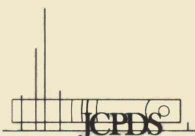
Powder Diffraction

H. Hermann and M. Ermrich	Microabsorption Correction of X-Ray Intensities Diffracted by Multiphase Powder Specimens	189
L.S. Zevin and Sh.L. Zevin	Standardless Quantitative X-Ray Phase Analysis – Estimation of Precision	196
B.L. Davis, D.K. Smith and M.A. Holomany	Tables of Experimental Reference Intensity Ratios. Table No. 2, December 1989	201
T.C. Huang and P.W. Wang	X-Ray Powder Diffraction Analysis of a Photoconductor Material p-Diethylaminobenzaldehyde Diphenylamine Hydrazone	206
J.A. Emig and D.K. Smith	The Detection and Quantification of Low Concentrations of Quartz in Dolostone by X-Ray Powder Diffraction	209
E. Goldish	X-Ray Diffraction Analysis of Barium-Strontium Sulfate (Barite-Celestite) Solid Solutions	214
A. Borgna, B. Moraweck and P. Fessler	X-Ray Diffraction and EXAFS Study of Palladium Tetrammine Dichromate, $[Pd(NH_3)_4]Cr_2O_7$	217
F.N. Blanchard	X-Ray Powder Data for $CaWO_4$, Synthetic Scheelite	220
Fang Zhou *et al.*	$(Na_{0.5}Bi_{0.5})TiO_3$: Synthesis and X-Ray Powder Diffraction Data	223
J.M. Amigó *et al.*	Crystal Data for Nickel Cimetidine Chloride: Ni $(CM)_2Cl_2 \cdot 2\ H_2O$	225
F.N. Blanchard	New X-Ray Powder Data for Gorceixite, $BaAl_3(PO_4)_2(OH)_5\ H_2O$, an Evaluation of d-Spacings and Intensities, Pseudosymmetry and its influence on the Figure of Merit	227
D.F. Rendle *et al.*	X-Ray Powder Diffraction Data for 2-nitro-1-phenyl-prop-1-ene	231
J.L. Garin and J.A. Costamagna	X-Ray Powder Diffraction Data for Two Ammonium Copper Molybdates	233
	International Report	236
	Calendar of Meetings	237
	Meeting Reports	238
	Correspondents Reports	240
	Short Courses and Workshops	240
	Book Reviews	241
	Computer Comments	242
	Commercial Announcements	245
	Volume 4, 1989 Contents	247
	Author Index	249



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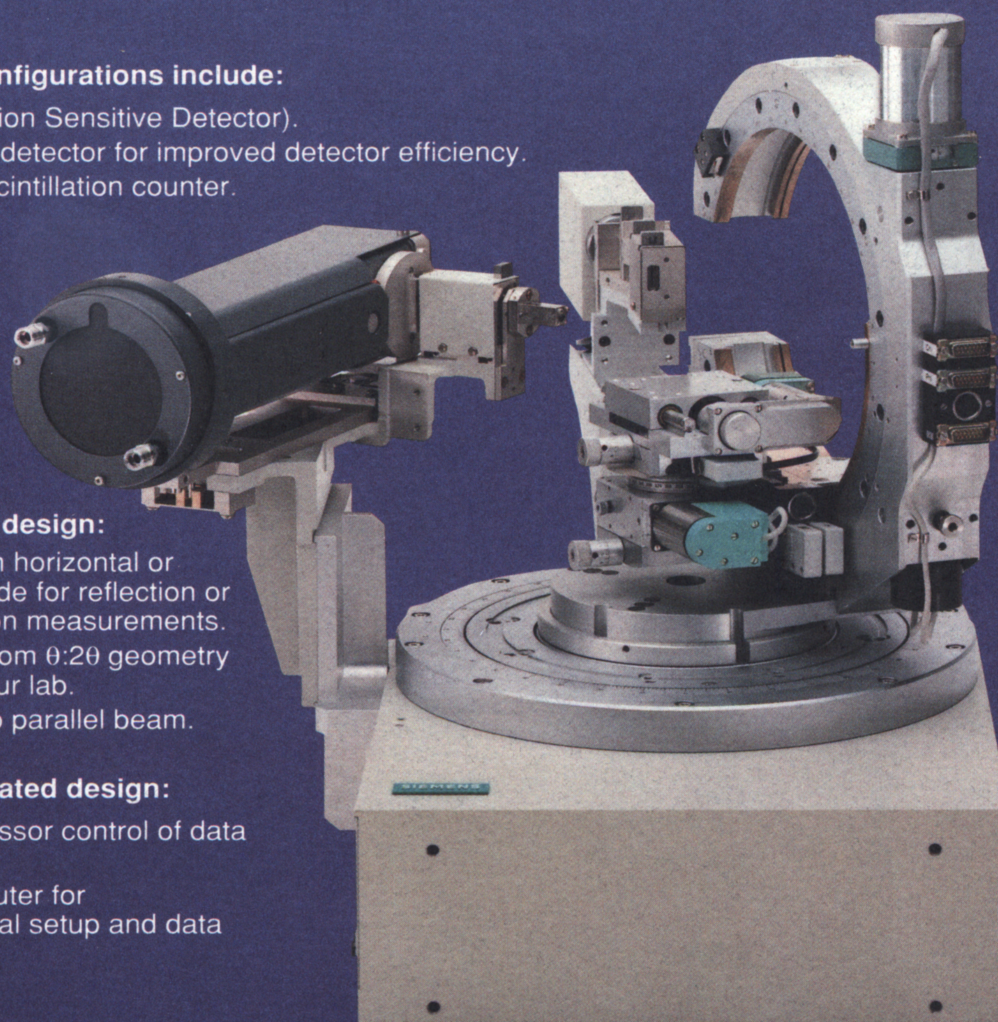

