

Commercial Announcements

Mineral Database & Manual for Personal Computers

Aleph Enterprises and CSIRO (Australia) have joined forces to create **MINERAL**, a computerized mineral reference book in a PC database format containing data for more than 3500 minerals. A user manual accompanying the computerized reference contains easily understood instructions for loading and using the system as well as a listing of the name and principal reference for all species present in the database.

MINERAL is designed to function with the recently introduced **TRACKER** program which allows very rapid searching of this database using:

- Species Name, Name Fragment or Synonym
- Elemental and/or Polyatomic Constituents
- Mineral Group Name
- Related Species Name(s)
- Crystal System and Space Group
- Lattice Parameters
- JCPDS Number
- Mineral Classification

Other information available for each species includes the chemical formula, two general references and an additional reference to the origin of the name.

The database comes with an on-line user help facility which explains the use of special Aleph function keys to conveniently search the **MINERAL** database. Also available is the ability to include your own information about each species such as catalogue number, locality, etc. as well as the ability to print, or view on the screen, summaries of those minerals that meet elemental or other criteria you have established.

The **MINERAL** database and its retrieval program require a hard disk and occupy approximately 4 megabytes of disk space. A minimum of 384 KB RAM is required as is IBM PC-DOS 2.0 or MS-DOS 2.02 or greater. A graphics adapter is not required for this system which uses either a monochrome or color CGA or EGA monitor.

MINERAL is available from Aleph for \$199 (Check with Aleph for prices outside the US). This price includes the **MINERAL** database, user manual with printed mineral summary, and the **TRACKER** retrieval system.

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μ PDSM Release 4.01 Supports CD-ROM

The latest release of μ PDSM, Fein-Marquart Associates' micro Powder Diffraction Search/Match system, fully supports retrieval, display, and manipulation of the JCPDS PDF-2 CD-ROM database.

The CD-ROM functions incorporated in μ PDSM include full Boolean logic retrieval using elemental composition, chemical and mineral names, and name fragments. A simplified language allows straightforward specification of complex queries; for example, "(Mn Mg) silicate not hydrate" locates all silicates containing either magnesium or manganese that are not hydrated. Both partial and exact name searches are supported, as well as incremental retrieval refinement, wherein a new retrieval can use prior retrievals' hit lists as search terms in the new request.

High speed browsing through any of the retrieved lists of PDF cards is provided. Full integration with the search/match function allows immediate testing of any retrieved pattern against the problem pattern with a single keystroke, and provides all of the search/match display and subtraction capabilities for the result. Similarly, the card image for any search/match result is instantly displayable, again with a single keystroke.

Use of the CD-ROM database is optional and automatic; μ PDSM detects its presence and adjusts its operation appropriately.

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Integrated PDF-2 on CD-ROM, Search/Match, Shown in Japan

The latest release of μ PDSM, micro Powder Diffraction Search/Match, by Fein-Marquart Associates, Inc., is now available in Japan through Sanyo Shuppan Boeki Company, Inc. This release of μ PDSM, described in the *Commercial Announcements* column, supports retrieval and display from the JCPDS PDF-2 database on CD-ROM, fully integrated with the search/match functions.

On March 18 and 19, a lecture and exhibit meeting on the effective use of CD-ROM in industry and science was sponsored by the Kansai Joho Center in Osaka, Japan. Sanyo Shuppan demonstrated the μ PDSM implementation of CD-ROM retrieval at this meeting. Additional presentations of this use of the JCPDS database have been made at various locations in Japan, and more are planned.

Philips PLUS³⁷, the First Total Access Diffraction Database on Compact Disc

Philips announces PLUS³⁷(TM), the first complete total access diffraction database available on compact disc. The PLUS³⁷ is a fully indexed and searchable data set containing every diffraction parameter in the 1987 JCPDS PDF-2 database (formerly Level III).

The JCPDS database in card image form has, for 36 years, supported diffractionists' needs for a reference set of known compounds. Through the use of JCPDS Search Manuals and applying the Hanawalt search technique, diffractionists were able to perform phase identifications of powder diffraction data from unknown materials. Now, with the availability of the expanded form of the JCPDS database as PDF-2, Sets 1-37, significantly more important crystallographic and material information is accessible.

Combining the diffraction database Sets 1-37 with state of the art data storage hardware and retrieval software, PLUS³⁷ allows rapid, comprehensive investigation for a variety of applications. Its new compact disc format offers the diffractionist, electron microscopist, and educator rapid access to over 200 unique data fields for each of nearly 50,000 compounds. The powerful retrieval software allows multiple field data searches using Boolean and relational logic. Previous databases, provided as ASCII text, offered only partial access to important data. The PLUS³⁷ database is provided in binary form, to give rapid, easy data access and unlimited search capability. Patterns satisfying the search criteria may be displayed as card images or in line format.

PLUS³⁷ allows the diffractionist to perform Hanawalt search/matches interactively, find patterns by PDF Reference Number, color, optical data, elemental content, single d-spacing, space group, or by hundreds of other criteria. The electron microscopist can also access patterns by d-spacing only, regardless of line intensity. Educators can use PLUS³⁷ to support crystallographic and diffraction education in geology and material research, with on-

line help screens guiding the user regardless of expertise level, through the entire retrieval process.

The PLUS³⁷ system operates as a stand-alone package on the IBM(TM) PC/AT, IBM-compatible systems or the DEC(TM) MicroVAX. When used in conjunction with Philips exclusive APD software, PLUS³⁷ can be used to create unique analytical subfiles to speed the Search/Match process, or to reprocess the Search/Match results with additional information.

