Powder Diffraction

JCPDS

Volume 1 Number 4 December 1986

Powder Diffraction An international journal of materials characterization

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The Siemens x-ray Diffraction Concept —

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Every aspect of the Siemens concept — its design, its price, and its application potential — allows you to start small and build big, assured each step of the way of Siemens' first-rate performance and complete support.

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Siemens' modular design lets you begin with the basic manual diffraction system, expand it with our DACO microcomputer, then take it to the limits of complete computer control with DIFFRAC, one of the largest and most versatile XRD user-oriented software systems.

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At Siemens, affordable means value. Because the cost of purchasing, upgrading and operating a Siemens system is so surprisingly low, you can expect your x-ray diffraction system to more than justify its initial investment.

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Siemens instrumentation is backed by a worldwide installation base of over 600 D 500 satisfied users, all more than willing to verify our system's superior performance.

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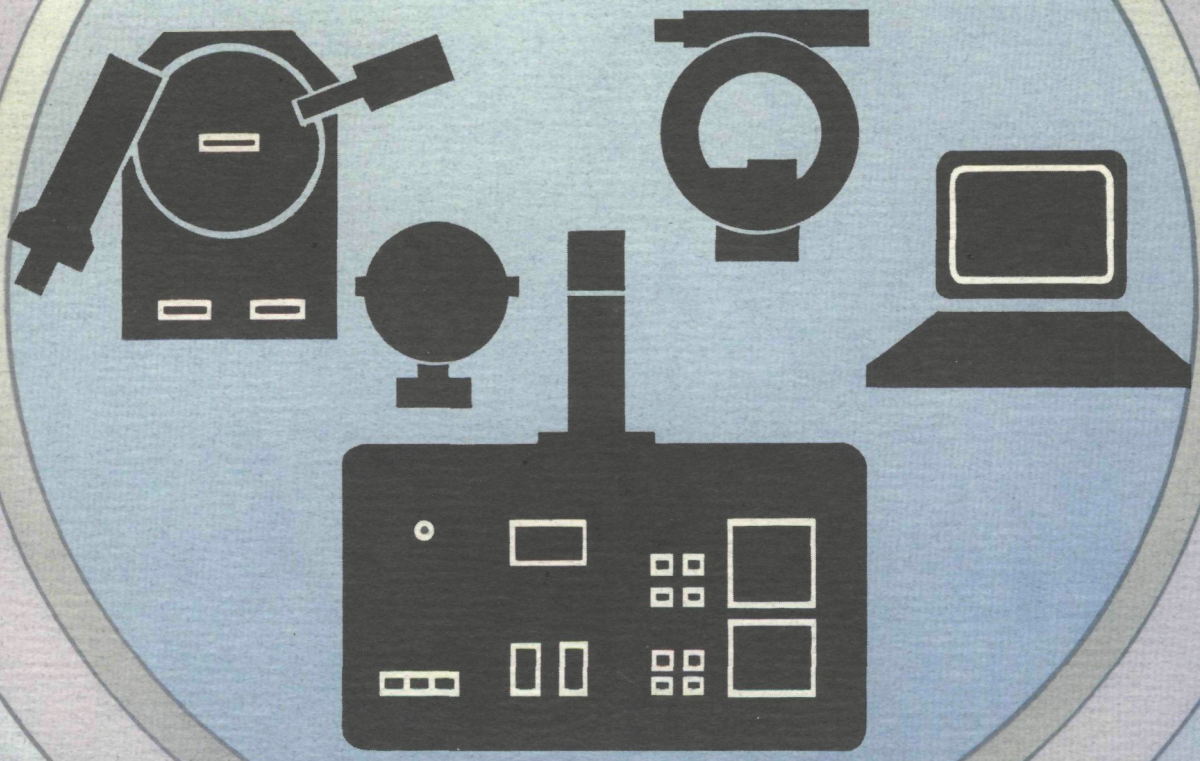

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μPDSM puts the world of XRD analysis at your finger tips.

Fein-Marquart has taken search/match out of the lab and literally put it at your finger tips with μPDSM—a full featured software program that gives you mainframe power for your IBM PC. Offering cost-effective stand-alone use, μPDSM allows you to analyze data from your diffractometer on your IBM PC. It delivers more accurate identification faster than any known alternative and gives you the 46,000-pattern JCPDS library plus the capability of developing your own library. Whether your x-ray diffractometer is manual, semiautomatic, or fully computer controlled, the μPDSM is the answer to your direct interaction in solving simple or complex diffraction patterns. For information or a presentation on μPDSM, call or write FMA.

