PDFEAPC Powder Diffraction editorial aids for the personal computer. Crystallographic evaluation of PD data according to criteria by the (U.S.) National Bureau of Standards and production of output in the form of powder diffraction data file card.

Available from: R. G. Garvey

Department of Chemistry North Dakota State University Fargo, ND 58105-5516 U.S.A. Type: Public Domain/Shareware

PDFPLOT Plots data from JCPDS CD-ROM in the form of simulated XRPD patterns.

Available from: S. P. Terblanche

Functional Ceramics Programme

DMST/CSIR

P.O. Box 395 Pretoria 0001 South

Africa

Type: Public Domain/Shareware

SHAPE Crystal drawing from keyboard input.

Available from: Shape

196 Beechwood Ave. Bogata, NJ 07603

U.S.A.

Type: Commercial

SIE112 XRPD diffractometer automation system. A diffractometer driver and data collection system. Can be interfaced with microPDSM search/match software or CSM-V. Graphic facility.

Available from: SIETRONICS

P.O. Box 84 Hawker ACT 2614 Australia Type: Commercial UNITCELL The program tries to find the unit cell parameters from a PD pattern using the algorithm proposed by deWolff (1968) and programmed by Visser (1969).

Available from: R. G. Garvey

Department of Chemistry North Dakota State University Fargo, ND 58105-5516 U.S.A. Type: Public Domain/Shareware

WYRIET The Rietveld powder pattern refinement program of Wiles & Young (1981) adapted to IBM AT computers. Graphic facility.

Available from: Dr. J. Schneider

Institute f. Kristallographie Universitat Munchen Theresienstrasse 41. D-800 Munchen 2 West Germany Type: Public Domain/Shareware

X-RAY ANALYSIS PROGRAM Graphical display of data generated by a diffractometer. Provides line or point display, difference plots, integrated intensity.

Available from: Fischer-Cripps Laboratories Pty. Ltd.

P.O.Box 890 Brookvale

NSW 2100 Australia Type: Commercial

microPDSM Micro powder diffraction search/match. Searches the data collected by the JCPDS - ICDD (both on floppy disk and CD-ROM) and matches them with the experimentally collected X-ray powder diffraction data patterns.

Available from: Fein-Marquart Associates, Inc.

7215 York Road

Baltimore, MD 21212 U.S.A.

Type: Commercial

Short Courses and Workshops

JCPDS - International Centre for Diffraction Data

Short Course on Search/Match Methods

The JCPDS-International Centre for Diffraction Data will continue to offer three-day short courses on Search/Match methods at the Swarthmore, PA, headquarters of the International Centre and elsewhere (see attached schedule).

The courses, which are now in their 5th year, are intended to build proficiency of the user in the interpretation of experimental data, especially in the application of the information provided in the *Powder Diffraction File.* The courses should be useful to the novice as well as the experienced powder diffractionist, and all discussions start with the basic principles leading on to useful laboratory procedures. Workbooks are provided to all attendees and these contain a number of experimentally obtained X-ray diffraction data sets which are used as class exercises. During the workbook sessions, the classes are subdivided to match the needs and experience of the attendees.

The course will emphasize the nature and organization of the information in the *Powder Diffraction File* and retrieval and use of this information for interpreting experimentally collected diffraction data. The implications of the accuracy of measurement of dspacings and intensities of experimental data with respect to use of the powder file will be discussed, as well as common instrumentation and specimen-induced errors. The use of both manual and computer search/match methods for phase identification will be practiced through the use of workbooks. Applications of File data for further characterizing phases will be illustrated using several mineralogical problems and a special X-ray diffraction minerals workbook. Other types of materials may be studied including organic and forensic materials, depending upon the needs of the participants.

Course Schedule

Optimization of data collection Evaluation of experimental data Instrumental induced errors Sample induced errors

Day 1 Afternoon: Introduction to the Powder Diffraction File

Role of the JCPDS-ICDD Alphabetic search procedures

The Hanawalt search/match procedure The Fink search/match procedure Classical powder diffraction problems

Phase identification

Analysis of polyphase materials

Day 2 Afternoon: Computer techniques in data collection

Use of the computer in qualitative analysis

Use of CD-ROM based systems

Day 3 Morning: Continuation of problem solving session

Use of the Crystal data file

Other data files (max-d; electron diffraction, etc)

Day 3 Afternoon: General question and answer session

For further information please contact:

Ms. Josephine Felizzi

JCPDS - International Centre for Diffraction Data

1601 Park Lane

Day 1 Morning:

Day 2 Morning:

Swarthmore, PA 19081, U.S.A. (215) 328-9403

The cost of a course is \$625.00 which includes textual materials and lunches. Lodging, transportation and other costs are at the expense of the attendee.

JCPDS - International Centre for Diffraction Data Course Schedules

1990

Oct. 30, 31, Nov. 1 San Jose, California