

# 40 CODATA / NEWSLETTER

**APRIL 1987**

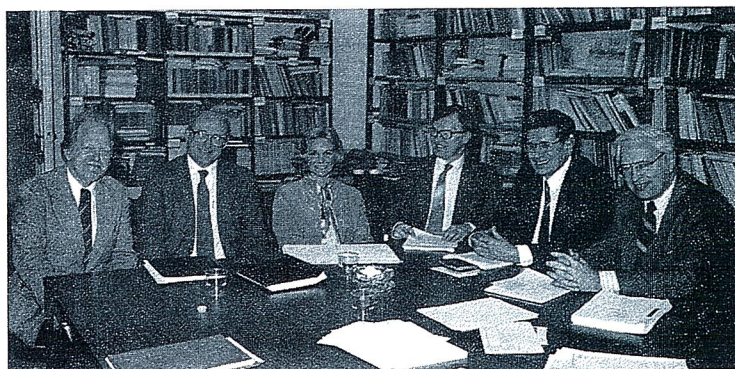
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### **CODATA Referral Database Task Group**

The CODATA Referral Database Task Group was created in 1986 with the cooperation of the Unesco General Information Program (PGI) and met most recently in January 1987. Its goals were reiterated then:

- The establishment of an electronic referral database which can be easily maintained and updated.
- The production of distributable versions of the database to be used as an information tool; these include both an on-line version to be used with vendor software and a self-contained package for microcomputers.
- The establishment of routine procedures for producing printed versions of CODATA Directories and of the Unesco Inventory as well as updates of extant documents.



*The Task Group meeting Paris, January 1987. (Left to right): Westrum, Lide, Molino, Smith, Dubois, and J.H. Westbrook, consultant.)*

The Directory and the Inventory provide access in book format to sources of data for science and technology. The master database is maintained and inverted in the highly structured ISIS software which lends itself to the maintenance updating, and printing operations of the database. For

*(continued on page 6)*

The **Committee on Data for Science and Technology (CODATA)** was established in 1966 by the International Council of Scientific Unions.

Working on an interdisciplinary basis, **CODATA** seeks to improve the quality, reliability, processing, management, and accessibility of data of importance to science and technology.



## Aerospace Materials Data Workshop

A workshop for the aerospace industry, "Computerized Materials Property and Design Data for Aerospace Technology" was held at El Segundo, California, June 23-25, 1986, and attended by 75 industrial and government aerospace materials experts and designers. The workshop was sponsored by: The Aerospace Corporation; American Institute of Aeronautics and Astronautics; National Bureau of Standards; National Materials Property Data Network; and the SDI Office of the Department of Defense. The participants in the Workshop concluded that the U.S. aerospace industry needs convenient and comprehensive access to computer databases of materials information to maintain its technical and economic leadership.

Other specific recommendations were as follows:

- The National Materials Property Data Network, Inc. (MPD Network) should be strongly supported in its effort to develop a network accessing materials databases. Immediate sponsorship by aerospace companies is urged.

- Industry should provide the major part of the investment needed by the MPD Network. The U.S. Government should also help, both directly and by supporting needed research on information technology and by supplying data to the Network.

- The Network should provide access to databases built and maintained by experts. Coverage should include the complete range of engineering materials and all relevant physical, mechanical, corrosion, and chemical properties. Optical and electrical properties should be added as supported.

- While no new technical committees are needed, technical and trade societies and standards groups should vigorously urge their groups to be as active as possible. The U.S. Government should ensure that materials property data generated by government contract research are made available through appropriate databases.

- A top priority is to convert to machine-readable form the principal print data references used by the aerospace industry: Mil Handbook 5 (metals), Mil Handbook 17 (composites), and Aerospace Structural Metals Handbook.

The proceedings of the Workshop were edited by J.H. Westbrook and L.R. McCreight.

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## Information Sources in Biotechnology

An update (1986) of the first (1983) edition of "Information Sources in Biotechnology" should help the multitudes who are aware of the impact of biotechnology, but seem thwarted in their attempt to find out more about it. Though glamour may have worn off a little, the flood of new information and the important ethical and ecological questions—plus the biological possibilities—still provoke a significant scientific challenge. Unfortunately, however, only English language publications have been included, individual journal publications have usually not been included. The 400-plus page volume is clearly a model of how a guide to literature sources in science and technology should be organized. After a definition of several aspects of biotechnology, the types of information sources—from newspapers through monographs with coverage on patents—are extensively reviewed and evaluated.

