

Powder Diffraction

S. Wang and X. Pu	General Expression of Quantitative Phase Analysis for Samples Containing Amorphous Phase	62
S. Ariely <i>et al.</i>	A Powder Diffractometry Study of γ' -Phase Formation	66
M.C. Osácar Soriano J. Besteiro Ráfales and J. González Martínez	X-Ray Diffraction Analysis of Strontium in Barites	70
R.J. Hill	Expanded Use of the Rietveld Method In Studies of Phase Abundance in Multiphase Mixtures	74
M.E. Bowden and M.J. Ryan	Comparison of Intensities from Fixed and Variable Divergence X-Ray Diffraction Experiments	78
J.-E. Jørgensen	Automation of FilmScanner for Evaluation of Guinier Films and Applications to Determination of Diffraction Data of $\text{Pb}_2\text{Sr}_2\text{Ho}_{0.625}\text{Ca}_{0.375}\text{Cu}_3\text{O}_8$ and Measurement of Thermal Expansion of GeO_2	82
T. Calvet <i>et al.</i>	Molecular Alloys in the Series of Para-Disubstituted Benzene Derivatives. Part V. The Para-Dibromobenzene Para-Chloriodobenzene	85
M. Gu and A. R. Marder	Quantitative Analysis of a Textured Coating by a New X-Ray Diffraction Method	89
R. Jenkins <i>et al.</i>	Nomenclature, Symbols, Units and their Usage in Spectrochemical Analysis – VIII Nomenclature System for X-Ray Spectroscopy	95
B. Lundtoft and S.E. Rasmussen	X-Ray Powder Diffraction Data for 2,2',2"-triaminotriethylamine-trihydrochloride	102
D.F. Rendle and E.J. Glazier	X-Ray Powder Diffraction Data for Two Antihistamines: Clemizole Hydrochloride and Cyclizine Hydrochloride	104
M. Garsche <i>et al.</i>	Powder Diffraction Data of Some Acentric Tartrates and Tartrato-Antimonates	107
M. Garsche <i>et al.</i>	Powder Diffraction Data of Four Complex Cesium Thiocyanates: $\text{Cs}_3\text{A}[\text{B}_2(\text{SCN})_7]$, with A = Sr, Ba and B = Ag, Cu	111
	Laboratory Note	114
	Letters to the Editor	115
	International Report	116
	Calendar of Meetings	117
	Correspondent's Report	118
	Book Reviews	119
	Short Courses and Workshops	120
	Commercial Announcements	121



Volume 6 Number 2 June 1991

Powder Diffraction An international journal of materials characterization

SIEMENS

Ask for performance - ask for the new D 5000 x-ray diffractometer

Detector configurations include:

- PSD (Position Sensitive Detector).
- Solid-state detector for improved detector efficiency.
- Standard scintillation counter.

Versatile goniometer design:

- Operates in horizontal or vertical mode for reflection or transmission measurements.
- Converts from $\theta:2\theta$ geometry to $\theta:\theta$ in your lab.
- Converts to parallel beam.

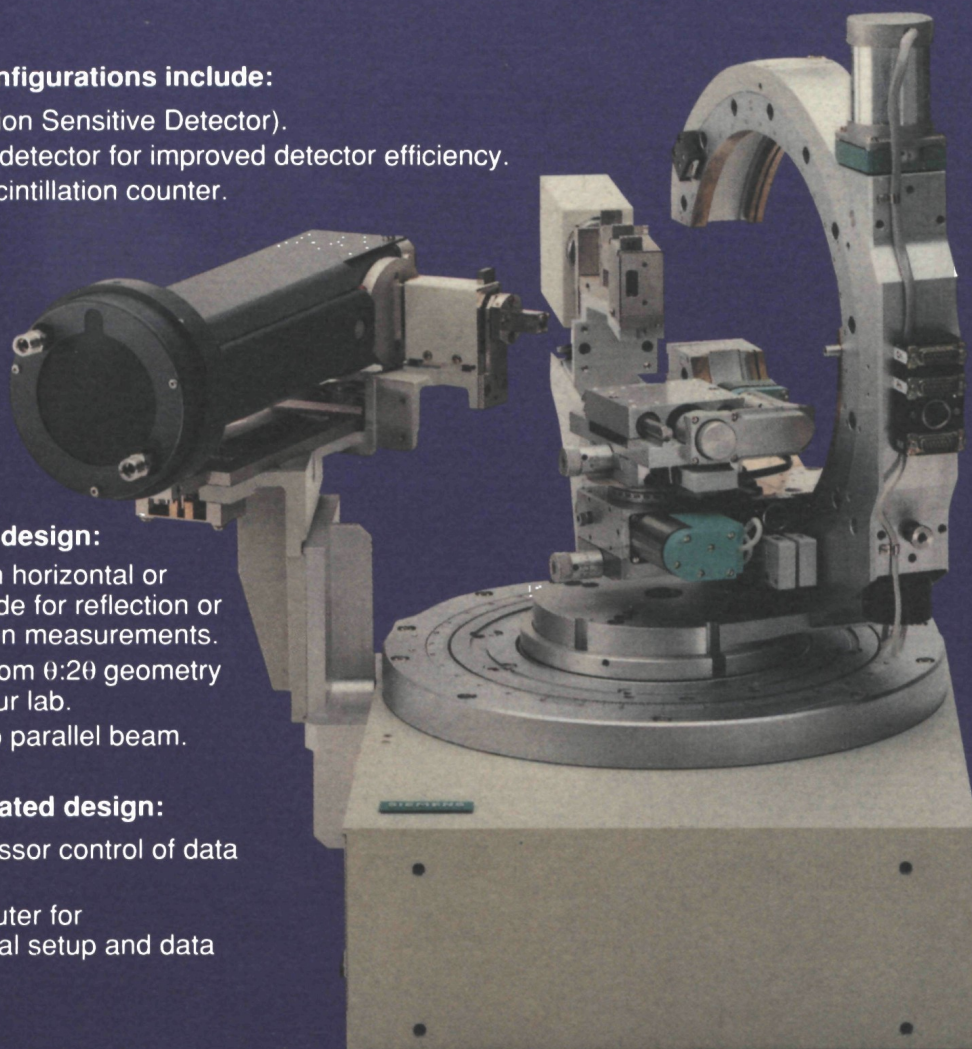
Fully automated design:

- Microprocessor control of data collection.
- Host computer for experimental setup and data analysis.