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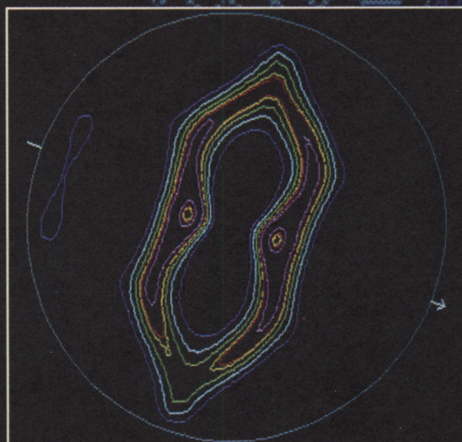

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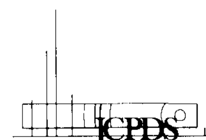

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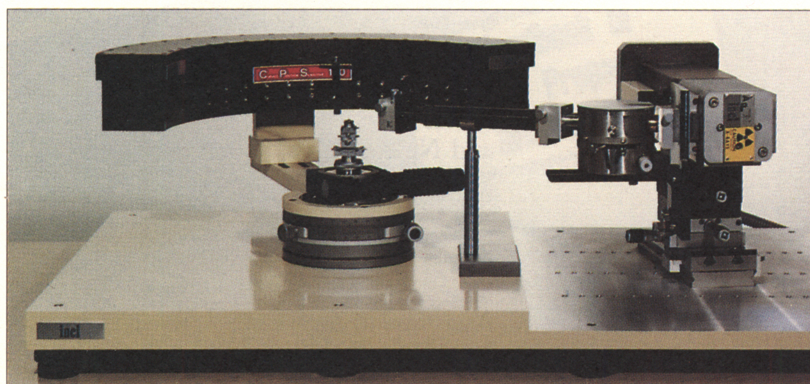

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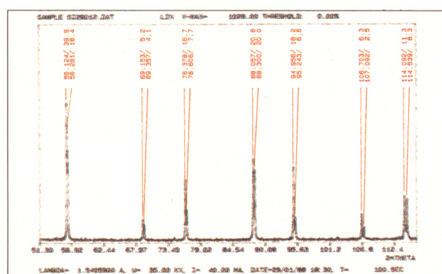

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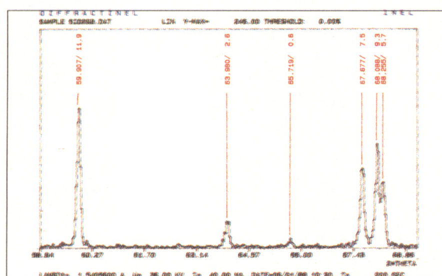

