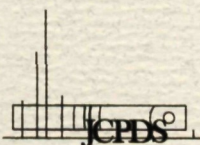


Powder Diffraction

B.H. O'Connor and M.D. Raven	Application of the Rietveld Refinement Procedure in Assaying Powdered Mixtures	2
E. Vila and A. Ruiz-Amil	Computer Program for Analysing Interstratified Structures by Fourier Transform Methods	7
W. Wong-Ng <i>et al</i>	Computerization of the ICDD Powder Diffraction Database Critical Review of Sets 1 to 32	12
J. Schlichter <i>et al</i>	The Influence of Emulsifiers on the Crystal Properties of Tristearin and Trilaurin	19
A. Amin and R.E. Newnham	Lattice Thermal Expansion of Lead Zirconate Titanate Piezoelectrics	23
L.S. Zevin	Bragg-Brentano and Seeman-Bohlin Diffractometers for Thin Films	25
J.J. Ritter	An Hermetically Sealed Inert Atmosphere Cell for X-Ray Powder Diffraction	30
D.G. Cameron and E.E. Armstrong	Optimization of Stepsize in X-Ray Powder Diffractogram Collection	32
G.J. McCarthy	Laboratory Note. A LOTUS 1-2-3 Spreadsheet to Aid in Data Reduction for Publication of X-Ray Powder Diffraction Data	39
E.H. Merrachi, F. Chassagneux et B.F. Mentzen	Données Cristallographiques sur le Trioxalato- Chromate (III) de Rubidium Trihydrate: $\text{Rb}_3(\text{Cr}(\text{C}_2\text{O}_4)_3) \cdot 3\text{H}_2\text{O}$	41
L.I. Haworth and R.D. Tomlinson	Crystal Data for CuInTe_2	43
W. Wong-Ng <i>et al</i>	Standard X-Ray Diffraction Powder Patterns of Fifteen Ceramic Phases	47
	Departments	
	Calendar of Meetings	57
	Meeting Reports	59
	JCPDS-ICDD Subcommittee Activities	61
	Short Courses and Workshops	62
	General Announcements	63
	Computer Comments	66
	Volume 2, 1987 Contents	70
	Author Index	72



Volume 3 Number 1 March 1988

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A detailed photograph of a Siemens D 500 x-ray diffractometer. The machine is a complex piece of industrial equipment with a large, circular goniometer in the center. The goniometer has several concentric rings and various mechanical components. A red digital display at the top shows the number '015.928'. The background is dark, and the lighting highlights the metallic surfaces of the machine.

