

# NBS Crystal Data

## Research and Routine Applications

**T**he NBS Crystal Data Center builds and maintains a large scientific database of evaluated chemical and crystallographic data. Scientists have long used the published Crystal Data Determinative Tables to help solve problems in materials science. Now the Crystal Data information is available as a computer-readable tape. The NBS Crystal Data Distribution Package includes information on over 60,000 materials as well as accompanying search software.

**F**urther information on the NBS Crystal Data Distribution Package is available from:

**JCPDS-International  
Centre for Diffraction  
Data**  
1601 Park Lane  
Swarthmore, PA 19081  
(215) 328-9400

The database is of interest to scientists of many disciplines.

- **Analytical Chemistry:** Identify chemical compounds using one tiny crystal, non-destructive
- **Materials Science:** Find materials having desired physical and structural properties and design new materials
- **Crystallography:** Save time and money. prevent redeterminations of crystal structures by checking to see if done previously
- **Mineralogy:** Study symmetry and pseudosymmetry of minerals with any given composition range
- **Ceramics and Metallurgy:** Identify phases even

with incomplete diffraction data

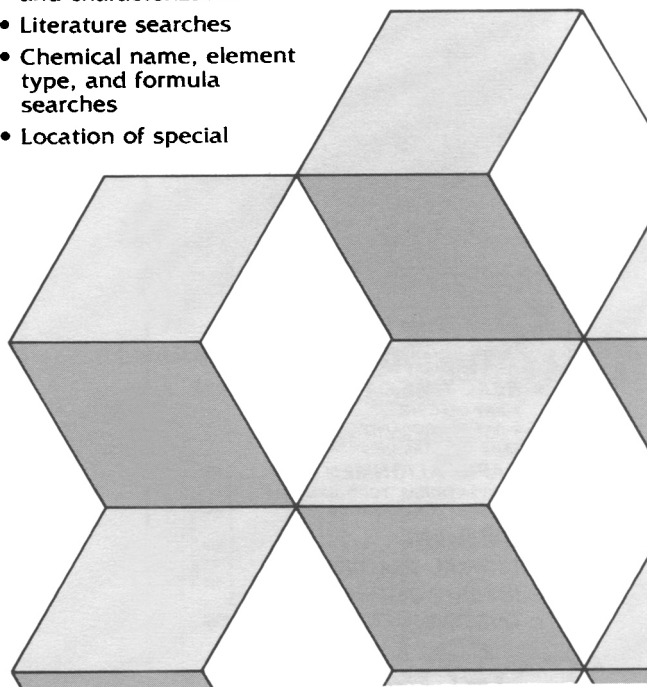
- **Inorganic and Organic Chemistry:** Characterize reaction products and intermediates uniquely and quickly

**T**he NBS Crystal Data Distribution Package is also of special interest to powder diffractionists, electron diffractionists, solid-state and structural chemists, and technical information specialists. Other typical uses include:

- Compound identification and characterization
- Literature searches
- Chemical name, element type, and formula searches
- Location of special

chemical classes or types of materials

- Identification of compounds having specified properties
- Source of data for scientific and statistical research studies
- Searches on space groups, density ranges, crystal systems, and many other parameters



PD21

# The 24th Annual X-RAY CLINIC, SUNYA 1987

## X-Ray Spectrometry

**Session I**  
Fundamentals

June 1-5

**Session II**

Advances, Fundamentals of  
Mathematical & Computer Methods

June 8-12

**Session III**

Mathematical &  
Computer Methods

August 17-21

### Tuition

Session I or II, \$1,100.00      Session III, \$1,200.00  
Sessions I & II, \$2,100.00      Sessions II & III, \$2,200.00

## X-Ray Powder Diffraction

**Session I**  
Fundamentals

June 15-19

**Session II**

Quantitative Methods and Advanced Techniques

June 22-26

### Tuition

Session I or II, \$1,100.00      Sessions I & II, \$2,100.00

For further information and to register:

Professor Henry Chessin  
X-Ray Clinic, SUNYA  
State University of New York at Albany  
Department of Physics  
1200 Washington Avenue  
Albany, New York 12222  
(518) 442-4512/442-4513

PD22

## PORTABLE IMAGE X-RAY INTENSIFIER



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- CUSTOM DESIGN SERVICES



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PD23

# X-RAY

applications software for easy,  
reliable data analysis in x-ray  
fluorescence and powder diffraction

Our programs run on Digital's LSI, PDP, and  
VAX computers, and we are planning for others.