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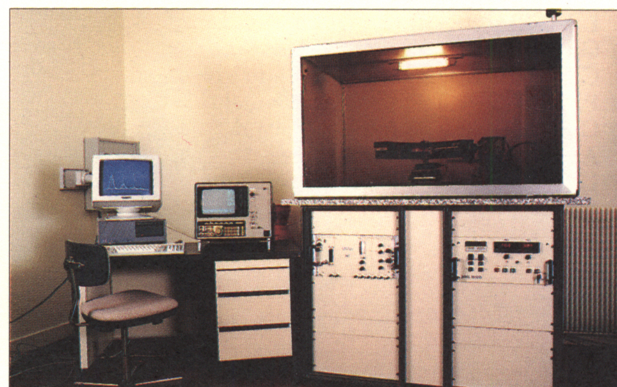

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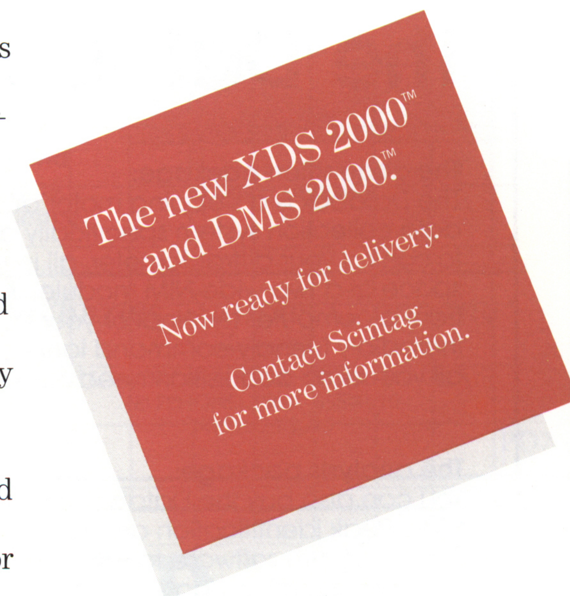

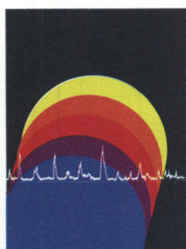

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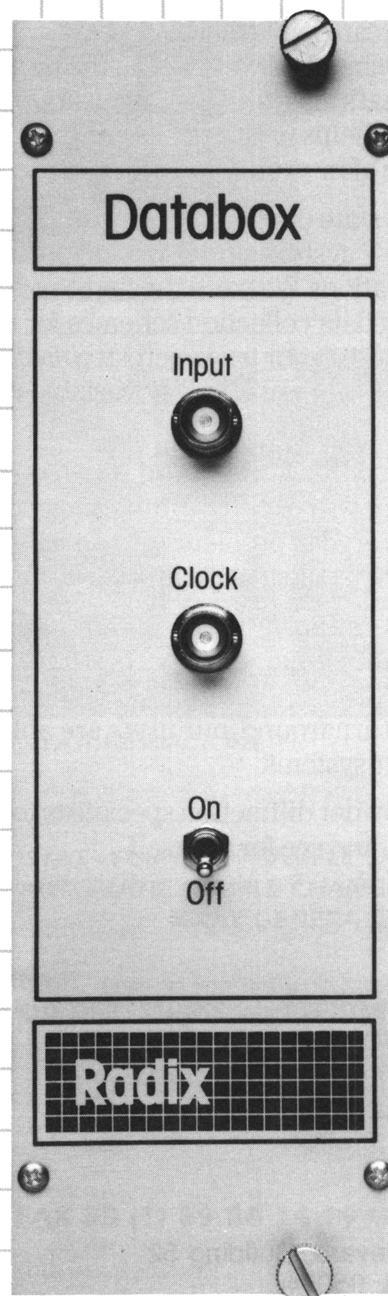

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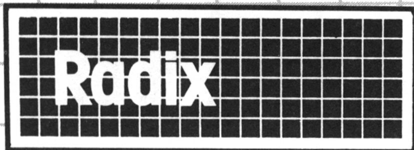

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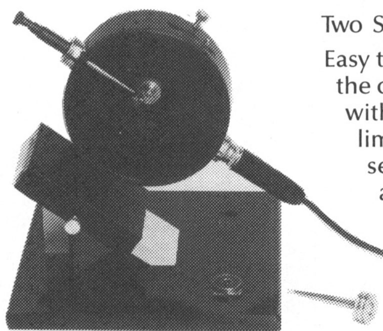