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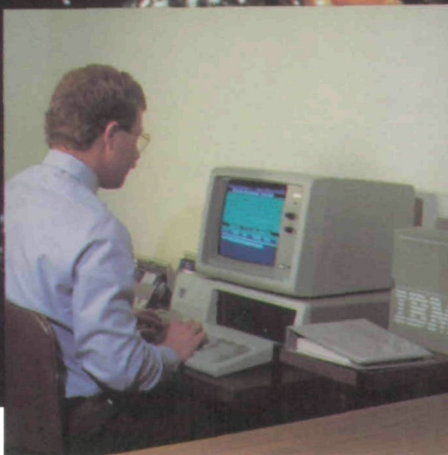
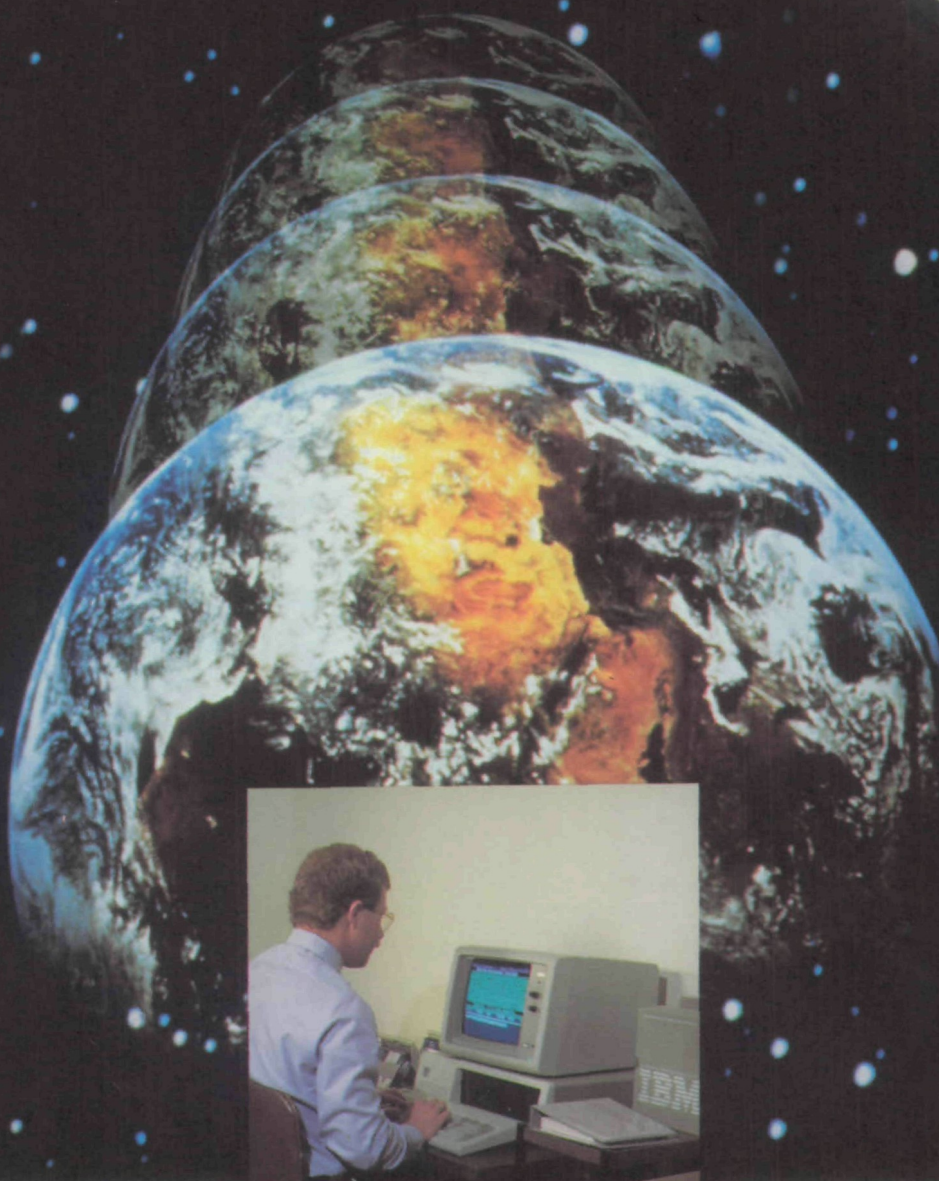
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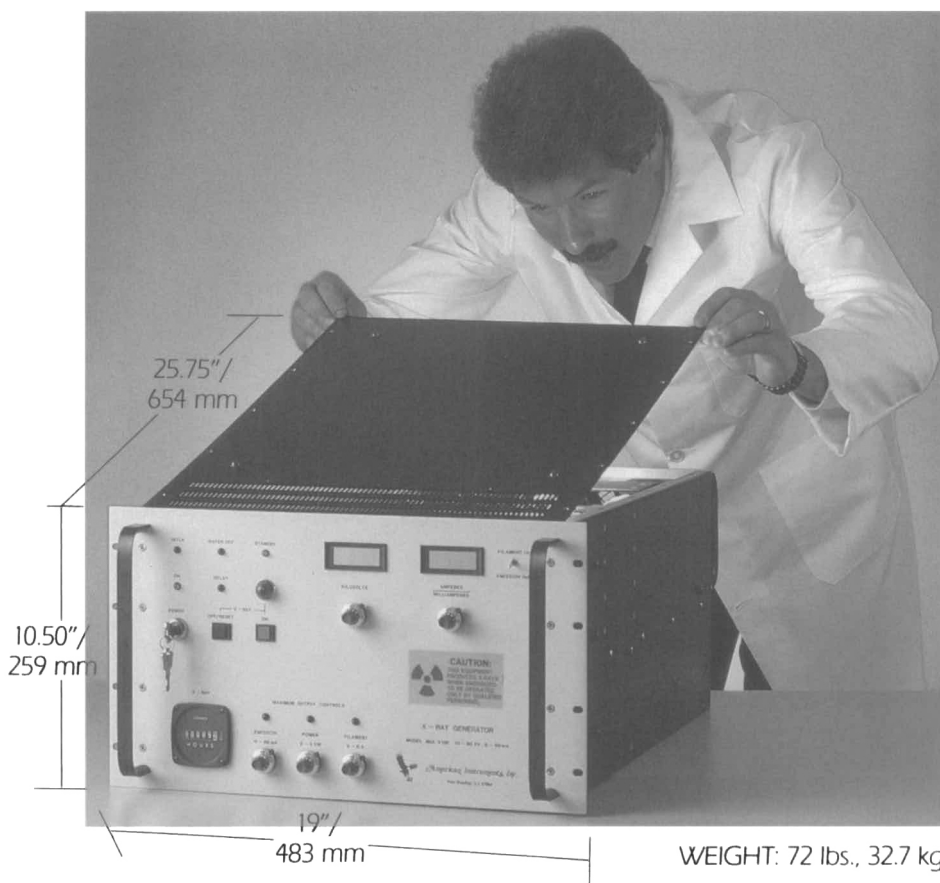