Fein-Marquart Associates, Inc.
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Baltimore, MD 21212
(301) 821-5980

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Powder Diffraction

An International Journal of Materials Characterization

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 epitactic 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.

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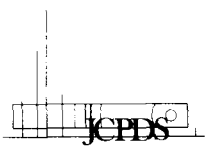

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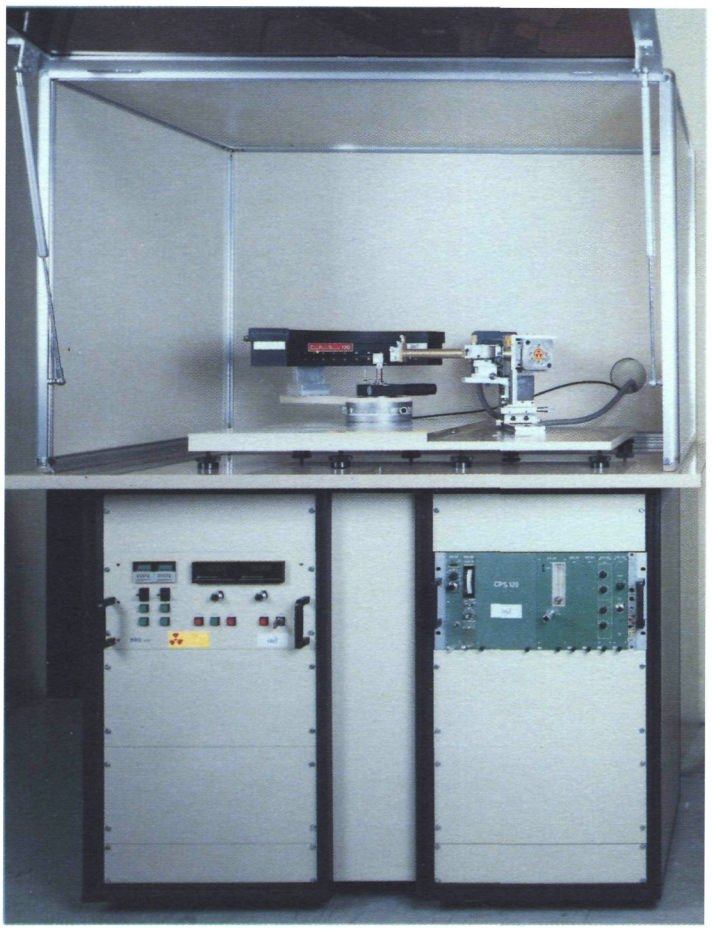


The Inel CPS Diffraction System.

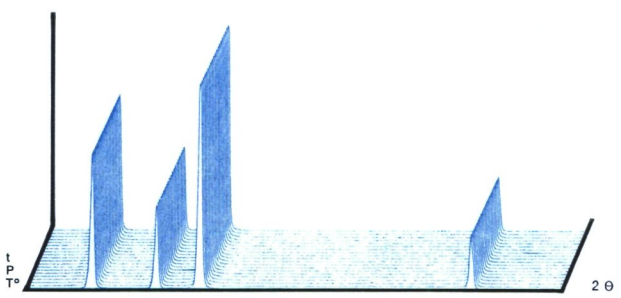
In Powder Analysis:

- No movement of detector or the sample.
- High-speed Data Collection displayed in Real Time.
- Extremely versatile horizontal or vertical configuration, addition of high temperature and other accessories.
- The Detector is easily adaptable to most existing Diffraction Systems.

In other applications:

- Texture analysis with simultaneous generation of 3 pole figures.
- Can be used for Single Crystal, Stress, Amorphous and Kinetic studies.

3-Dimensional Graphic Output of a Kinetic Study.



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NBS Crystal Data

The 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.

