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

PLUS37 from Philips Analytical is a fully indexed and searchable data set containing every diffraction parameter in the 1987 JCPDS PDF-2 database. Combining the diffraction database Sets 1–37 with state-of-the-art storage hardware and retrieval software, PLUS37 allows rapid and comprehensive crystallographic and materials investigation for a variety of applications.

The new compact disc format of PLUS37 offers the diffraction user and electron microscopist access to over 200 unique data fields for nearly 50 000 compounds. Powerful retrieval software allows multiple-field data searches using Boolean and relational logic – while the binary form database gives rapid and easy data access with unlimited search capability. Patterns satisfying the search criteria may be displayed as card images or in line format.

PLUS37 allows the diffraction user to perform Hanawalt search/matches interactively, find patterns by PDF Reference Number, colour, optical data, elemental content, a 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. In teaching applications, on-line help screens will guide the novice and expert alike through the entire retrieval process.

The PLUS37 system operates as a stand-alone package on the IBM PC/AT, IBM compatible systems or the DEC 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.

Jeff Grimes, Philips Scientific, York Street, Cambridge CB1 2PX, England

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Chem-X/AMBER Interface

Chemical Design is happy to announce that the **Chem-X molecular modelling system** now offers a **transparent interface to AMBER**, the leading molecular-dynamics simulation program. Version 3 of AMBER, written by staff of the University of California at San Francisco, is now also available directly from Chemical Design.

The new interface allows AMBER's advanced molecular mechanics and molecular-dynamics calculations to be run on macromolecular systems constructed quickly and easily within Chem-X. AMBER is also one of the very few molecular-dynamics programs capable of calculating changes in Gibbs free energies, which can be of great utility in protein and drug design. Typical applications include studying solvation effects in proteins, looking at drug-receptor interactions and calculating the best 3D structure of proteins.

The Chem-X/AMBER interface provides a link between two of the most popular computational chemistry programs on the market. A major advantage is that data for structures built in Chem-X are automatically converted to the correct format before transfer to AMBER. This overcomes the problem of data input often encountered when AMBER is employed as a stand-alone program, making it significantly easier to use.

To make the most of this new development, Chemical Design has enhanced its graphics facilities to allow dynamic simulations to be played back in real time on high-performance devices such as the Graphicon 1700. In addition, it will soon be possible to run AMBER on Chemical Design's powerful transputer-based MITIE superworkstation, which is ideally suited to computationally intensive tasks of this type.

With more than 270 installations of its Chem-X software worldwide, Chemical Design is a leading supplier of molecular modelling systems. Customers include divisions of most multinational chemical companies and any leading academic research centres. As well as the modular Chem-X system, Chemical Design also offers a range of customized workstations and graphics terminals for molecular modelling.

Chem-X runs on DEC VAX computers under VMS.

Helen Gasking, Chemical Design Ltd, Unit 12, 7 West Way, Oxford OX2 0JB, England

Book Reviews

Works intended for notice in this column should be sent direct to the Book-Review Editor (R. O. Gould, Department of Chemistry, University of Edinburgh, West Mains Road, Edinburgh EH9 3JJ, Scotland). As far as practicable books will be reviewed in a country different from that of publication.

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Gem and crystal treasures. By *P. Bancroft.* Pp. 488. Western Enterprises/Mineralogical Record Co-publication (3538 Oak Cliff Drive, Fallbrook, CA 92028, USA), 1984. Price US$60.00

The dust-cover blurb which accompanies this weighty coffee-table tome is distinctly off-putting:

> ... Experience human drama as it was – incredible good fortune, stark tragedy ... Marvel at a wealth of gemstones ... surely among God's greatest treasures ... Meet those who worked in and about the mines – shopkeepers, sheriffs, miners, prostitutes and bad men ...

– and more in like vein, all calculated instantly to put off an Englishman educated to sniff at purple prose and to recoil at consecutive imperatives whenever he encounters them.

Let it be said at once that this is *not* a book to be sniffed at. Dr Bancroft is a reputable educationalist and an experienced museum curator. His book is planned around precisely 100 mining areas notable for the production of gemstones and crystals. The author has visited most of the locations, the spread of which is world-wide. Each location has one chapter, and each chapter has precisely two references. Only one mineral is dealt with for each location, and there are some 320 colour illustrations of a very high standard. So far as I have been able to judge, the attributions are accurate.

The orderliness of the plan reflects the mind of the museum curator, but the spirit of the book is essentially romantic. Two previous generations of Bancrofts were associated with mining activities in Nevada, Arizona, California and Mexico, and their spirit is the true motivation for the enterprise. The real treasures of the book are the 667 mainly black-and-white photographs, largely 19th and early 20th century, but interlaced with sometimes disturbingly equivalent scenes of more recent provenance.