XRF-11 treats matrix effects in XRF  
analysis, using just one standard or many.

PDPEAK calculates d, I, and FWHM for  
powder-diffraction peaks, with corrections.

Other programs are also available or  
being developed. Call us at 202/249-7522.

## CRISS SOFTWARE

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PD24

# 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:

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(Manufacturer)  
2 McCrone Mews, Belsize Lane  
London NW3 5BG.  
Phone: 435-2282  
Telex: 8952387 McResearch

Tintometer GmbH  
Westfalendamm 73  
D-4600 Dortmund 1  
West Germany  
Phone: (0231) 435051  
Telex: 822-605-lovib d

**McCrone Accessories & Components**  
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Chicago, Illinois 60616. U.S.A.  
Phone: (312) 842-7100  
Cables: Chemicrone

**Selby Anax**  
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Notting Hill, Melbourne  
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Telex: 30889



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PD25

**•2-D/1-D •1-D •DNA & IMAGE ANALYSIS**  
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FOR SCANNING: X-RAY DIFFRACTION, EMISSION PLATES, TWO DIMENSIONAL & 1-D SLAB GELS, TLC PLATES, TUBES & BLOTS ON NITRO CELLULOSE.

**X-RAY DIFFRACTION**

**DENSITOMETRIC TRACING**  
(Various computer programs for analysis)

**2-D**

Peak	(X, Y)	Size	Base Area	%Size	Amount
91	(115, 29)	39141	478	14.3	1.2298
92	(140, 46)	33928	774	12.4	1.7654
93	(4, 50)	5890	144	2.2	1.922
94	(96, 81)	5157	124	1.9	1.634
95	(162, 100)	35202	358	12.9	1.1094
96	(228, 100)	7875	195	2.9	1.2494
97	(26, 108)	17103	243	6.2	0.532
98	(134, 111)				
99	(18, 120)				

**PICTORIAL**

**1-D**

**MOLECULAR WEIGHT**

PEAK #	POS.	MOL. WT.
1	07	61 07
2	23	77 64
3	28	85 08
4	37	97 55
5	44	107 84

**Automatic DNA-SEQUENCING**

```

DATA1 (A)
DATA2 (T)
DATA3 (C)
DATA4 (G)
    
```

**SUPERIMPOSITION**  
Graph & Quantitation Difference

**FROM THIS** **YOU GET THIS**

Prices: 2-D: \$12,995 & up 1-D: \$1,895 & up **REPRESENTATIVES NEEDED.**

**1-D Complete System (Laser scanner, computer, disk drive, monitor, printer) \$6,990**

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**BIOMED INSTRUMENTS INC.**  
1020 South Raymond Avenue, #B, Fullerton, California 92631, U.S.A. Tlx 692430

PD26

## Materials Data, Inc. Has Software for Your IBM-PC!

**Micro-Peak** Data reduction including smoothing, background subtraction, peak finding, graphical compare and more.

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(415) 449-1084

PD27

# Mineral Powder Diffraction File Data Book & Search Manual

## 850 *new* patterns

### 3400 patterns total

### 2700 species

#### Data Book

- Enlarged and revised for Sets 1–35
- Ordered alphabetically on mineral name

#### Search Manual contains sections on

- Chemical Name
- Hanawalt Numerical
- Fink Numerical
- Mineral Name

Since its inception almost 50 years ago, the Powder Diffraction File has always been well served in the area of mineral species. In 1974 the first special mineral based publication was produced, this being in the form of a book of minerals containing about 2,600 selected patterns in numerical sequence. A supplement to this edition was produced in 1981. In 1980 an alphabetically ordered data book was produced followed by a group data book in 1983. Each of these products has proven very popular both with the community of mineralogists as well as others involved in general qualitative phase identification.

The International Centre for Diffraction Data is now pleased to announce a new Mineral Powder Diffraction File containing about 2,700 species represented by 3,400 patterns. This selection includes about 850 new patterns added since 1980. This revision of the mineral file has been produced by the Editors of the International Centre for Diffraction Data in cooperation with the Minerals Subcommittee, and has been further guided by nomenclature recommendations of the International Mineralogical Association.

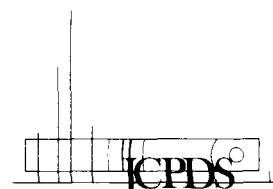
The Mineral Powder Diffraction File Data Book is ordered alphabetically on mineral name, thus grouping together patterns of the same mineral including hydrates, polytypes, order-disorder and chemical varieties, and obviating the need for an index. All data have been reedited with special reference to nomenclature, chemical formula, indexing and other crystallographic data. Physical data is also recorded including opaque optical data where available.