The growing hoard of biotechnology databases are discussed in a 10-page section, and information on companies (34 pp.) and on organizational sources (7 pp.) culminates in a short discussion on the management of library and information sources in biotechnology. Extensive tables and lists provide identification of sources.

The author, Anita Crafts-Lightly, is a trained microbial biochemist and researcher, as well as Managing Director of BioCommerce Data Ltd., and senior editor of "Abstracts in BioCommerce." More details on the procurement of this Macmillan Publisher's Ltd. volume is provided in the Book Section of this Newsletter.

## Mixed-Media Scientific Communication

The National Science Foundation (NSF) has announced an award of \$3 million to the University of Michigan (U-M) for a project that will help scholars exchange information on-line. The award will fund research to enable generation and communication of mixed-media documents among differing computing environments.

Such documents include text, mathematical notation, graphics, and images, and eventually could include or interact with voice, animation, sound and video media, and remote computational servers.

The program, called EXPRES, will initially yield a system that researchers can use to prepare and submit proposals to NSF. EXPRES will provide a basis for very general electronic information interchange and collaboration among the nation's geographically dispersed science and engineering community.

The U-M project includes teams from BBN Laboratories, Inc. of Cambridge, Massachusetts, and ArborText of Ann Arbor, building on BBN work in multimedia electronic mail technology and ArborText work in document composition systems. The ArborText team is led by Dave Rodgers. The U-M team consists of faculty, staff, and students from Electrical Engineering and Computer Science and many other campus units, including the Center for Information Technology Integration (CITI), the College of Engineering's Program in Technical Communication, the School of Business Administration, the Department of Cognitive Psychology, and the Division of Research Development and Administration (DRDA).

The project is receiving an additional \$2.5 million in equipment grants and technical support from Apollo, DEC, IBM, and Sun Microsystems. Many universities will be involved as active U-M/EXPRES test sites. The EXPRES technology also has the potential to greatly enhance information exchange between the university community and industry.

A focal point of the U-M work is design and propagation not only of EXPRES technology, but also of appropriate new patterns for using the technology. "Imagine interacting with a figure in a document, to see an animated demo, or conduct a remote experiment, or collaborate with a distant colleague to redesign the figure itself—it's often easier to create such a technical capability than to create and propagate shared patterns for using it. Thus we must create new cultural forms along with the new technological forms," says Lynn Conway, EXPRES Principal Investigator, Professor of EECS, and Associate Dean of the College of Engineering at U-M.

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## Coding Microbiological Data

A 1986 book "Coding Microbiological Data for Computers" by Rogosa, Krichevsky, and Colwell presents an open ended system in which computer techniques facilitate encoding, entry, management, and analysis of microbiological data derived from the study of bacteria, algae, fungi, and protozoa. Since the system is not constrained by any taxonomic point of view or by proprietary computer technology and is freely and easily adaptable to the special needs of special problems, investigators are thus enabled to deal efficiently with unforeseen areas of their investigation or with new data generated by old or new technology.

In their document entitled "Method for Coding Data on Microbial Strains for Computers", Rogosa, Krichevsky, and Colwell (1971) proposed the use of computers in microbial identification and classification and recommended the establishment of an international data bank or network for microbiology. The argument offered was that the experience of microbiologists with computers was sufficient and computer technology adequate for current and foreseeable demands. Indeed, models of computers available to major universities and research centers in many countries at that time had storage capacities, software

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## Coordination of Protein Sequence Data

The Task Group meeting, chaired by Prof. B. Keil, in Nice, France 23-27 January 1987, reviewed their achievements and planned for the future as recorded by Prof. A. Tsugita, Secretary. The TG has completed the "Directory of Protein Sequence and Nucleic Acid Sequence Data" and will publish it in several months as a CODATA Bulletin.

Dr. A. Lesk reported that the book "Introduction to Computing in Molecular Biology," to be published by Oxford University Press, is virtually complete. He reported further that many comments on the "Common Format for Sequence Data Exchange" had been received and considered for a final version.