Complete set of attachments for specific applications:

- Eulerian cradle for texture.
- Open Eulerian cradle for texture/stress.
- Automatic sample changer.
- High and low temperature stages.
- Programmable sample rotation.

Available with computer-controlled variable aperture slits in incident and diffracted beam paths to control divergence and reduce background.



For maximum performance in your lab, Siemens has engineered a new generation of x-ray diffractometer designed to meet your requirements. The D 5000 features a new goniometer design manufactured to the strictest tolerances. Complete with application-specific attachments and advanced software routines, the D 5000 has the precision and flexibility to outperform other systems in every x-ray application.

Your Solution is Siemens

In USA & Canada: contact Siemens Analytical X-Ray Instruments, Inc. • 6300 Enterprise Lane • Madison, WI 53719-1173 • (608) 276-3000 • FAX (608) 276-3015
Worldwide Contact: Siemens AG, Analytical Systems E 689 • D 7500 Karlsruhe 21 • P.O. Box 21 1262 • Federal Republic of Germany • Tel. (0721) 595-4295



Look into μ PDSM . . . It's more than accuracy. It's performance.

Performance makes μ 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 μ PDSM's reputation.

The utility of function and clarity of content in μ PDSM's graphics go beyond merely attractive presentation, to give you a valuable addition to the analytic power μ 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, μ PDSM

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

The universal applicability and continuing enhancement of μ 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 μ PDSM. It takes you beyond accuracy into the next generation of search/match performance.

PD2



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

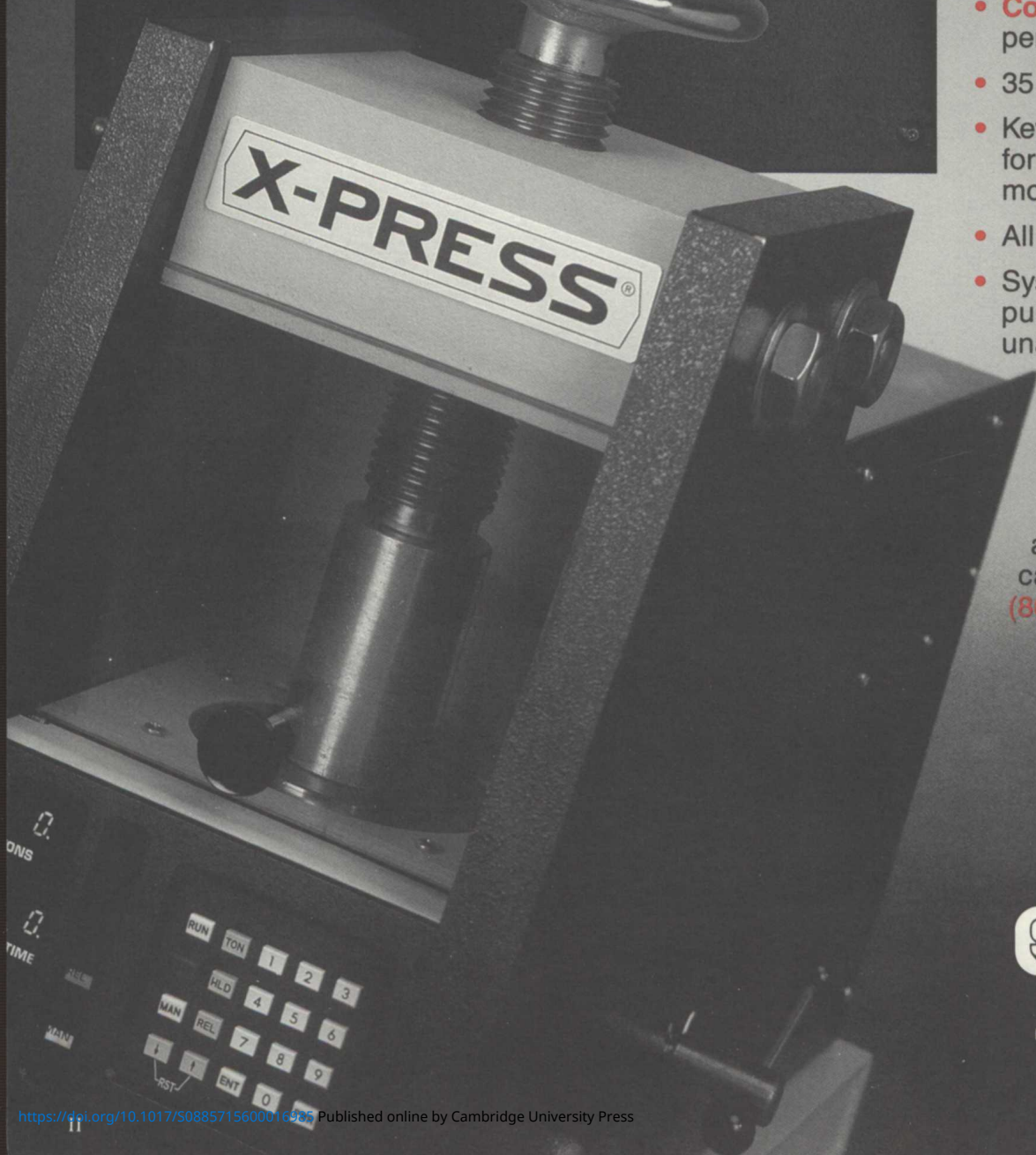
Pressed for Time?