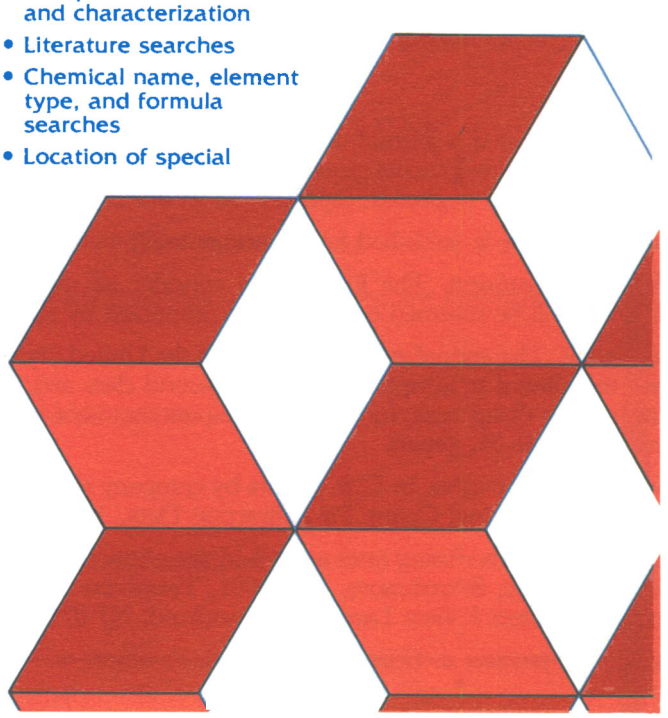
Research and Routine Applications

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

The 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



Further information on the NBS Crystal Data Distribution Package is available from:

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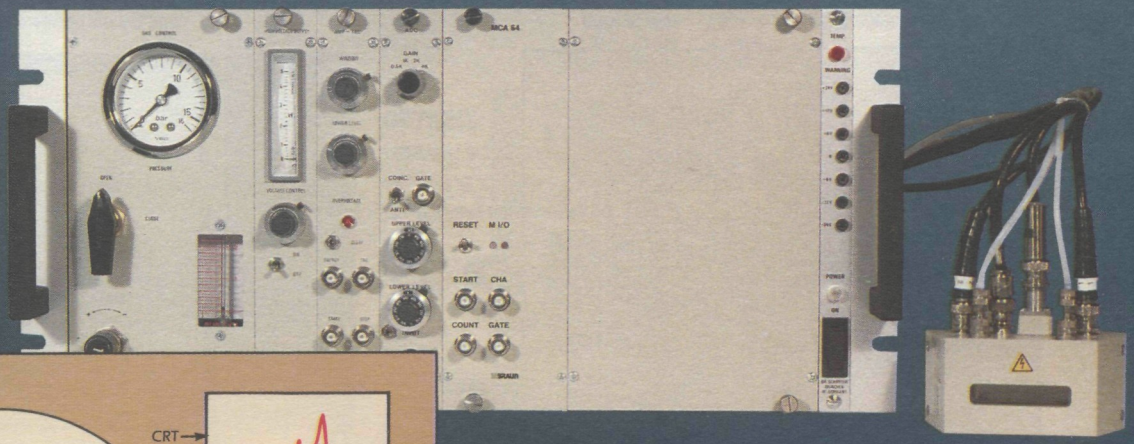
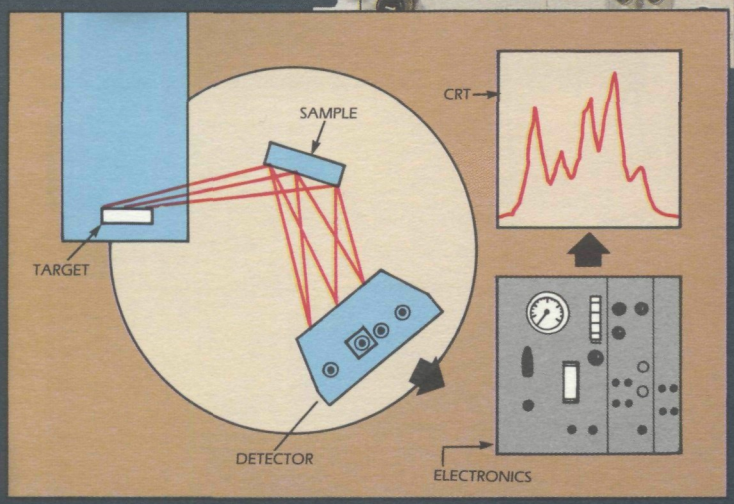
M BRAUN Position Sensitive Proportional Counter

for Simultaneous Detection of X-ray Diffraction Data





The M Braun Position Sensitive Proportional Counter is the most innovative product for rapid collection of X-ray diffraction data available. It enables the diffractionist to collect data at a rate 100 times faster than conventional scintillation counter/step scanning modes.