Prof. Tsugita noted that eight papers so far had been received for the Journal, "Protein Sequences and Data Analysis." The first issue of this bi-monthly Springer-Verlag publication is scheduled to appear in March. Although not officially a CODATA journal, it will have members of the CODATA Task Group in the key positions. The journal will have as Editor-in-Chief, Prof. A. Tsugita; as Executive Editors: Dr. W.C. Barker and Dr. A. Henschen, and as Managing Editor: Dr. H.W. Mewes.

Dr. Barker proposed that the Second Edition of "Directory of Sources of Protein and Nucleic Acid Sequence Data" be made available as a computer database so that it may be easily accessible, easily updated, and used for referral; a printed version might appear in two years.

The motion "The CODATA Task Group on the Coordination of Protein Sequence Data Banks recommends that "A Standardized Format for Sequence Data Exchange" written by D. George, H.W. Mewes, and Hiroshi Kihara be used for the exchange of amino acid sequences between databases." was unanimously approved by the Task Group.

Task Group concerns will be well represented at the 1988 International CODATA Conference, Karlsruhe, where Lois Blaine will organize a special session on nomenclature problems.

The Task Group composition is at present: Prof. B. Keil, Chairman; Prof. A. Tsugita, Secretary. Members: Drs. W.C. Barker, A. Henschen, A. Lesk, R. Simpson, Prof. M. Kotani. Consulting Members: Drs. G. Cameron (to be confirmed), J.-M. Claverie, D. George, K. Loehning, H.W. Mewes, T. Ooi, Prof. A.S. Kolaskar. Corresponding Members: Drs. A.P. Kyne, J.R. Rodgers, S. Sakakibara. Observer: Dr. Z. Wang.

## JANAF Thermochemical Tables

The Third Edition of the JANAF Thermochemical Tables represents a revision of the 1971 Second Edition, an update of four supplements from 1974-82, plus a number of previously unpublished tables. Thus, the tables of thermodynamic properties for more than 1800 inorganic substances, and for organic substances containing not more than two carbon atoms, have been brought together into a two volume set.

The historical origin of these tables stem from the wartime need to conduct rigorous performance calculations for propellant systems that gave multiphase combustion products characterized by complex chemical and thermal equilibrium. The Joint-Army-Navy-Air-Force (JANAF) panel initiated this endeavor to provide the essential data. The work began at Midland, Michigan, at the Dow Chemical Company under the direction of Daniel R. Stull. In more recent years, although the U.S. Air Force continues its support of the preparation of the tables, the Department of Energy entered the scene with different reactors and reagents of interest. Malcolm W. Chase, Jr., has been the project director since late 1982.

These tables cover the thermodynamic properties over a wide temperature range with single-phase and multiphase tables for the crystal, liquid, and ideal gas state. The properties tabulated are heat capacity, entropy, Gibbs energy function, enthalpy, enthalpy of formation, Gibbs energy of formation, and the logarithm of the equilibrium

## CODATA Calendar...

1987

### April

20-25 Chemical Thermodynamic Tables Task Group, Moscow, U.S.S.R.

20-25 Geothermodynamic Data Task Group, Leningrad, U.S.S.R.

### May

3-6 First CODATA Workshop on Nucleic Acid and Protein Sequence Data, Gaithersburg, Maryland, U.S.A.

27-29 Conference on Integrating Data for Decisionmaking: USNC CODATA, Integrated Users Workshop, National Governor's Association, Shoreham Hotel, Washington, DC, U.S.A.

### June

1-2 Hybridoma Data Bank Task Group, Paris, France

1-6 Conference and Training Course on Geomathematics and Geostatistics, Wroclaw, Poland

10-11 Task Group on Materials Database Management, Paris, France

### September

6-8 Third CODATA/IUPAC Symposium on Phase Equilibrium, Budapest, Hungary

9-11 Third International IUPAC Workshop on Vapor-Liquid Equilibria, Budapest, Hungary

1988

### March

3-5 CODATA Task Group on Coordination of Protein Sequence Data Banks, Paris, France.

3-5 32nd CODATA Executive Committee, Paris, France

### July

— First International Symposium on Thermodynamics of Natural Processes, Strasbourg, France

### September

26-29 11th International CODATA Conference, Karlsruhe, F.R.G.