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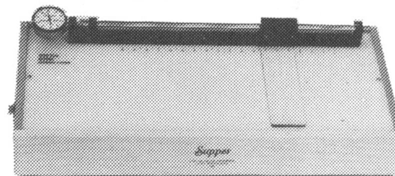

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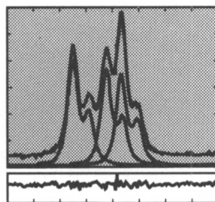

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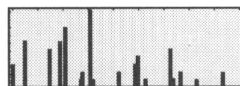

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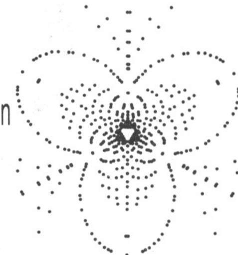

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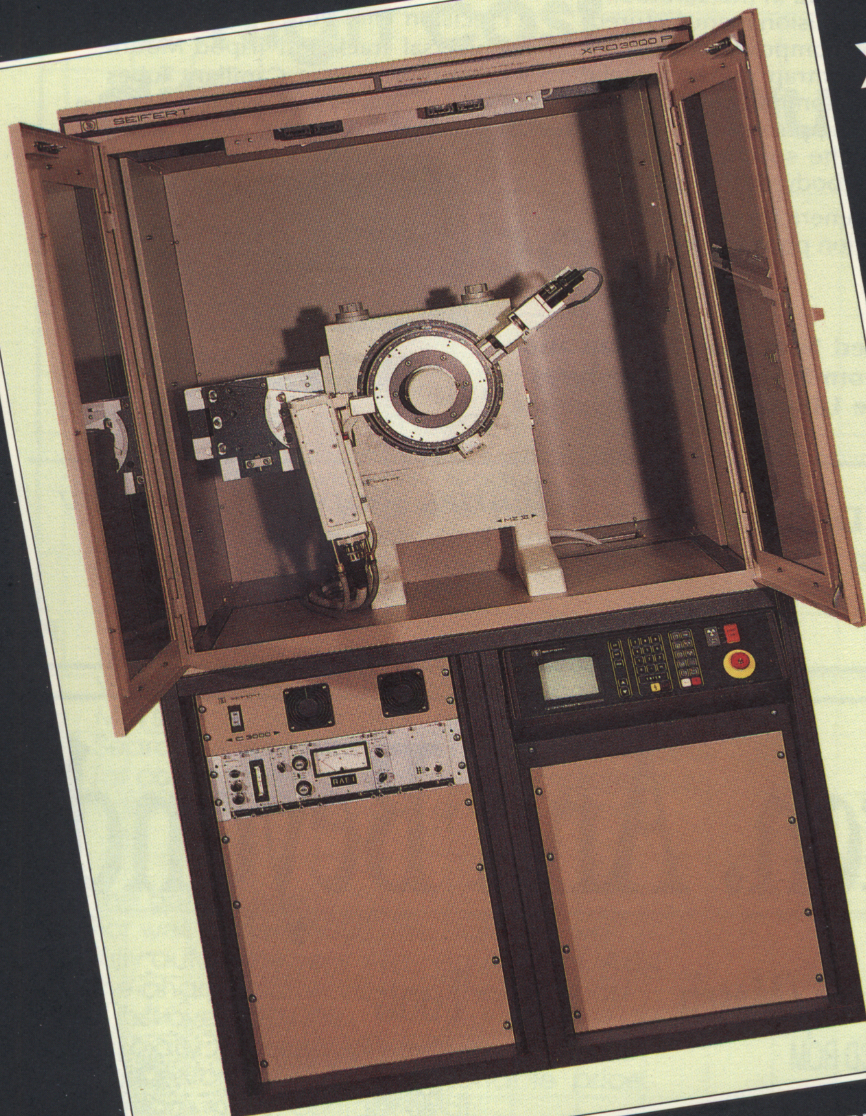