The detector has an inherent resolution of .01° FWHM, thereby providing data equivalent to standard counting techniques. However, since it acquires data over 10° 2-theta simultaneously, it dramatically increases throughput. Detectors can be utilized in a stationary mode or can scan rapidly to collect data over the entire 2-theta range.

Additionally, the detectors are gas proportional counters and exhibit excellent energy resolution. Choose between a straight or curved configuration to match the diffractometer radius.

Complete systems, with DEC-PDP-11 computers and software, can be provided including detector mounts, vertical divergence slits and filter holders. An 8K × 32 bit MCA is standard and includes a baud rate selectable RS232C interface. A 64K × 16 bit MCA is also available for time resolved diffraction studies. Software to interface the detector to your PDP-11 under RT-11, RSX11M or VMS may be selected to include peak search for D/I pairs.

Some typical applications include:

• Small angle X-ray scattering • Wide angle powder diffraction • High pressure studies • Guinier diffractometer • Scattering experiments • Time resolved diffraction.

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Keyboard and CRT for local control of the detector and spectrum display.

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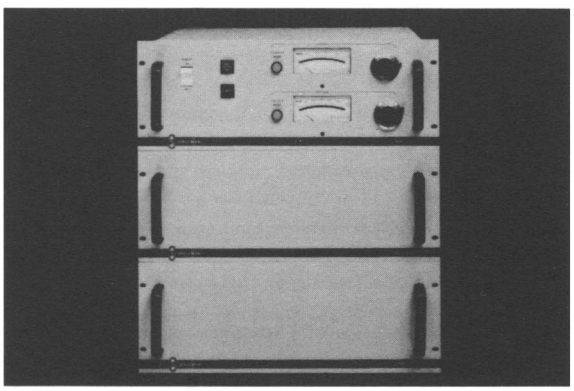
A New Generation Of X-Ray Generators

Spellman, a leader in high voltage technology, has developed a power supply with the features diffraction scientists require. The DXR 3000 offers a unique combination of low cost, high performance, and compact size. These features are achieved through Spellman's experience in high frequency resonant inverter technology.



FEATURES:

- Greater than 90% efficiency.
- High stability through precision feedback control circuits.
- Solid encapsulants insure maintenance-free operation.
- System fault diagnostics and display, including arc detection, filament short, overvoltage, and tube water flow interlock.
- Automatic slew of the high voltage and emission current to preset values.
- Current source provides automatic matching of the filament current to X-Ray tubes with various heater voltages.
- Continuous adjustment for both high voltage and emission current.

TECHNICAL DATA: MODEL DXR3000

Output Power	3KW
High Voltage Output	0-60KV
Emission Current	0-50mA
Emission Current Regulation	±0.1% for a 50% voltage change
Emission Current Accuracy	±1%
Line Regulation	±0.01%
Ripple	0.1% RMS
Input Voltage	220V ±10%/50 or 60Hz single phase
Input Power	4.3KVA
Filament Output	0-6A/20VDC Compliance
Dimensions	Three chassis each 7"H × 19"W × 20"D
Weight	180 lbs total

OPTIONS:

- 6KW and 9KW available.
- Outputs up to 100KV available.
- 208V 3 phase model available.
- Remote interface for all analog and digital functions available.
- Fast emission current response (stable to 0.1% within 50mS) available.