Philips Launches XRD Software for Personal Computers

PC-APD is an easy-to-use analytical software package for the Philips IPD Integrated Powder Diffractometer, MPD1880 Multi-Purpose Diffractometer system and CPD Compact Powder Diffractometer. Developed for IBM XT/AT/PS2 or compatible computers such as the Philips P3200 Series, it offers an economical yet powerful means of system automation for powder diffraction applications. Extensive use of menus and input forms make it simple for a user to set up automatic analysis programs very quickly, without need to consult lengthy operating manuals.

Peak searching employs a proven multi-pass search algorithm, as incorporated in Philips' powerful APD1700 software. Output options include listings and plots of raw data, DI (peaks and intensities), background, smoothed data and second derivative files - while the availability of a high resolution color graphics display with zoom function facilitates results interpretation.

A sophisticated search/match routine is based on the CIF (Compound identification with Inverted search and Fuzzy sets) program. This provides for rapid comparison of DI files with data bases containing up to 500 reference patterns. Sub-files can also be created, allowing further reductions in search time. And as any number of data bases can be assembled and stored on disc, the package is capable of meeting wide-ranging application needs.

As one of many utility options, data can be converted to ASCII file format - allowing extended processing using the many commercially available programs for PCs.

Multi-Purpose Diffractometer Offers Performance and Versatility

The MPD1880 multi-purpose X-ray diffractometer from Philips combines modularity with top performance for the most demanding research and industrial application requirements. Two goniometers, two generators, two instrument enclosures, a choice of X-ray tubes and a broad selection of accessories give freedom to assemble individual installations according to specific needs.

Configuration Choice

The PW1820 vertical goniometer is the preferred choice for phase, stress and texture analysis on standard samples. An optional sample stage enables objects weighing up to 1 kg to be loaded. Unattended batch analysis of standard samples is also possible, with a choice of 35- or 21/42-position automatic changers.

An open-architecture design makes the PW1835 horizontal goniometer ideal for phase and stress analysis on bulky samples weighing up to 20 kg. This also can be equipped with a multi-purpose sample stage, accepting loadings of up to 4 kg. Additional sample rotation and translation movement permits easy and accurate positioning for measurement at areas of interest. A slot-in sample holder makes it a simple matter to adapt the system at any time for analysis on small powder and sheet specimens.

Both generators - the microprocessor-programmable PW1825 and the more economical, compact PW1830 - employ 400 Hz resonant technology to produce a highly stable 3 kW, 60 kV output. Single- or double-width instrument enclosures provide fail-safe radiation protection when working with open-beam systems, and offer generous space for mounting multiple experiments on either generator. Full system control is provided by a microprocessor module, which also acts as an interface to external computers for analytical programming and results calculation.

Powerful Software

By adding a DEC computer, users can benefit from Philips' APD1700 software, which offers extremely sophisticated diffraction data processing capability.

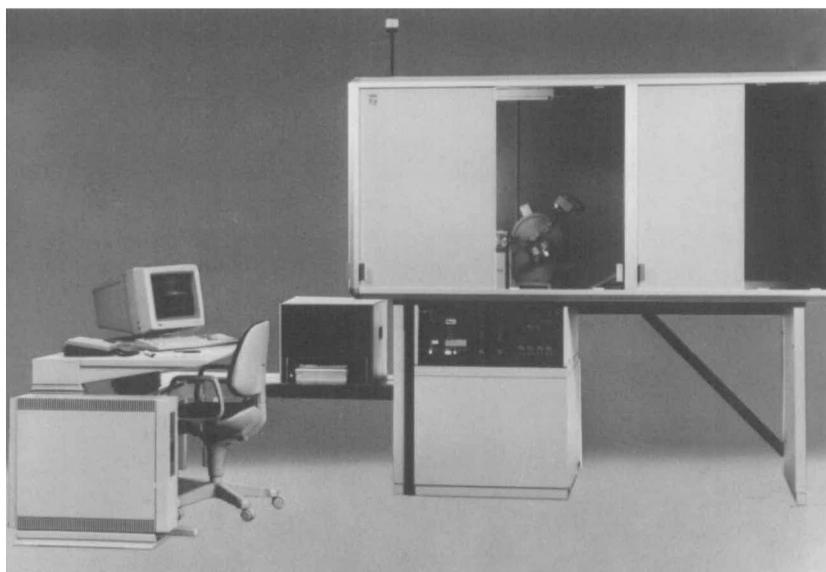
Qualitative analysis is based on a unique multi-pass search procedure for accurate peak detection. Data interpretation is simplified by provision of the complete JCPDS Powder Diffraction File on disc, while a search/match program allows fully automatic phase identification. Modules for quantitative, stress, texture, crystallography and line profile analysis complete this powerful package.

The alternative PC-APD software for IBM XT, AT, PS2 and compatible computers provides a low cost, flexible solution for many qualitative phase analysis requirements.

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The modular MPD1880 Multi-Purpose Diffractometer system enables installations to be specifically tailored for individual users' requirements in research and industry. The system shown employs the vertical goniometer, compact generator and double instrument enclosure.



This horizontal goniometer and multi-purpose sample stage makes the MPD1880 Multi-Purpose Diffractometer system from Philips particularly useful for stress and phase measurements on bulky objects up to 4 kg.