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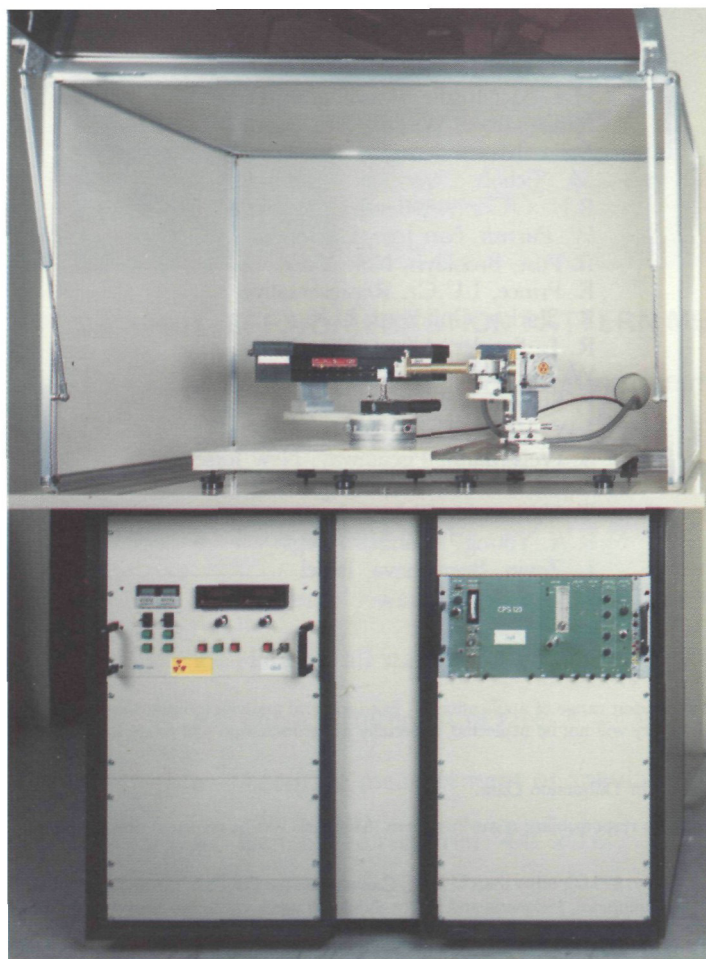
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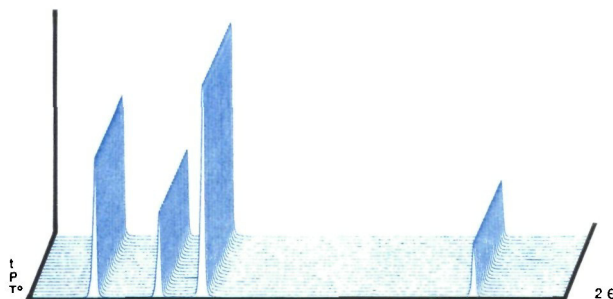
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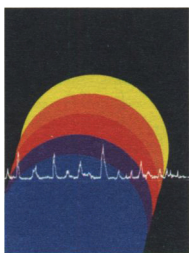
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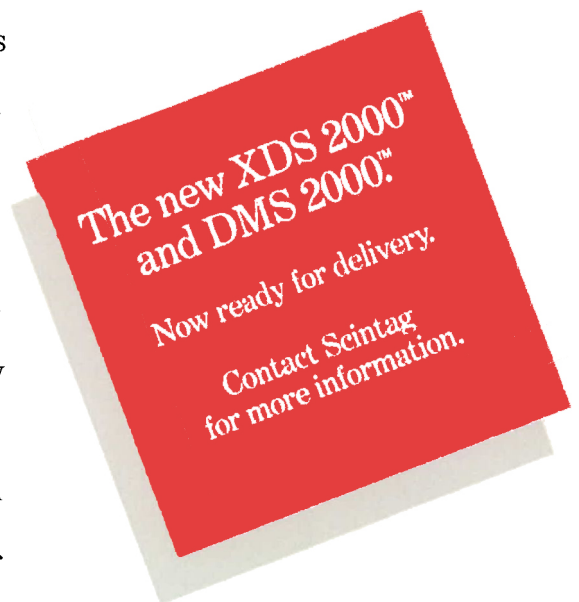
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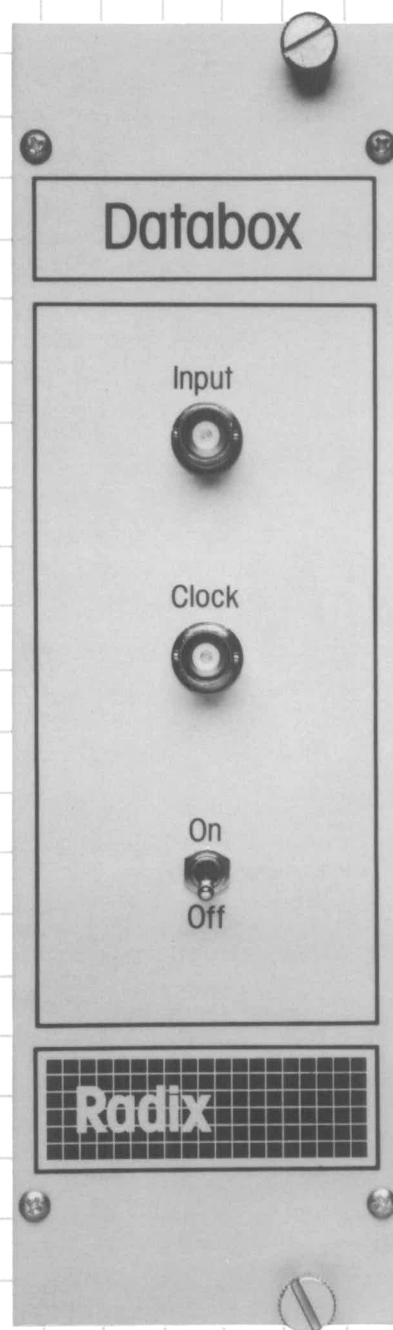
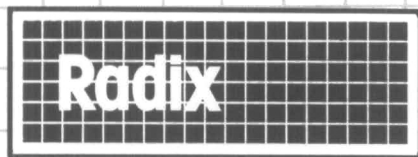
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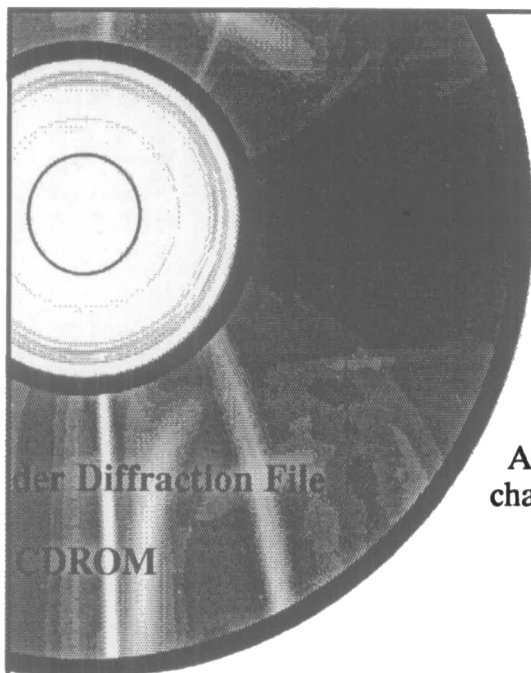
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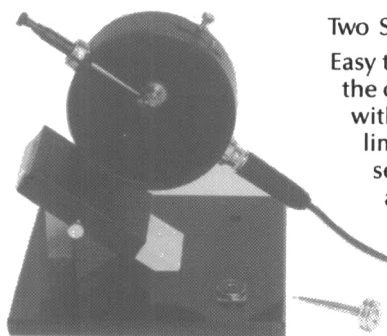