A splendid specimen of native silver on quartz (which could have been the product of a French silversmith of around 1910) is juxtaposed with the Virginia City cemetery photographed in 1972. 20 000 miners had staked 16 000 claims on the Comstock Lode in the period 1858–1864. The Hale and Norcross mine was controlled financially by four Irishmen (Freemasons to a man), and managed by Dr Bancroft's great-uncle. The cemetery reflects not only the incidence of underground fatalities, but also some of the perils of organized prostitution in that environment.

A photograph of a ragged horde of emerald miners (surely 19th century) turns out to be Muzo (Colombia) in 1978.

An illustration of wolframite from Llallagua (Bolivia) is accompanied by photographs from Pinkerton's Detective Agency of Butch Cassidy and the Sundance Kid, who had robbed the Llallagua payrolls in 1900 (and neither of whom I would have liked to meet on a dark

night). It was here also in 1903 that an unemployed debt-collector, Simon Iturbi Patino, began to lay the foundations of one of the great mining fortunes of this century.

All good, stirring stuff, but has it any use? This may be a largely irrelevant question, but I can answer in the affirmative. Dutch settlers knew that the Lenni Lenape Indians (in what is now New Jersey) used brightly coloured zinc minerals as pigments, and this led them to discover the Sterling Hill zinc deposit in 1640. In 1838 the United States Customs Department demanded the use of brass weights, leading eventually to the development of the Sterling–Franklin mines, and the establishment of the great New Jersey Zinc Company (now, alas, deceased and subsumed into one of the newer faceless energy/raw materials conglomerates). From these mines came chlorophoenicite, glaucochroite, leucophoenicite, margarosanite, norbergite, zincite and franklinite (this last with echoes of Benjamin Franklin and of Pierre Berthier). The reviewer has found this information fascinating, and has obtained samples of minerals from this locality for structural investigations relevant to the production of artificial pigments.

What more can you ask: good bed-time reading and commercial utility!

P. A. YOUNG

Department of Mining and Mineral Engineering
University of Leeds
Leeds LS2 9JT
England

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Quartz. By *Michael O'Donoghue.* Pp. ix + 110. London: Butterworths, 1987. Price £20.00.

This monograph is published in Butterworth's *Gem Book Series* with the intention of providing all necessary information on one particular gem species to dealers and collectors. In nine chapters the author deals with the origin of quartz, the chemistry of silicon dioxide, colour in quartz and physical and optical properties. There are three chapters on the occurrence of the mineral in Europe, America and the rest of the world and, finally, testing and fashioning of quartz.

Though most of the book is concerned with the description of exceptional occurrences of the quartz family, coarse and fine crystalline varieties throughout the world, the author has spent a fair amount of effort introducing the reader to crystallography, petrology, physics and chemistry of quartz. Since the book is meant for a general audience, these chapters are kept on an introductory level. Unfortunately, these first four chapters contain many imprecise statements and errors.

On page IX, O'Donoghue summarizes 'constants and characteristics' for silica minerals crystallizing in the quartz structure type and has subdivided into quartz and chalcedony instead of using the established classification where coarse (rock-crystal, amethyst *etc.*) and microcrystalline (chalcedony, agate, onyx *etc.*) varieties are distinguished. On page 8, tridymite is cited as a stable polymorph of silica. On page 9, 'polymorphism', 'form' and 'habit' are used with different and misleading meanings. On page 10, the room-temperature symmetry of quartz (point group 32) is discussed in the text, but reference is given to figures depicting the high-symmetry form. On page 22, 'In some quartz trivalent aluminium may be substituted by tetravalent silicon' occurs instead of the substitution of silicon by aluminium. On page 34, reaction equations with 'NH^-' ions and 'NH_4' or 'HF_2' molecules are introduced. Furthermore, symbols for crystal faces, directions and forms are mixed up, 'molecules' and 'atoms' are interchanged, imperial and metric measures are used together and citation of references seems to be arbitrary. This is only to mention a few of the most obvious errors.

Overall, I had the impression that the author was addressing these subjects without the required familiarity and the necessary care and precision (in particular for his chapter on colour in quartz).

The three chapters on occurrences of members of the quartz family report many interesting localities from all over the world. Here, for the more scientifically interested collector, many helpful references to unusual occurrences will be found.

In conclusion, I regret that the author missed the occasion to present a valuable and popular introduction to solid-state science and petrology of quartz for amateur collectors and gemmologists.

H. GIES

Mineralogisch-Petrographisches Institut
Olshausenstrasse 40–60
2300 *Kiel*
Federal Republic of Germany