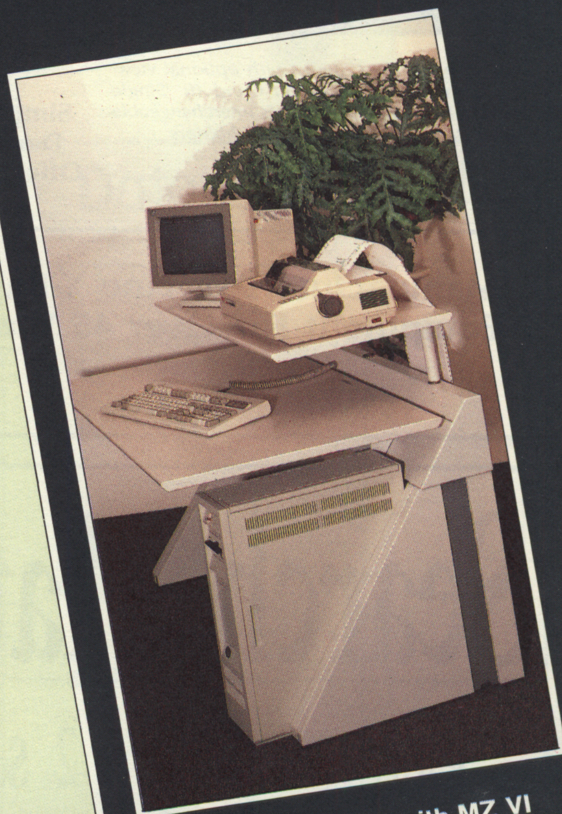

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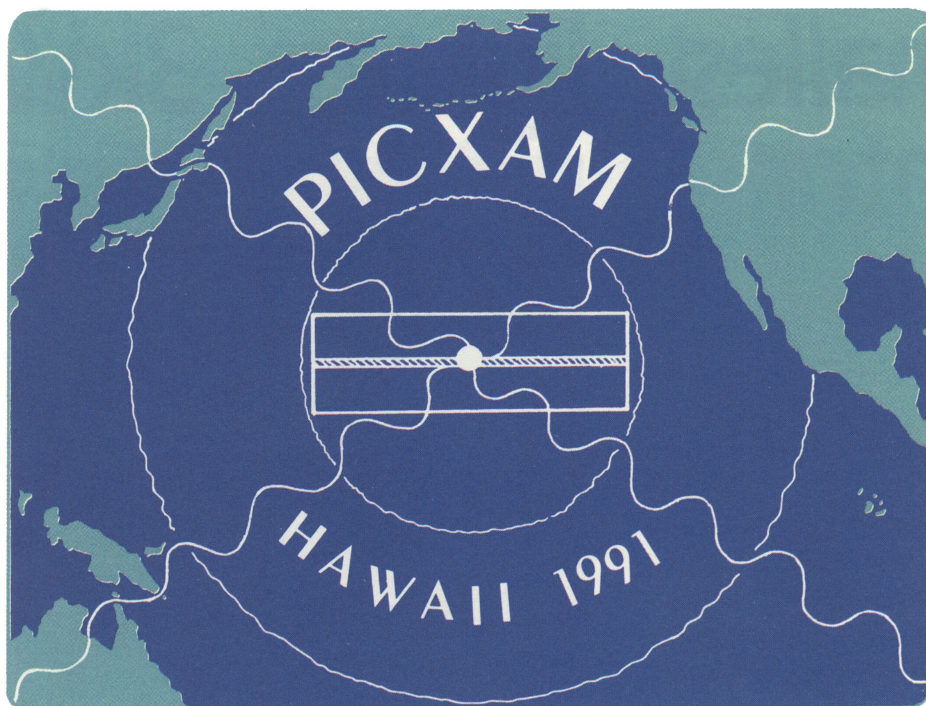

Second Announcement...

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:

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X-ray Chemical Analysis Group/
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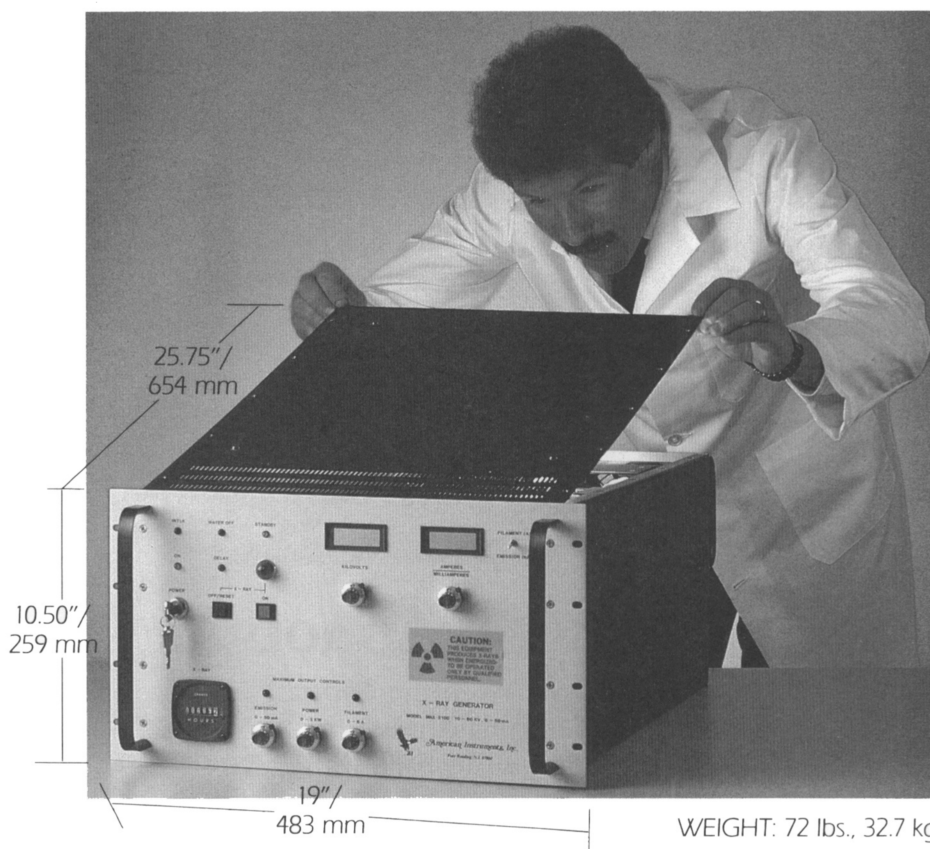

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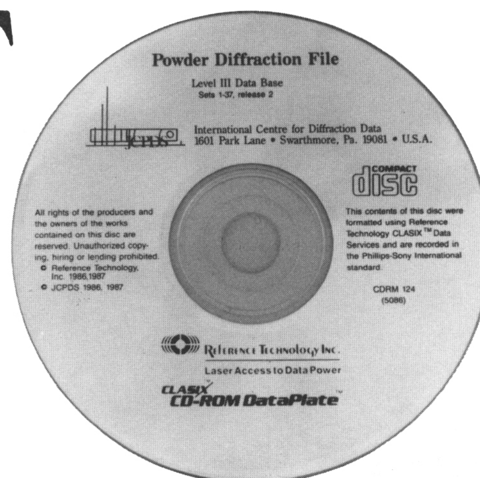

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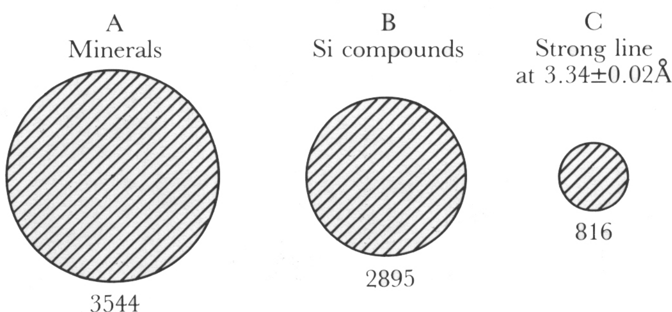

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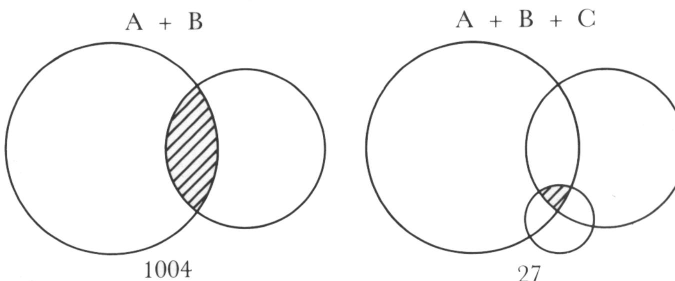

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1601 Park Lane, Swarthmore, PA 19081–2389 USA
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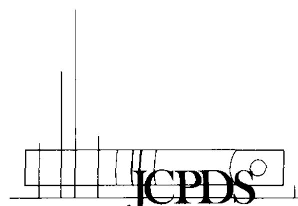

PD-12

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Introducing the world's fastest, high resolution powder diffractometry system ...