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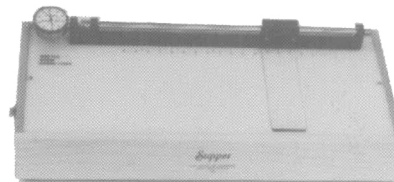
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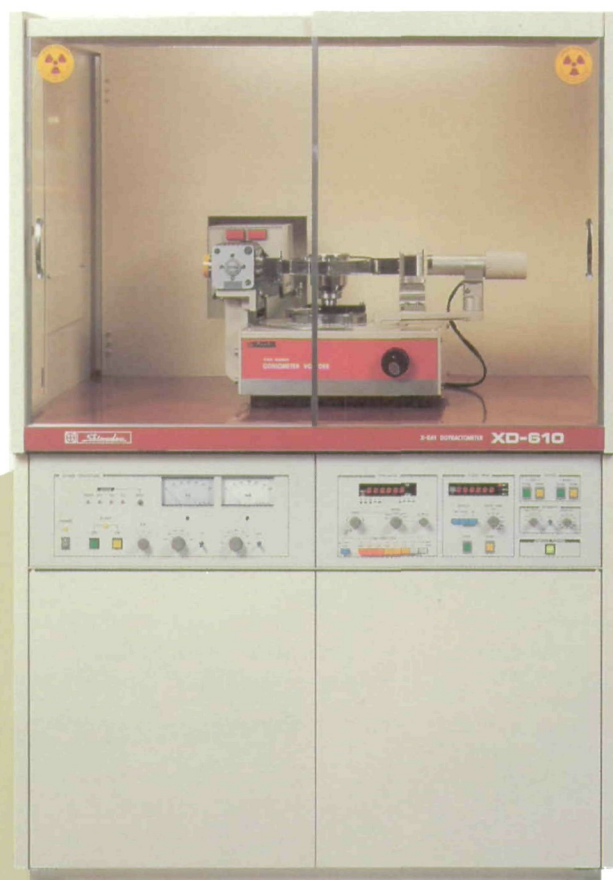
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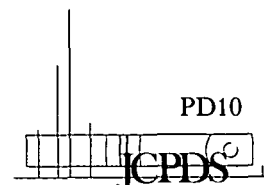
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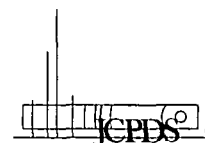
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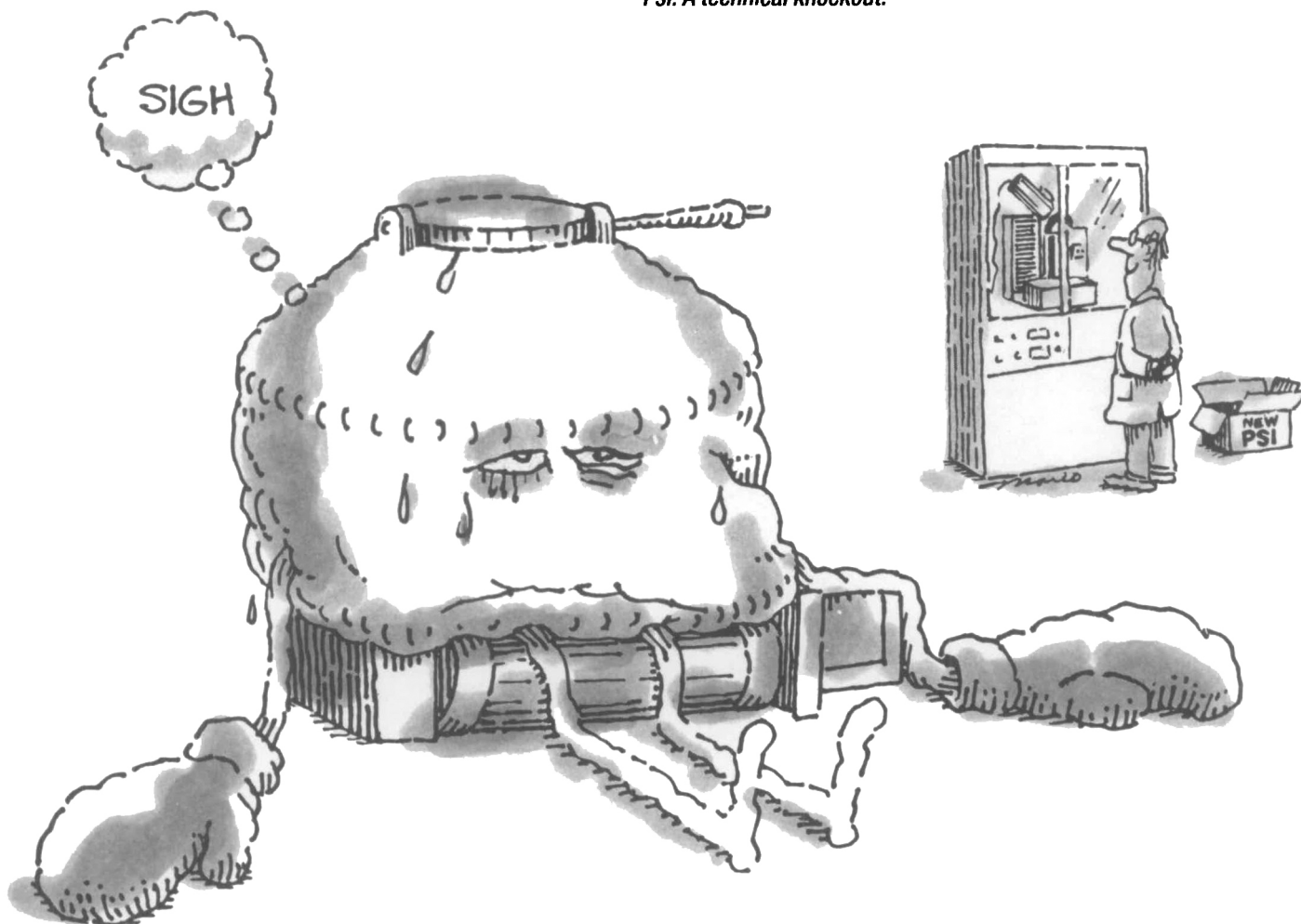
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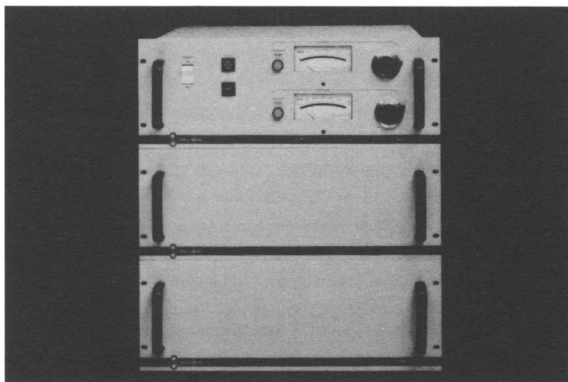
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June 13-17