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

Richard N. Rose

Assistant Editor and
Manager of Publication

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

Gregory J. McCarthy

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

Helein D. Hitchcock

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

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, Nyköping, 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
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 \$45.00; Library; \$85.00; other than U.S.A., Canada and the Far East, the annual subscription is \$65.00. 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).

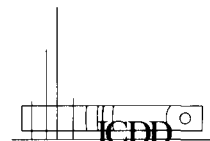
Payment may be made in U.S. dollars by company check, MasterCard, Visa or international money order. Please address communications to the publisher's office.

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.

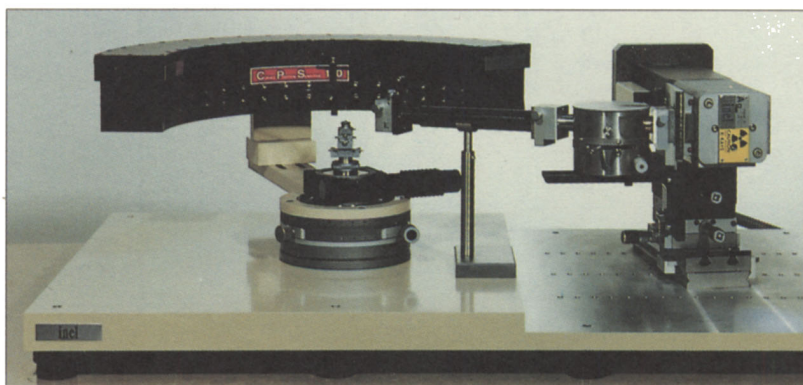
Reprints and permissions. Contact the Publisher's office.

Postal Information. Powder Diffraction (ISSN 0885-7156) is published quarterly for \$45.00 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.

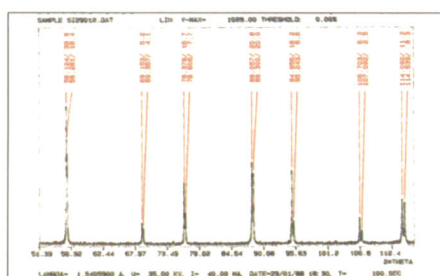
International CODEN Service (Intercode): PODIE2
ISSN 0885-7156
Telex 847170
FAX 215 328 2503



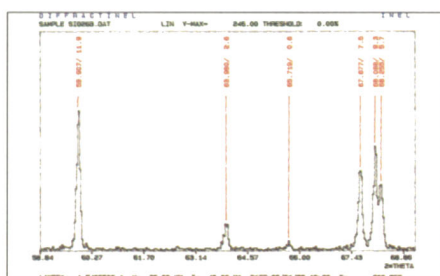
THE CHOICE OF THE FUTURE
SIMULTANEOUS XRD
OVER 120° - 2 THETA
- FAST - ACCURATE - RELIABLE -



CPS 120 MOUNTED ON TGS (TRANSMISSION AND REFLECTION MODE)



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



QUARTZ 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

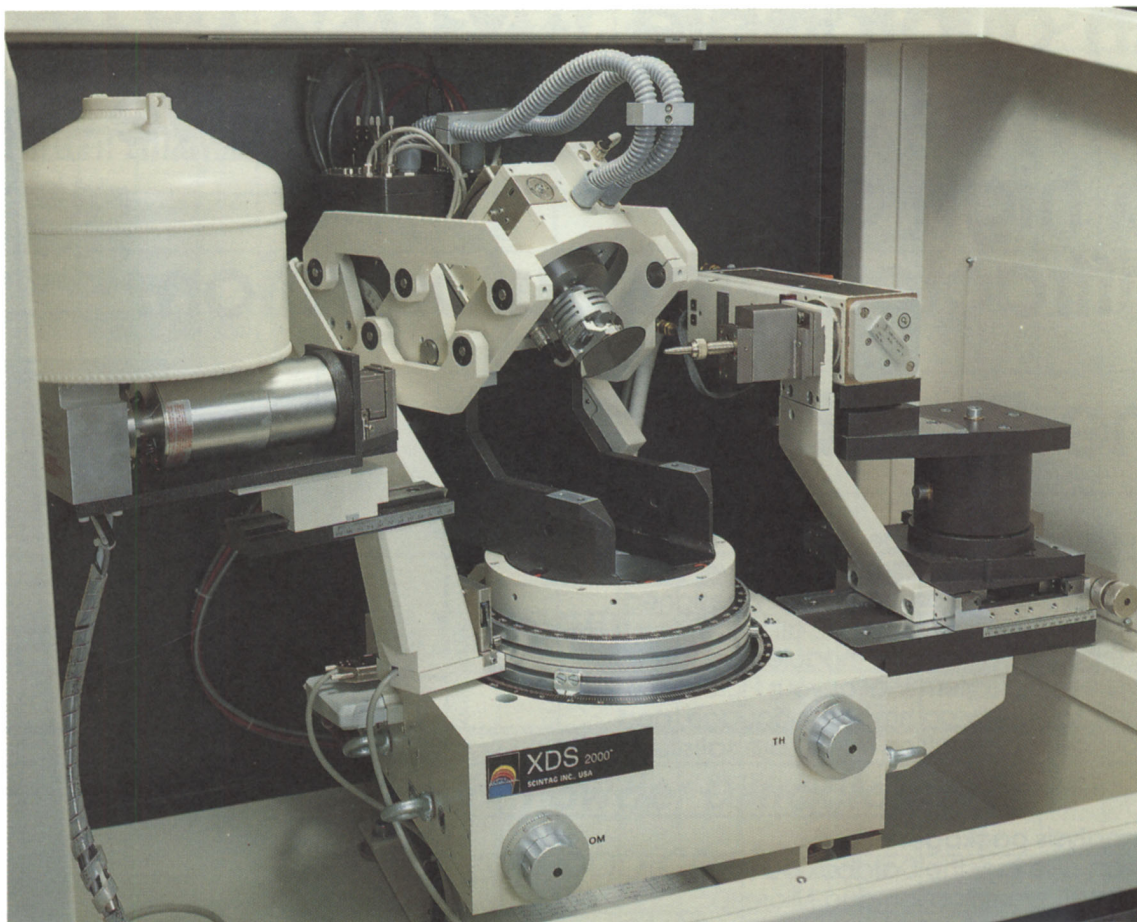
12, avenue de Scandinavie
 91953 LES ULIS CEDEX FRANCE
 PHONE 33 (1) 69.86.13.30
 FAX 33 (1) 69.86 14 19
 TELEX 603965