The new PDS120 is a complete, integrated system that provides superior results quickly and easily. It is the product of close cooperation between Enraf-Nonius, the world-leader in single-crystal X-ray diffractometry, and Inel, the manufacturer of a unique curved position sensitive detector.

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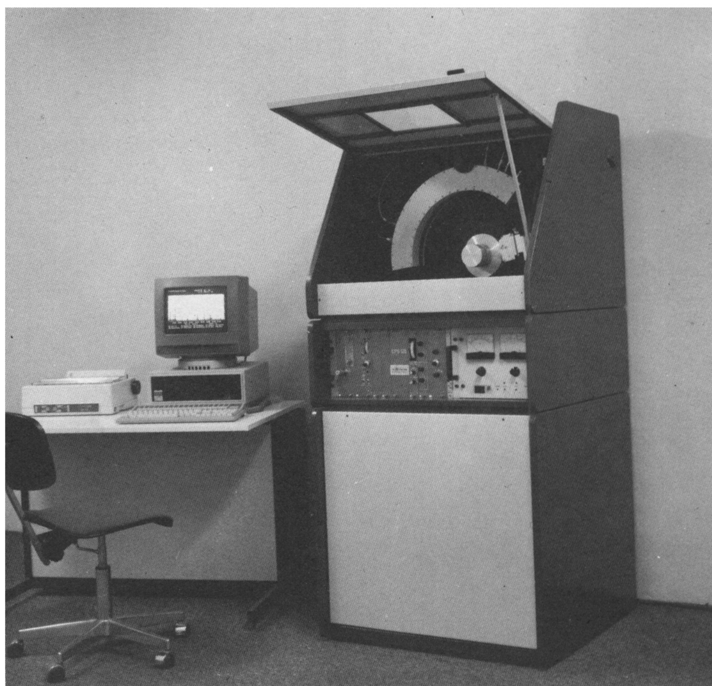
A new class of diffractometer with X-RED



X RED... an X Ray Electronic Diffractometer based on a Curved Position Sensitive detector ranging 120 degrees with a resolution of better than 0.03 dg. and its associated electronic, X-ray generator, water refrigerator unit, all included in an indipendent X-ray proof cabinet. Of course linked to a PC Olivetti Computer with its fine graphic performance, to display in real time a diffraction pattern. And more, automatic sample exchanger for capillaries, liquid, high, low temperature attachment.
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PD-15

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For further information contact:
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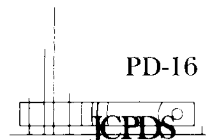
JCPDS-ICDD
1601 Park Lane, Swarthmore, PA 19081
USA (215) 328-9400 Telex: 847170



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SieRay 112

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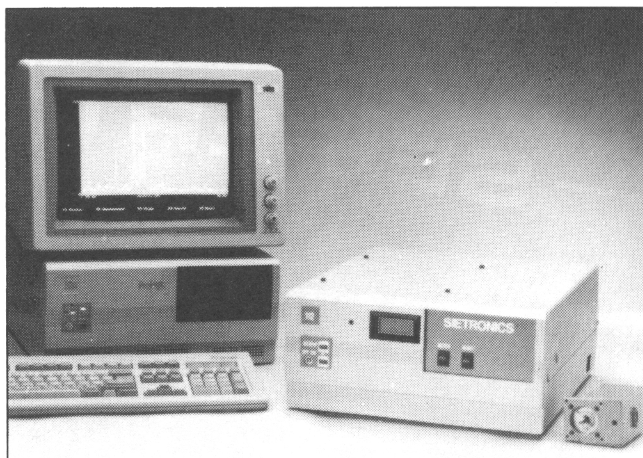
(For a lot less than you thought)