Session III

**Mathematical &
Computer Methods**

August 15-19

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 20-24

Session II

Quantitative Methods and Advanced Techniques

June 27-July 1

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

PD17

Set **37** 1987-1988

Powder Diffraction File

Set 37 Pattern Profile:

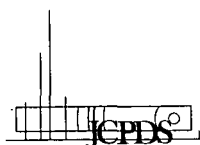
- 150 Replacements
- 32 New NBS
- 83 New Minerals
- 231 New Metals & Alloys
- 34 New Common Phases
- New Inorganics & Organics
- NBS*AIDS83 Review

New:

- CD-ROM
- Set 37 Data Book
- Sets 29-30 Book Form
- Methods & Practices in X-Ray Powder Diffraction

For further information contact:

JCPDS
International Centre for Diffraction Data
1606 Park Lane, Swarthmore, PA 19081
USA (215) 328-9400 Telex: 847170



PD18

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.

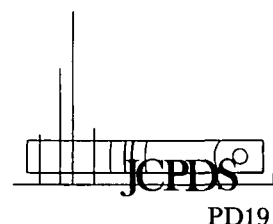
The Mineral Powder Diffraction File Data Book is ordered alphabetically on mineral name, thus grouping together patterns of the same mineral including hydrates, polytypes, order-disorder and chemical varieties, and obviating the need for an index. All data have been reedited with special reference to 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.