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

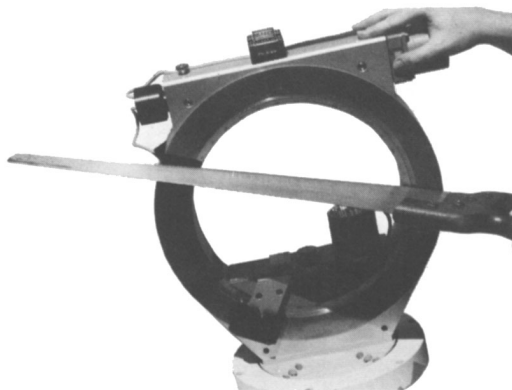
PD4

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

PD5

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

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:

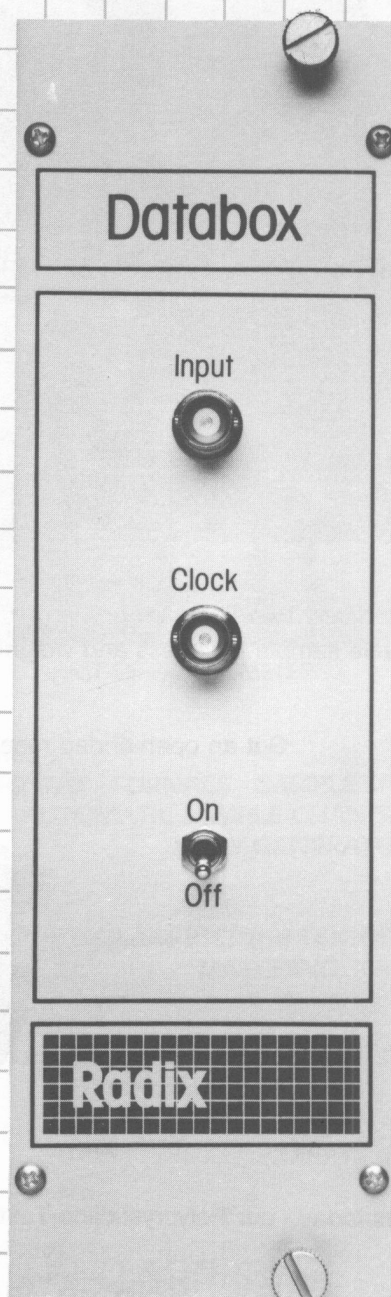
You can also buy the Databox bundled with MDI's Peak Identification and Micro-ID Search/Match software to run on your IBM PC (or compatible), giving you a complete x-ray control, acquisition, and analysis system.

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:

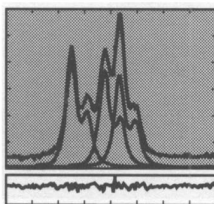
Radix Instruments
3312 Febo Court
Carlsbad, California 92009
Phone/FAX: (619) 753-4646



Search Match. And Beyond.

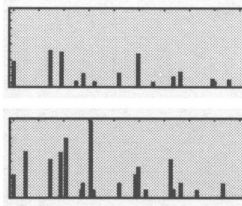
1. Pattern Analysis

- ◆ Peak finding
- ◆ Profile fitting
- ◆ Size/Strain analysis
- ◆ Fast, interactive, complete



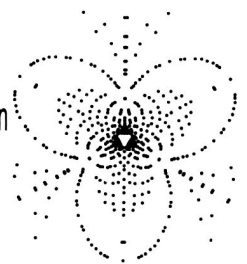
2. Search/Match

- ◆ CD ROM
- ◆ Subfiles
- ◆ User files



3. Tools

- ◆ Pattern simulation
- ◆ Indexing
- ◆ Cell refinement
- ◆ Laue patterns
- ◆ Others



Complete XRD Analysis Software For Your PC. MDI.

Materials Data, Inc.
Post Office Box 791
Livermore, California 94550
415/449/1084
FAX 415/373/1659 PD7

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.