The Search Manual supplied with the new Data Book is based on the latest Hanawalt search/matching techniques including special provisions for finding patterns recorded using the Debye-Scherrer technique and data from highly oriented materials.

We feel that with the large number of new patterns, along with the improved quality of many of the older data, this new product should prove invaluable to both existing users of the Mineral Data products as well as to those new to the field.

Price: \$550.00    Terms: Domestic — 30 days net  
Foreign — Prepayment in U.S. currency

Please address all inquires and orders to:  
JCPDS—International Centre for Diffraction Data  
1601 Park Lane  
Swarthmore, Pennsylvania 19081  
U.S.A.  
Telephone: (215) 328-9400



PD28

# 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.

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(914) 962-2477

*We're the Specialists in XRD*

PD29

# Powder Diffraction File 27-28

Now available in book form sets

**Inorganic Volume:**

2882 numeric diffraction patterns of inorganic phases, metals, alloys and minerals.

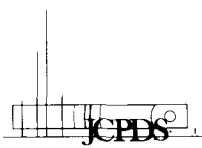
**Organic Volume:**

992 numeric diffraction patterns of organic and organometallic phases.

Crystallographic evaluation data made with program NBS\* EXAIDS83. Figure of merit for completeness and accuracy of interplanar spacings is assigned to each indexed pattern.

For further information write or call:

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

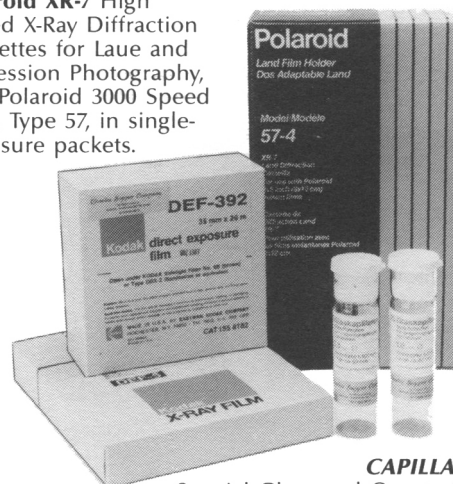


PD 30

## Capillary Tubes and Laboratory Supplies for X-Ray Diffraction Use

**Kodak Direct Exposure Film** especially developed for X-ray diffraction analysis. Available in 35mm x 20m rolls and in 50 sheet boxes.

**Polaroid XR-7 High Speed X-Ray Diffraction Cassettes** for Laue and Precession Photography, and Polaroid 3000 Speed Film, Type 57, in single-exposure packets.



### CAPILLARY TUBES

Special Glass and Quartz in 15 sizes from 0.1mm to 3.5mm O.D. Uniform 89mm length and funnel shaped at the top. 0.01mm wall thickness.

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PD31

**Notice:**

Back issues of Powder Diffraction, Volume 1 1986 are available.  
\$15.00 (U.S.) each; complete set, \$45.00 (U.S.)  
Prices include postage by air.