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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

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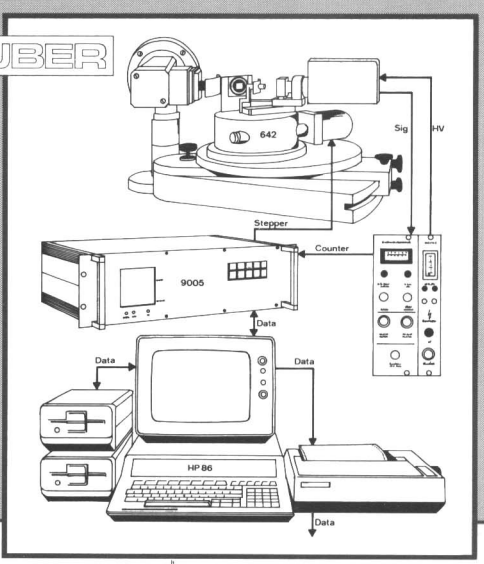
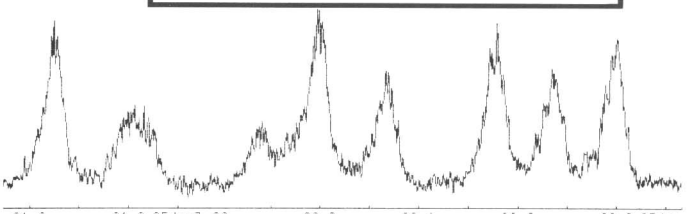
PD12

GUINIER DIFFRACTOMETER
FOR POWDER AND THIN FILM TECHNIQUE





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PD13

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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:

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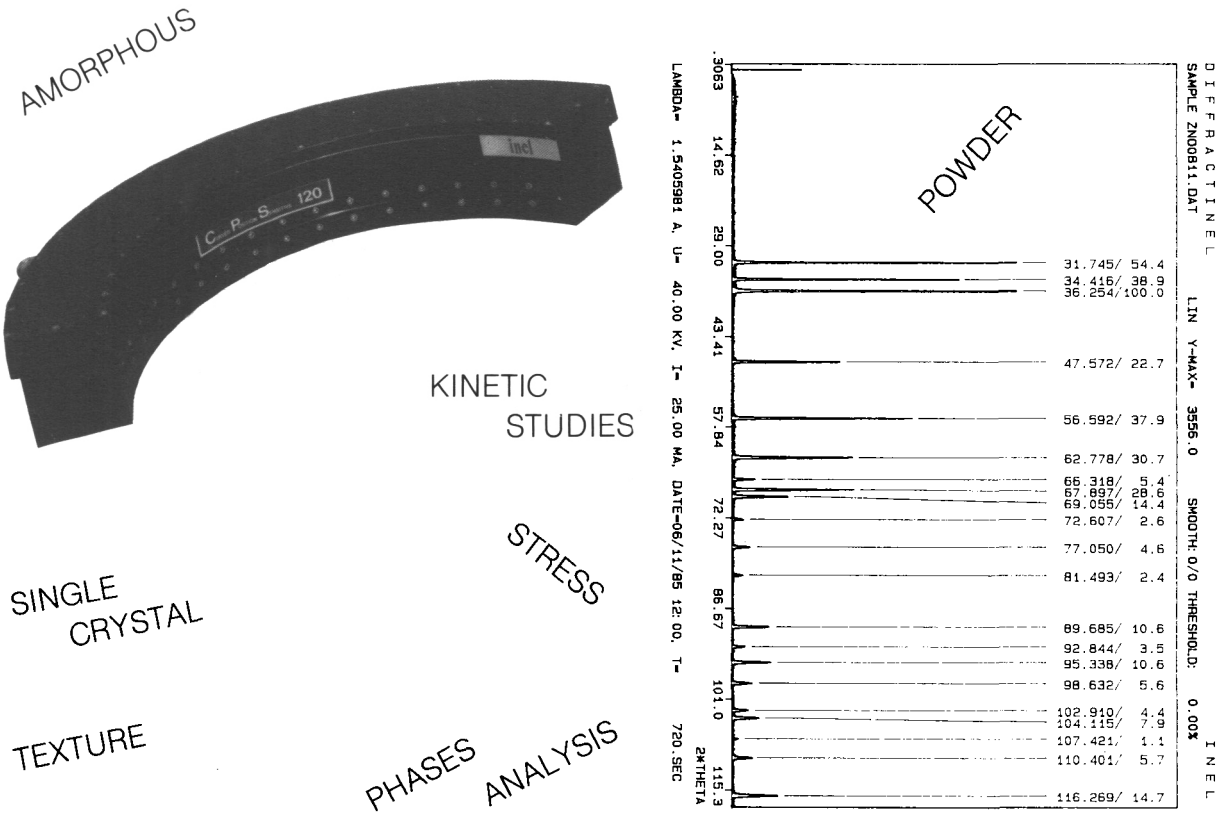
THE WAY OF THE FUTURE FOR X RAY DIFFRACTION