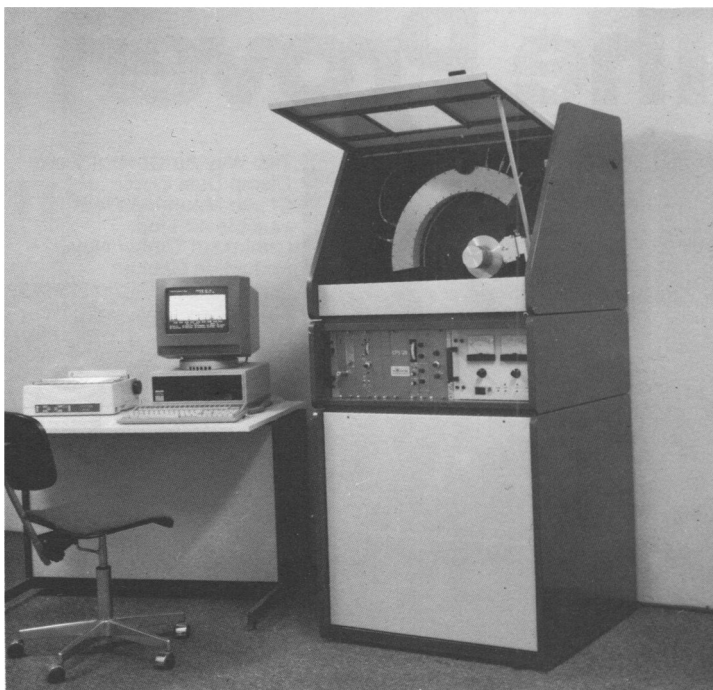
Price: \$550.00 Terms: Domestic — 30 days net
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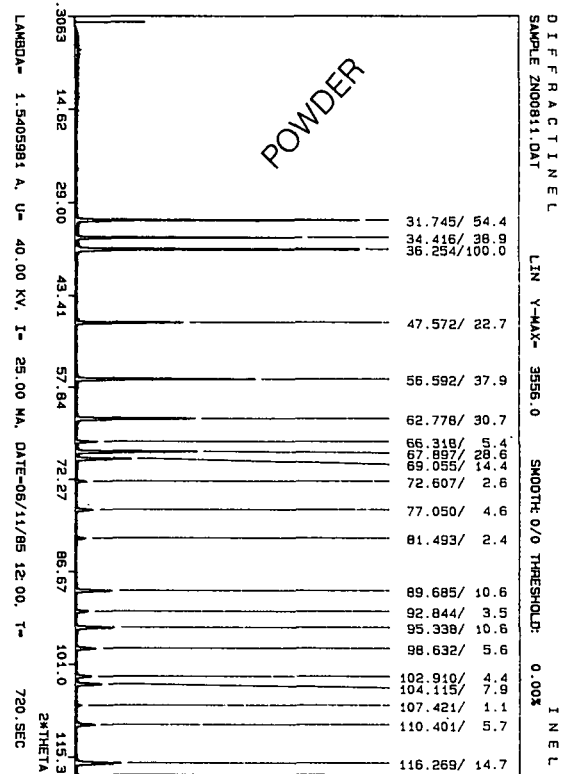
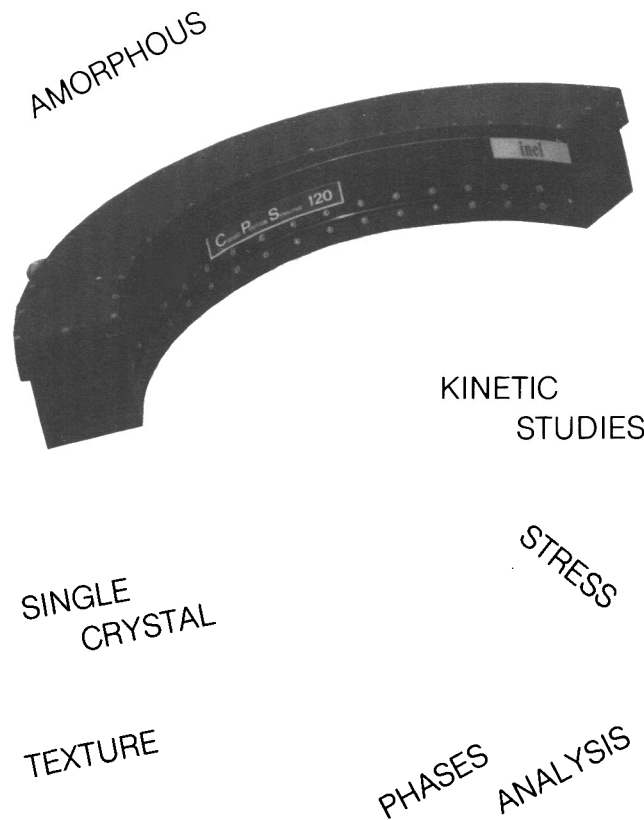