PD8

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

APD 2000 Diffractometric System

GD 2000 Goniometer

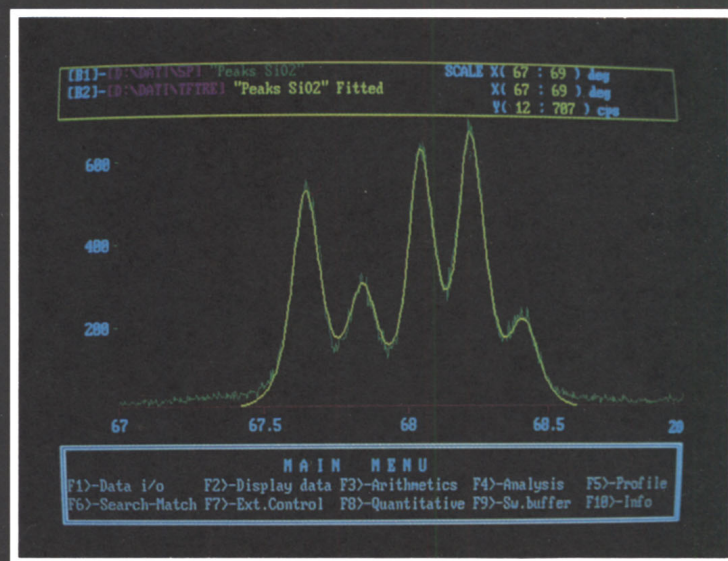
- High resolution
- 2 step motors
- Horizontal and vertical configuration

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

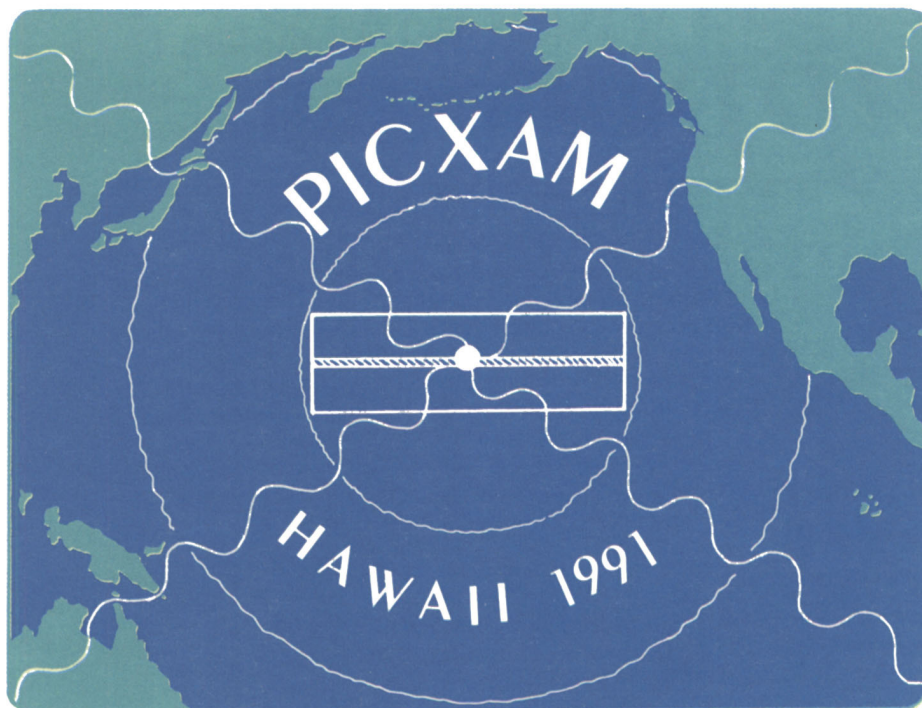
Accessories

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



PD9

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



Second Announcement...

The first international congress on X-ray Analytical Methods for Materials Analysis will be held in Honolulu, August 12-16, 1991, at the Hilton Hawaiian Village.

Congress Theme...

The major thrust of this meeting will be related to the practical aspects involved in X-ray methods for materials analysis. This will be in keeping with the tradition of the Australian X-Ray Analytical Association (AXAA), the Denver X-Ray Conference and the X-Ray Chemical Analysis Group of the Japan Society of Analytical Chemistry.

To be discussed will be the use of X-ray methods based on Powder Diffraction, Fluorescence, Surface Analysis, Absorptiometry, Column Electron Diffraction and Thin Film Characterization by X-ray Diffraction, and Trace Analysis and Thin Film Characterization by X-Ray Fluorescence.

A two day pre-congress workshop program will be held at the University of Hawaii at Hilo, on August 8 and 9.

PICXAM is organized by:

The Australian X-ray Analytical Association
The Denver X-ray Conference
X-ray Chemical Analysis Group/
Japan Society for Analytical Chemistry

PICXAM is cosponsored by:

The International Centre for Diffraction Data
The University of Denver
The University of Hawaii

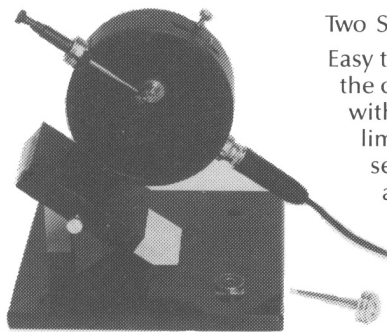
PICXAM

PD10

Pacific-International Congress on X-Ray Analytical Methods

Supper

Complete Debye-Scherrer Powder Camera Systems Accessories, and Film

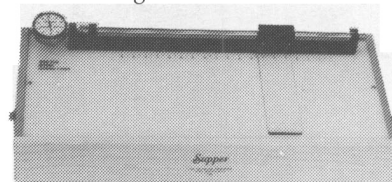


114.6mm Powder Camera with optional viewing stand, illuminator, and Gandolfi "Single Crystal Randomizer" which is interchangeable with standard powder sample holders

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.