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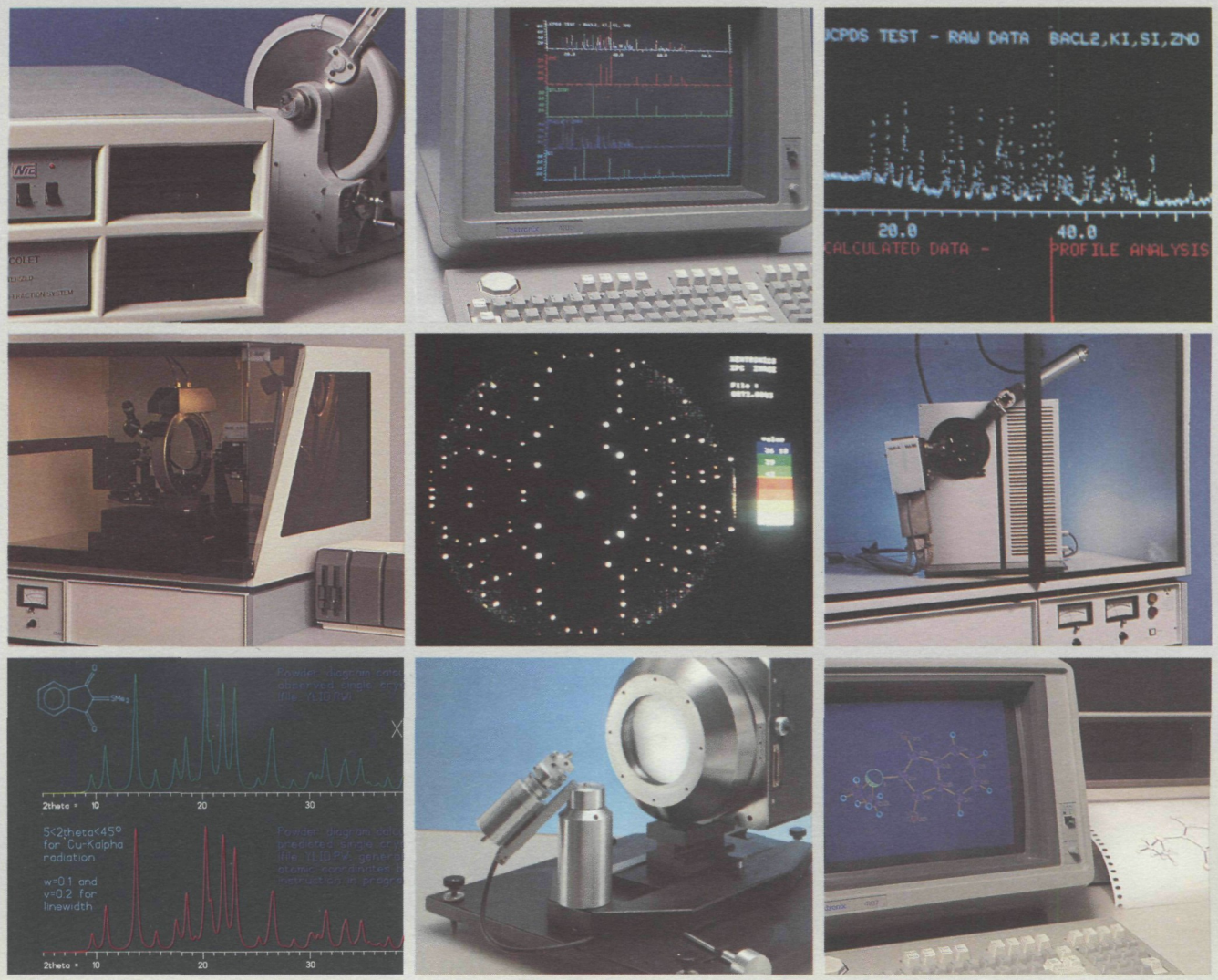
Nicolet X-ray Diffraction



Nicolet X-ray Instruments brings together state-of-the-art instrumentation to meet your x-ray diffraction needs: in large and small molecule x-ray crystallography, in x-ray analysis of polycrystalline materials, as well as general materials analysis applications. Our commitment to advanced instrumentation provides higher productivity and performance whether you are upgrading existing instrumentation or adding new fully automated systems to the laboratory.