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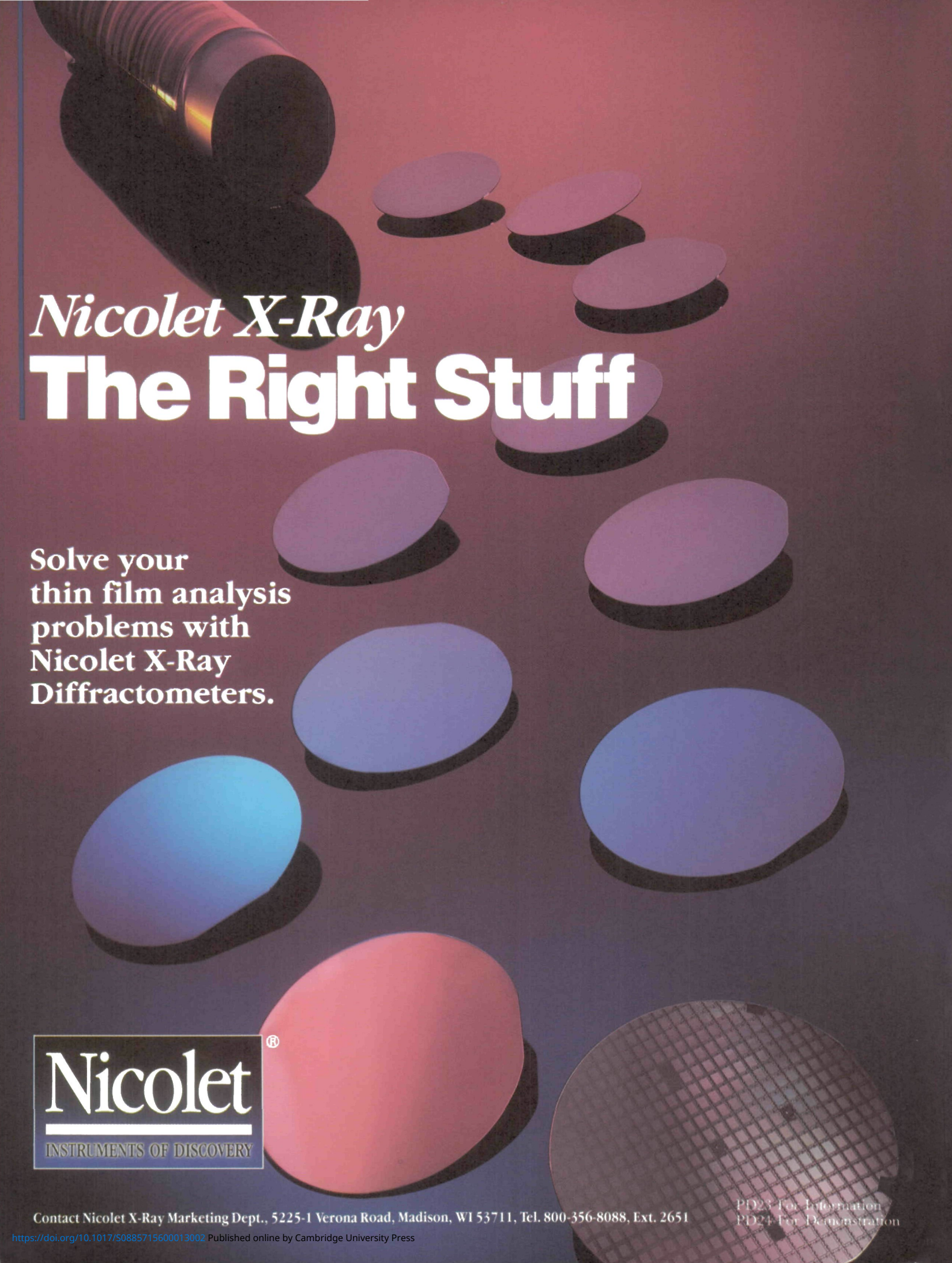
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PD23 For Information
PD24 For Demonstration