- 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

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

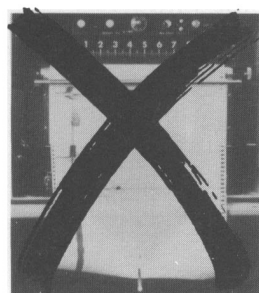
Manufacturers of Fine X-Ray Diffraction Equipment For Over 45 Years

Charles Supper Company
INCORPORATED

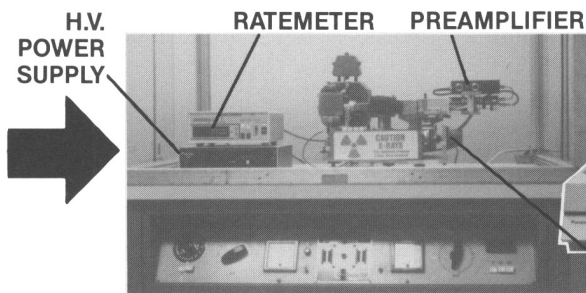
15 TECH CIRCLE, NATICK, MA 01760, U.S.A.
TELEPHONE: (508) 655-4610
1-800-323-9645

PD11

DIFFRACTOMETER AUTOMATION FOR ONLY \$4600



Why Struggle with This?



When You Should be Using This!



Let your PC operate your diffractometer for you!

	CHART RECORDER	SDAC-10
OPERATION:	Manual	Automated (unattended).
OUTPUT:	Strip chart spectrum with written notes	High resolution "strip chart" like spectrum printout. Data stored on disk for future processing.
DATA PROCESSING:	Manual measurements	Data ready for import to data analysis program.
ADVANTAGES:	None	Unattended data acquisition with multiple section scans. Ideal for production analysis.

Basic system consists of a digital ratemeter, fast computer interface with stepping motor driver, stepping motor, and menu driven acquisition software, all for only \$4600.

PD12

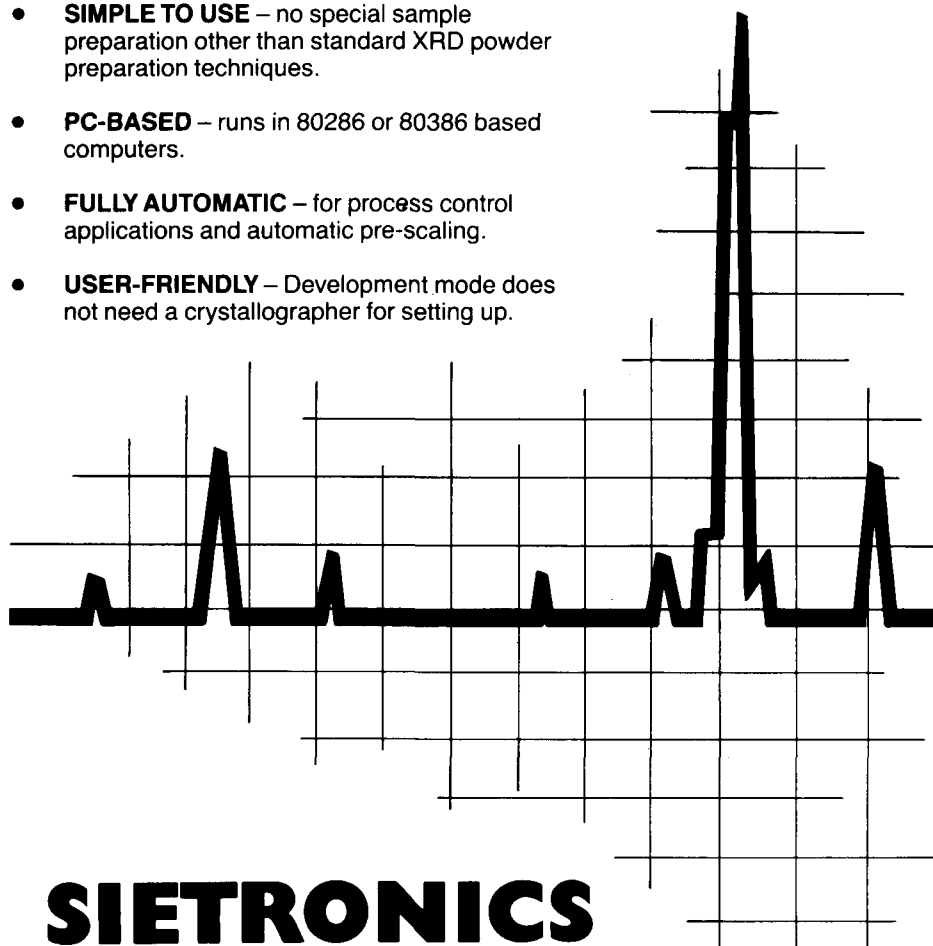
For more information, call (303) 449-2288 or write MIT Corp. 2434 30th Street, Boulder, CO 80301

SIROQUANT^(c)

STANDARDLESS QUANTITATIVE XRD PHASE ANALYSIS SOFTWARE

SIROQUANT^(c) 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

PD13

XI

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) 842-7100
FAX: (708) 887-7417

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

PD14

For 1991 from ICDD...



Set 40 PDF

In all current media

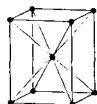
CD-ROM & Mag Tape... Microfiche ... Book
Over 200 new &/or updated entries in PDF-1
and PDF-2†



EDD Electron Diffraction Data Base

(NIST/Sandia/ICDD)

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



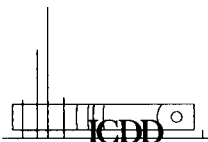
NIST Crystal Data File

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

In book form now

PDF Sets 35-36

Inorganic volume

2955 numeric dif-
fraction pat-
terns of inorganic phas-
es, metals, alloys and
minerals.

Organic volume

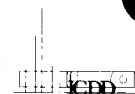
992 numeric diffrac-
tion patterns of
organic and organometallic
phases.

Crystallographic data evaluation uses
NBS*AIDS83. Figure of merit for complete-
ness and accuracy of interplanar spacings
is assigned to each indexed pattern.

For further information contact:

PD16

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



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.