Nicolet's developments in new computer hardware, diffractometer design, and our unequaled SHELXTL software provide simultaneous data collection and structure determination to solve virtually every crystal sample analyzed to date. And now, the addition of the Xentronics™ high-resolution area detector, with its ten-fold increase in data collection speed, significantly expands previously limited research studies of macromolecular structures, and promises extensive new capabilities in the immediate future for powder diffraction, thin film and polymer analysis, and Laue crystal orientation studies.

For more information on Nicolet's new developments in x-ray diffraction, write to us on your company or department letterhead for a copy of our RefleXions Newsletter. Send your request, attention Barbara Brink, to:

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Nicolet X-ray Instruments 5225-5 Verona Road, Madison, WI 53711 608/273-5048 PD21

Editorial

Presentation of Reference Data in *Powder Diffraction*

One of the purposes for creating *Powder Diffraction* was to provide a medium for the publication of new diffraction data. The first three issues have included data produced by the Research Associateship of the International Centre for Diffraction Data and other laboratories. The papers illustrate several formats which can be followed in the presentation of powder data.

Many compounds examined in the modern laboratory produce patterns superior to those presently in the Powder Diffraction File. Often, there is little time in the rush of the project to devote much effort to preparing a formalized description of compound, the data, and the documentation. Consequently, much useful data is lost to the scientific community. I would like to suggest a procedure to rescue these data and provide recognition to the experimentalist who collects the data.

The data published by the Research Associateship exemplifies the useful documentation organized in a concise manner along with the complete listing of the diffraction pattern. These tables can serve as a model to diffractionists who wish to prepare data sets for submission. Of course, the diffraction data is the most important component of the information, but it is more valuable with as much documentation as is possible. Conditions and diffraction parameters for the data collection and the description of the compound, both its chemistry and synthesis, need to be supplied by the submitter. Crystallographic data should also be supplied as far as it is known. If the pattern can be indexed and refined to determine the best-fit cell parameters, the information is desirable. However, all patterns submitted will be processed through the EXAIDS review program, and this check will confirm the indexing as well as much of the other information supplied and produce a refined cell along with the figures-of-merit. For any diffractionist who will take the time to supply this basic data to the editorial staff, we will process the data through EXAIDS and prepare the data tables and supporting information for a short article in *Powder Diffraction* if the data prove to be an improvement on the existing pattern.

The International Centre for Diffraction Data does have a standard form which is used by many diffractionists for submission of data. Copies of this form will be supplied on request. The Notes for Authors published in the first issue also contains guidelines for documenting powder data. These guidelines were prepared by a committee of the American Crystallographic Association and accepted by the International Union of Crystallography. They were published in detail in National Bureau of Standards Special Publication 567 (1980). These guidelines resulted when a committee examined the quality of powder data available at the time and made recommendations to improve the status of these data. One of the major recommendations was the preservation of the original diffraction data, i.e. the 2θ values, and the analysis of errors based on these values. This decision was based on the linearity of errors on the 2θ scale and on the non-linearity of errors on the d-spacing scale. The effect is to require that the 2θ values be reported along with the rest of the data, so that EXAIDS can properly evaluate the accuracy of the data.

Diffractionists should not be discouraged from submitting data just because it does not meet all the requirements listed in the guidelines or match the quality of the data produced by the Research Associateship. This quality of data demands a considerable amount of time in the data collection. Any data set which is an improvement of existing data is useful. Some compounds may never yield this quality of data. For experimentalists who have a stock of compounds for which data should be collected, but who have no support for the time, may wish to consider the Grant-in-Aid program of the International Centre. It is designed to provide funding to support the data collection in just such situations.

This request for submission of experimental data is not meant to discourage the preparation of more detailed papers describing crystal-chemical studies and data analysis. It is not the desire of *Powder Diffraction* to establish a required format for all data presentation. However, such a format may encourage a lot of diffractionists to publish data which they would not otherwise take the time to prepare. If this effort does prove successful, we will start a section devoted to data sets and assign this section to a special editor for data. Go to your files, pull out those data sets and send in the necessary information.

Deane K. Smith
Editor-in-Chief

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