Editorial

Powder Diffraction in Education

The identification and characterization of materials by powder diffraction is a topic which should be taught in all chemistry, physics, material science and geology departments. Unfortunately, not all departments include the topic in their undergraduate curricula, and, when they do, it is rarely more than a single experiment in a laboratory type course. Only the material science programs may regularly offer a series of experiments or a full course in X-ray diffraction analysis, ... even here theory is rarely involved. Chemistry departments, in particular, due to their emphasis on the organic field and its many new instrumental methods of identification, often ignore powder diffraction to the point where it is seldom mentioned.

Recognizing that there is a lack of training of analysts in the academic environment, the International Centre for Diffraction Data has made efforts to fill this gap. For over ten years now the International Centre has had an Education Subcommittee whose goals have included the setting up and running of short courses in identification and in the preparation of teaching aids for inclusion in these courses; courses have also been run in industry and academia. The educational materials have been made available, essentially at cost, to anyone desiring to use them. Both the materials and the short course have evolved over the years through use in the International Centre's own courses and in those taught by some Subcommittee members at their own universities. The short course currently given includes the evaluation of diffraction data as well as the identification of phases using the Powder Diffraction File in both manual and computer forms. Separate, special courses, taught from time to time, have been developed for mineralogy and forensic materials. As a supplement to the phase identification course material the International Centre has prepared a *Methods and Practices Manual*, available to short course attendees, on all aspects of experimental techniques. In addition to the products of the International Centre, members of the Subcommittee have assisted in preparing the Audio Short Course on X-Ray Diffraction distributed by the American Chemical Society.

The success of the short course program is indicated by the attendance and responses of the attendees. For over ten years courses have been presented several times each year at the International Centre Headquarters as well as at various facilities around the United States and overseas. Attendees range, typically, from new analysts to very experienced diffractionists; the design of the course has allowed all to learn new material of benefit to their analytical assignments. New diffractionists learn the basis of phase identification and the interaction of diffraction information and chemical information in the confirmation of results. Experienced diffractionists learn the need for accuracy and methods for achieving it plus other applications of powder diffraction analysis, such as quantitative analysis. This course augments the several experimental courses provided at various universities for the training of technologists in the diffraction laboratory.

In spite of the success of the short courses, there is a need to reinstall the teaching of X-ray powder diffraction into the curricula of academic programs. All scientists need to know the value of X-ray diffraction methods and their uses and limitations. They are the requestors who supply most of the samples submitted to the diffraction laboratory. Many do not appreciate the difficulties in the full characterization of a material. I have had requestors respond to my question for background information on the sample, with "you do not need any information as it will bias your results." They did not realize how much time might be needed to fully analyze a pattern. And, when these requestors returned for results, the answers they sought were usually the hardest to explain.

The revived interest in superconducting materials has also reaffirmed the recognition that there are problems for which powder diffraction may be the only suitable technique. For example, the structure of the superconducting phases has been determined by X-ray and neutron powder diffraction. Or again, it is absolutely necessary to confirm the presence of the appropriate phase by powder diffraction prior to expending time measuring properties on incorrectly prepared samples. One of the continuing problems of this research is educating the experimentalists that their material must be properly characterized. The need for courses in diffraction analysis is apparent.

The present educational problem is not that material is not available for present courses, but rather the lack of availability of time in busy curricula for the adequate instruction of students in diffraction analysis. One alternative is to have video materials prepared for individual instruction at a user's convenience. This approach is excellent where it is employed for explaining the use of equipment, but falls short where it involves the interpretation of results, if there is also no chance for interaction with a competent instructor. Experience and practice are the best teachers in this field, but the availability of some personal assistance is invaluable in the early learning stages of any course.

The International Centre continues to have interest in the development of instructional material for training in the use of powder diffraction data. Suggestions as to how to improve the present instruction packages and for new materials that would be useful in courses are very welcome and should be sent to Ron Anderson, Departments Editor of this Journal, who is Chairman of the Education Subcommittee. Contributions for the *Methods and Practices Manual* should be submitted to this Journal; most of the contents of the Manual are reprints of articles which have appeared here.

Deane K. Smith
Editor-in-Chief