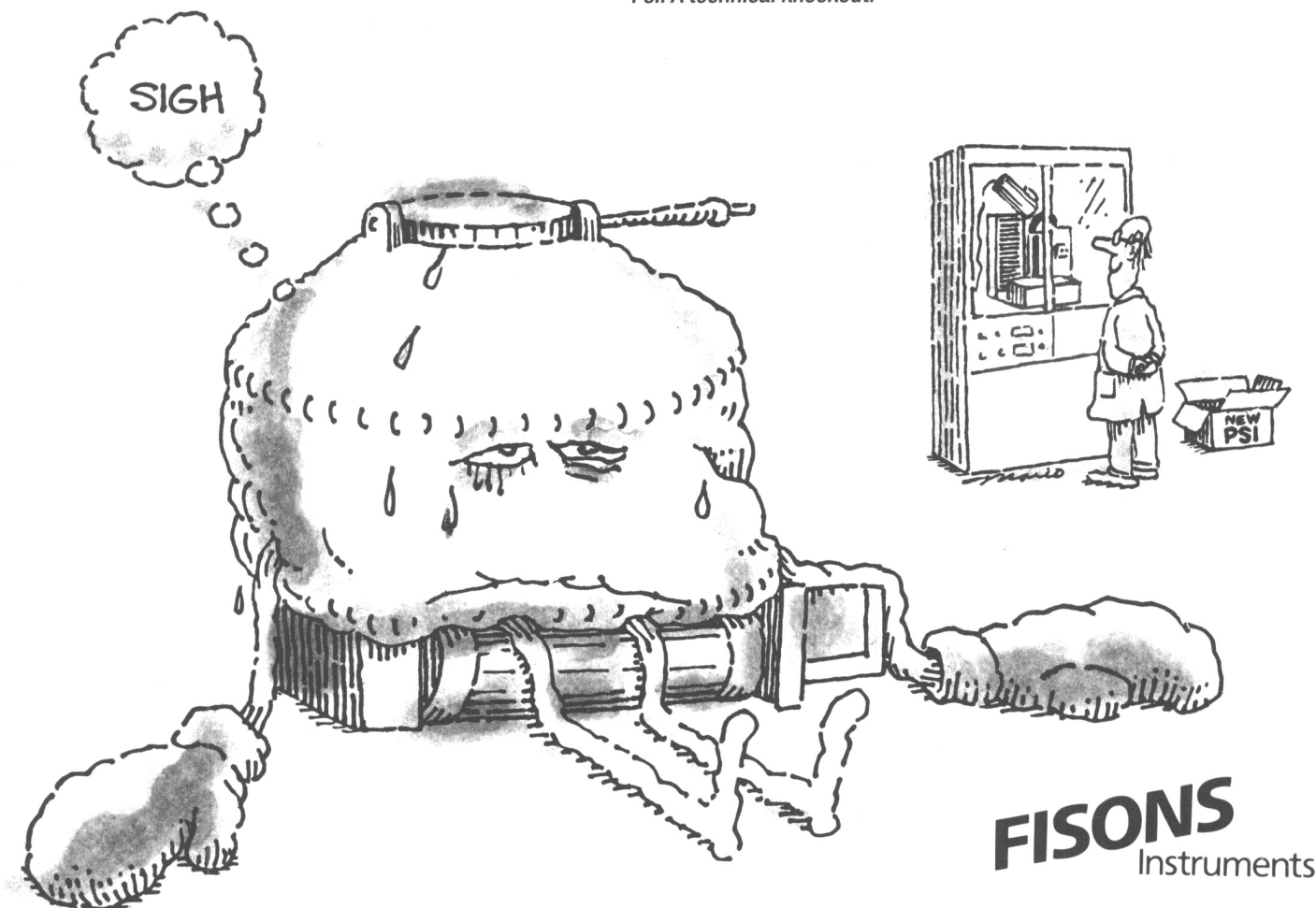
With Psi, you get 3 to 5 times faster throughput, 10 times better energy resolution. And the best diffraction patterns you've ever seen. Psi is like having an electronic monochromator. You get clear $K\alpha$ or $K\beta$ patterns from any tube anode.

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

PD17

Theta.XRD™ ThetaPlus™

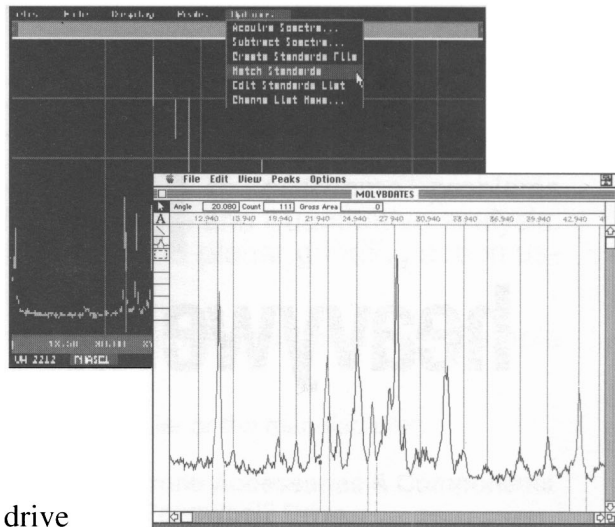
X-ray Diffractometer Automation
from Dapple Systems

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

PD18

**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

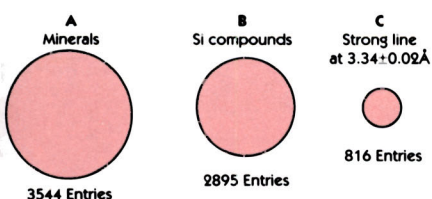
The background of the advertisement features a grayscale X-ray diffraction pattern plot. The y-axis is labeled with values 90, 150, 250, and 350. The x-axis is labeled with values 12.00 and 56.00. The plot shows a series of peaks of varying heights and widths.

