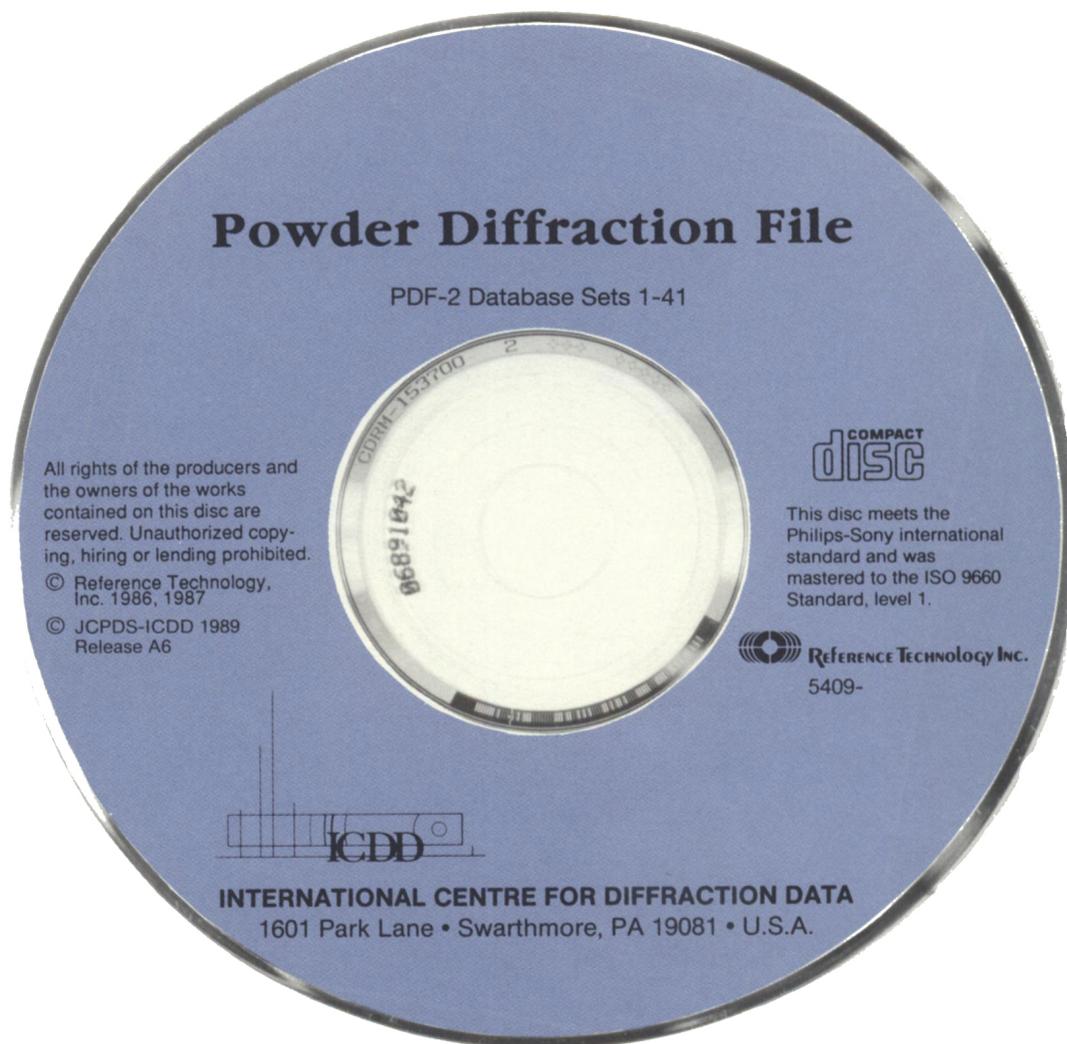
**Display** results within seconds.

**PC-PDF**, a low cost personal computer based system, makes the entire Powder Diffraction File available on a single CD-ROM disk and, through use of optimum packing and access algorithms, displays results within seconds.

- Use with an IBM-XT or equivalent system.
- Annually updated disks will be made from the full data base and will include all additions and corrections.
- Space saving: One disk contains data equivalent to a file cabinet full of Data Cards.

You can now enhance your present system for search, retrieval and display. For additional descriptive material and ordering information, contact:

JCPDS-International Centre for Diffraction Data  
1601 Park Lane, Swarthmore, PA 19081-2389 USA  
(215)328-9400 Telex: 847170



Also available for  
 $\mu$ VAX & Macintosh



# SEIFERT

## X-RAY TUBES



The SEIFERT diffraction X-ray tubes SN 60 with normal focus and SF 60 with fine focus are featured by a high primary intensity at a homogeneous intensity distribution, spectral purity, and a long lifetime.



**SEIFERT X-RAY CORPORATION**  
2551 Industry Lane, P.O. Box 294, Fairview Village, Pennsylvania 19409  
TEL: 215-539-4700 TWX: 510-660-0568 FAX: 215-539-6031

# Editorial

## Accuracy in Powder Diffraction

The first Symposium on Accuracy in Powder Diffraction was held at the U.S. Bureau of Standards in May 1979 under the sponsorship of NBS, the International Union of Crystallography and the International Centre for Diffraction Data. The proceedings of this successful meeting were published as "Accuracy in Powder Diffraction" (NIST Special Publication 567) and have been widely cited in the literature as resource material for further developments in powder diffraction. It has been over 12 years since this symposium, and the importance of powder diffraction in modern materials research has continued to increase. A second Symposium on this important topic has been organized for May 1992 at the same location.

Accuracy in Powder Diffraction II will be held at the National Institute of Standards and Technology in Gaithersburg, Maryland, on 26-29 May 1992. This symposium is being organized by the Commission on Powder Diffraction of the International Union of Crystallography along with NIST and is cosponsored by the International Centre for Diffraction Data. The topics for this meeting include:

- William Parrish Memorial Session
- Accuracy and standards
- Phase identification and quantification
- Profile fitting and total pattern decomposition
  - Microstructure and orientation effects
- New developments in software and data processing
- Structure determination and refinement
  - Phase transitions and novel applications
- New developments in hardware
  - Non-ambient conditions

The program will include keynote invited papers and contributed oral presentations along with posters and workshops. Further program information may be obtained from Program Chairman Rod Hill, CSIRO Division of Mineral Products, 339 Williamstown Road, Port Melbourne, Victoria 3207, Australia. (E-mail address is rodh@dmp.csiro.au). Papers on all the above topics are solicited.

The Local Chairman is Edward Prince, Reactor Radiation Division, E151 Reactor Division, NIST, Gaithersburg, Maryland 20899, U.S.A. (E-mail address is prince@enh.nist.gov or prince@nbsenh). Limited financial assistance is available for young scientists (under age 30), and applications for this assistance are available through the Local Chairman. To get on the mailing list for further announcements of this meeting, interest should be indicated to Carol O'Connor at the same address. Be sure to include E-mail or FAX information.

This symposium should be of interest to all researchers who use powder diffraction to study materials. It promises to bring together scientists from all over the world to interact on this important field.

Deane K. Smith  
Editor in Chief