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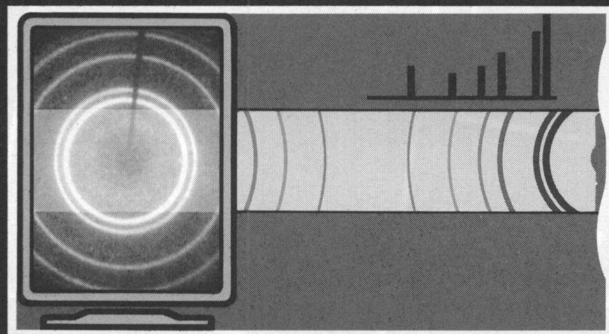
PD-17

X-RAY DIFFRACTION SERVICES



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PD-18

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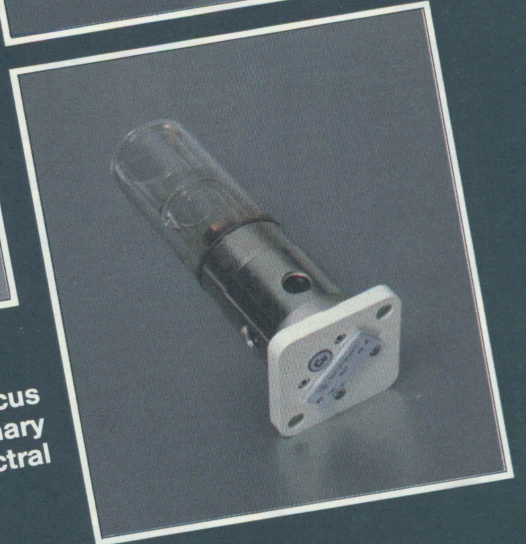

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Editorial

Short Course on Advanced Powder Diffraction Methods

The Mineralogical Society of America held a short course on advanced powder diffraction methods in St. Louis, Missouri, November 4-5. The organizers were David L. Bish and Jeffrey E. Post who also edited the course notes which have been published by MSA. Other participants included R.C. Reynolds, Jr., R. Jenkins, R.L. Snyder, D.K. Smith, S.A. Howard, L.W. Finger and R.B. Von Dreele. The course included topics of considerable interest in research and materials characterization whose applications reached well beyond the mineralogical community.

Following the introductory material on the principles of diffraction, there was considerable discussion on instrument alignment and experimental procedures with modern equipment. Special topics included sample preparation, quantitative analysis, diffraction by small and disordered crystals, powder diffraction software, profile refinement methods, Rietveld refinement, synchrotron and neutron powder diffraction. The presentations emphasized the modern applications and advances in techniques and equipment. Experiments with neutron diffraction and synchrotron sources were also presented. Many of the presentations emphasized the use of sources with high intensities and digitized data traces.

With the increasing availability and widespread use of computer-controlled instrumentation and the availability of more intense sources, powder diffraction has expanded its role in materials analysis very rapidly in recent years. One good example of significant improvement is the use of the entire digitized diffraction trace for analysis rather than just the derived ds and Is. Applications to quantitative analysis, crystal structure refinement, and crystal perfection studies were emphasized in the MSA presentations. Use of the full digitized trace as raw or processed data will become increasingly important in the future. These early applications will be enhanced as new procedures are developed.

In addition to using the full trace as a basis for analysis, there has been considerable emphasis on the fitting of selected profiles to the digitized data to achieve the most accurate position and intensity information and in the unravelling of complex clusters of diffraction peaks. Not only have there been additional analytical profiles evaluated, but the computational methods in the fitting procedures have been optimized for rapid calculations. Profile fitting is an easier procedure than deconvolution, and the results are proving to be as useful in the determination of crystallinity parameters on imperfect materials.

One section of the MSA program, prepared by this editor, was a review of the available computer programs for analyzing diffraction information. This list contains over 100 programs, including many not discussed elsewhere in the course, along with the names of individuals to contact for copies. The programs are classified according to application, and similar programs are compared with respect to the type of algorithm used and the information produced. They are not compared for efficiency or ease of use. PC, mini and mainframe programs were considered. This list will be valuable to any diffractionist.

Although the course was designed and presented by mineralogists for mineralogists, the material is of general interest to any materials scientist. The course notes were prepared to be used as text material for advanced diffraction instruction or as a reference source for techniques and articles on general and special topics. This publication was issued in November 1989 and is available from the Mineralogical Society of America, 1625 I Street N.W., Suite 414, Washington, D.C. 20006, U.S.A. The cost of the publication is $20.00 U.S.

Deane K. Smith
Editor-in-Chief

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