PD19

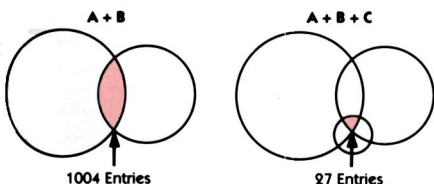
PC-PDF

The Powder Diffraction File on CD-ROM

Search on key fields within the data base.



Search on combinations of fields.



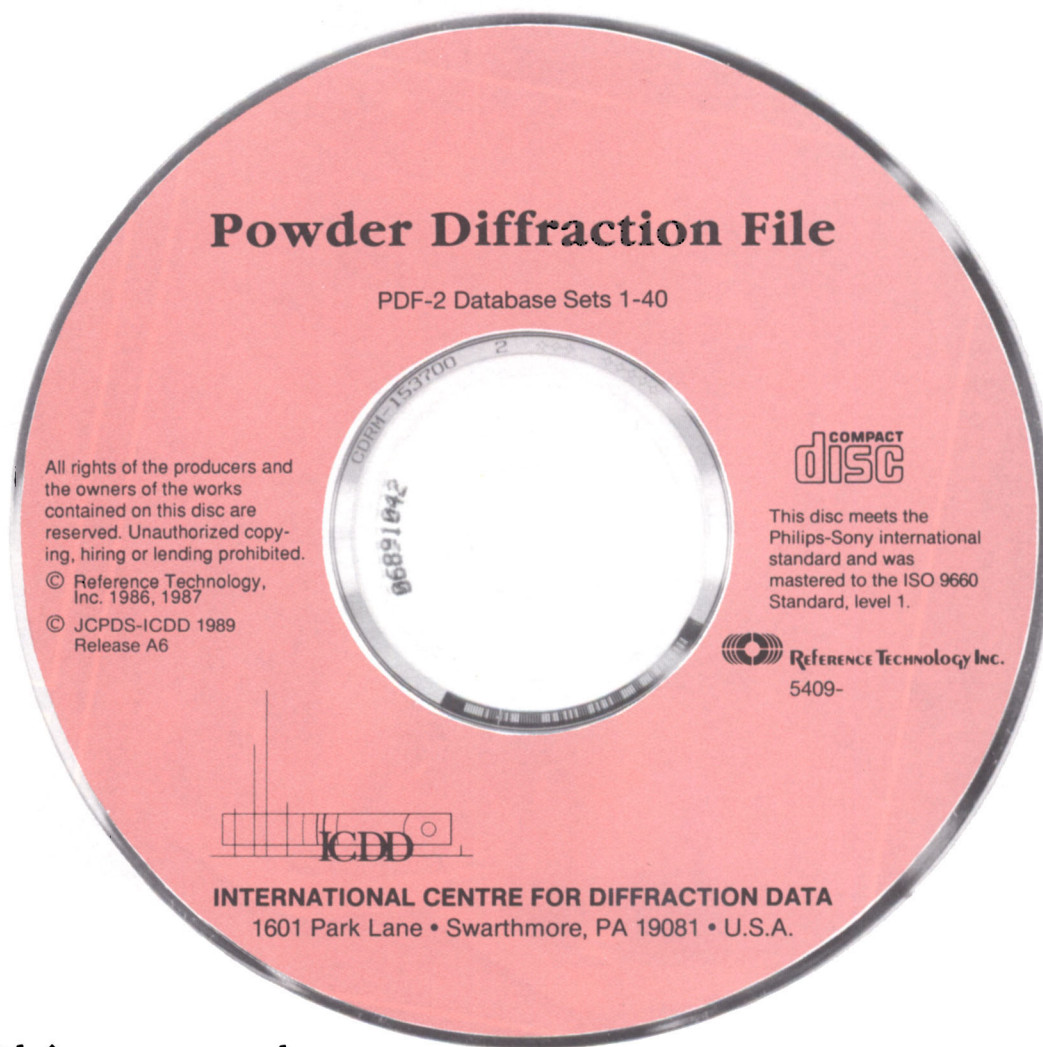
Display results within seconds.

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
μVAX & Macintosh

PD20



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

Few would question, though some might regret, that we live in a world of rapid change. Not the least in our rapidly reshaping life-style is our languages, and especially our scientific vernacular. It seems that, almost daily, new particles, phenomena and devices come along which stretch our rhetoric to the very limit. The broad field encompassing the various aspects of materials analysis by means of X-radiation is certainly no exception and inter-disciplinary communication problems are frequently exacerbated by the growing tendency among instrumental analysts to specialize. In recent years we have fought for the retention of the Angstrom unit and won, but have begged for world-wide acceptance of the metric system and lost.

The *International Union of Pure and Applied Chemistry*, through its *Analytical Chemistry Division on Spectrochemical and Other Optical Procedures for Analysis*, has labored faithfully for more than two decades to bring order to a chaotic situation.

The latest of their series of recommendations is "*Part VIII – Nomenclature system for X-ray Spectroscopy*". Their report is reprinted in this issue of *Powder Diffraction* on pages 95-101.

Current difficulties in the use of the Siegbahn notation for X-ray lines are well known, and stem mainly from problems in attempting to define closely a system not yet completely understood. After all, Siegbahn, who introduced his wavelength nomenclature system in the 1920's can hardly be blamed for not having the foresight to allow for recently resolved multiplets and multipole lines. The fact remains, however, that complications with the use of the Siegbahn system do abound and for a period of almost ten years, Commission V4 of the IUPAC struggled to come up with a more logical system. The result of their labors is called the *IUPAC Notation*. It is to be hoped that the X-ray community as a whole will be swift to implement the new system.

Ron Jenkins