PD32

# Rigaku's Thin Film Diffractometer Attachment

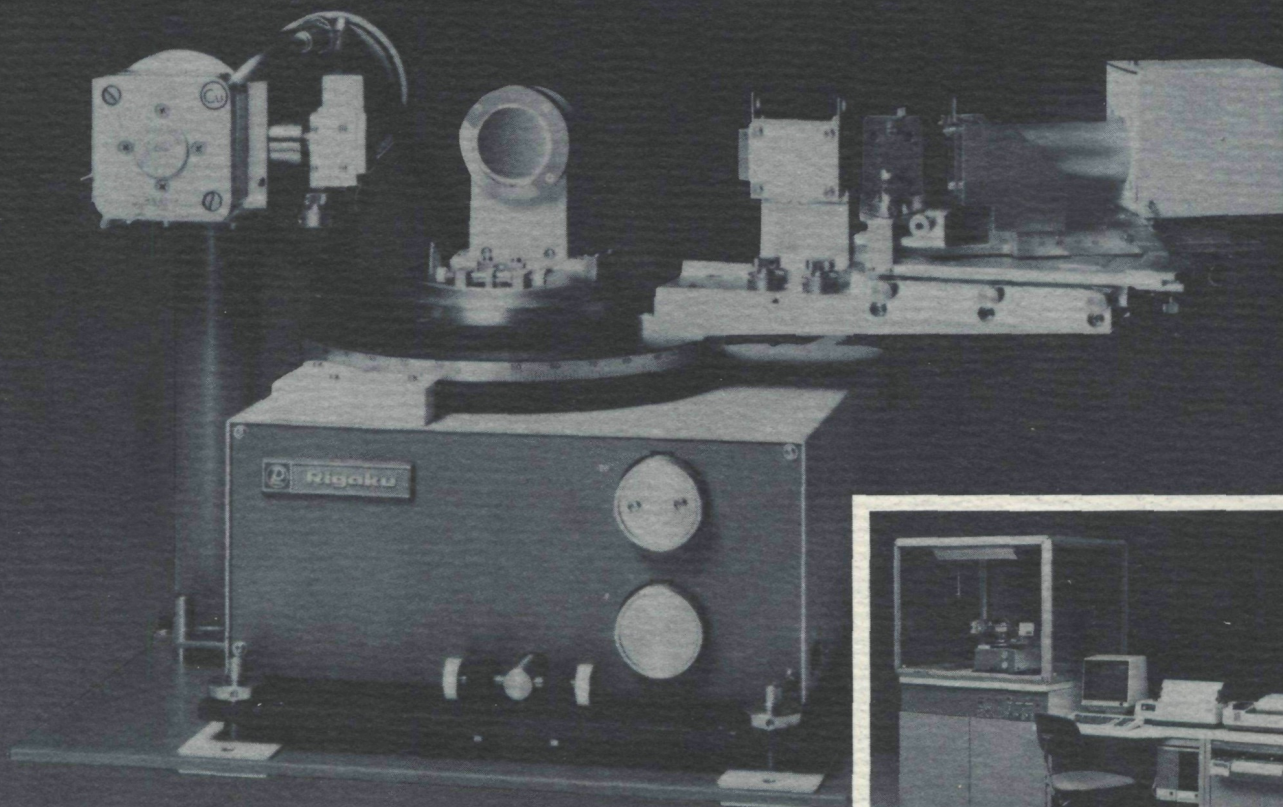
...Throwing light  
on 100Å film.

X-ray diffractometry of thin films, which has so far been exceedingly difficult, is now possible with Rigaku's Thin Film Attachment.

Up to now, obtaining a sharp X-ray diffraction profile of a thin film has been a problem; the extremely thin sample weakens the intensity of the diffracted rays, resulting in relatively low signals and high backgrounds. Moreover, since the conventional diffractometer is designed for a  $\theta$ - $2\theta$  coupled scan, intense diffracted rays from the substrate material overwhelm the diffracted rays from the thin film sample, making it difficult to obtain reliable data.

The dilemma has now been solved by newly developed optics from Rigaku (pat. pend.). Used in conjunction with our wide angle diffractometer, the Thin Film Attachment employs a low-angle incidence method with parallel beam optics that increase the diffraction intensities of thin film samples. A scan system for  $2\theta$  alone and an intraplane sample rotation mechanism enhance efficiency. Rigaku has thus made thin film measurement feasible with only the X-ray flux available from a conventional sealed-off X-ray tube.

Throwing light on 100Å ... only Rigaku has the technology to make it happen!



D/Max-B Wide Angle Diffraction System



For information write or call: Rigaku/U.S.A., Inc.,  
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Telephone: (617) 777-2446



# Spot the difference, win a prize

The truth is, these groups of industrial raw materials and finished products are visually identical. And even the differences that do exist may be too subtle for easy detection by many analytical procedures.

But now there's a new answer. The PW1800 automated powder diffractometer from Philips, designed specifically for high volume sample monitoring in the research and plant laboratory.

A host of innovative features make the PW1800 a brilliant performer – one that will quickly bring real rewards through increased efficiency and more competitive production.

There's a new high precision goniometer, totally enclosed for optimum contamination protection and radiation safety. Its two-collimator, four-slit optics allow outstanding analytical accuracy and resolution for all kinds of powder and fused bead samples.

The compact, high efficiency generator cuts power consumption by up to 40%, while electronic control ensures stable excitation.

For the first time, built-in robotics give smooth, trouble-free handling of even delicate materials, singly or in batches.

Five-microprocessors provide distributed intelligence for automated operation, supervision and diagnostics.

Permanent alignment means fast start-up and reliable long-term operation.

And the addition of a DEC computer gives you access to the world's most sophisticated diffraction software, opening the door to a huge range of data processing and reporting possibilities for qualitative, quantitative and crystallographic analysis.



For more information contact your local Philips office or:

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