30- Oct.1 CODATA General Assembly, Karlsruhe, F.R.G.

constant for formation of each compound from the elements in their standard reference states. All values are given in SI units and are for a standard-state pressure of 100,000 Pa(1 bar). Each tabulation is accompanied by a critical evaluation of the literature upon which the thermochemical table is based. Literature references are given. All tabulations have been rewritten in a consistent style; many, but not all, have been revised as a result of a reevaluation of the data.

The high standards initially established, despite the urgent need for the data, have been enhanced over the quarter century elapsed, and at present, the tables are a prime example of the results of truly critical evaluation of high quality. The quantity of material is also large—over 1890 pages.

The authors of the present edition are: M.W. Chase, Jr., C.A. Davies, J.R. Downey, Jr., D.J. Frurip, R.A. McDonald, and A.N. Syverud. Other details, including ordering information, are to be found under Books in Newsletter 39.



# Software Directory for Molecular Biologists

A guide to the selection of computer software for the management and analysis of molecular sequences by Christopher J. Rawlings has been provided as a tool for the management and analysis of data generated during molecular sequencing and genetic engineering projects.

It also responds to needs of neophytes to computerized methods, in demonstrating how software developed on microcomputers for business applications may be exploited in a scientific environment and provides a glossary of computer jargon and terms. For example, the Directory describes spreadsheet systems which can be used to keep and demonstrate cell growth curves. Other kinds of software highlighted in this section include text processing, database management systems, terminal emulators, graphics, financial planning, file transfer, and integrated software systems.

A second part of the Directory deals in specialist software. It examines, compares and critically appraises a wealth of state-of-the-art software for scientists engaged in the collection, management, and analysis of DNA, RNA, and protein sequences. Each entry covers functional features, machine type, computer manufacturer, operating system, and author or company. Unlike current

research reports which are not only widely scattered, but also rarely offer comparative or critical appraisals or describe the limitations of particular software, it provides comparison and evaluations.

The third part provides indexes and ample cross-referencing to the software listed. The indexing is so thorough that you can track down a specific software package seven different ways: by functional feature, by machine type-mainframe/mini/micro/work station, by computer manufacturer, by operating system, by author or company, by package name, by keywords.

Dr. Christopher Rawlings is a research fellow in the Biomedical Computing Unit at the Imperial Cancer Research Fund investigating the applications of artificial intelligence to computational problems in data analysis and management in molecular biology.

More than 200 pages are devoted to the discussion of specialist software in considerable detail. References, cross-referencing, and indexing are generously adequate.

The book "Software Directory for Molecular Biologists" is available from the Stockton Press. Further facts, identification and details are available in the Books section of this Newsletter.

## FOOTNOTES for BOOKS - (page 5)

(a) Selected papers from the 10th International CODATA Conference, Ottawa, Canada, July 1986. Subscription and advertising enquiries from customers in North America should be sent to: Pergamon Journals, Inc., Maxwell House, Fairview Park, Elmsford, NY 10523, U.S.A. and for the remainder of the world to: Pergamon Journals Ltd., Headington Hill Hall, Oxford, U.K.; CXC 0807. Annual institutional subscription rate (1987/88): DM 195.00, two-year institutional rate (1987/88): DM 370.50 (including postage and insurance). Subscriptions for personal use by individuals may be obtained for DM 42.00 per annum. ISSN 0266-737X.

(b) This book presents an open ended system in which computer techniques facilitate encoding, entry, management, and analysis of microbiological data derived from the study of bacteria, algae, fungi, and protozoa. The system is not constrained by any taxonomic point of view or proprietary computer technology and is freely and easily adaptable to the special needs of special problems. This enables investigators to deal efficiently with unforeseen areas of their investigation or with new data generated by old or new technology. xi + 299 pp. 1986. Springer Verlag, 175 Fifth Avenue, New York, 10010. U.S.A. ISBN 0-387-96417-7.

(c) A volume in the CODATA Series on Thermodynamic Properties. A Report of the CODATA Task Group on Chemical Thermodynamic Tables. 1987. 559.50. Hardbound. Hemisphere Publishing Corporation, 79 Madison Avenue, New York, N.Y. 10016-7892. U.S.A. ISBN 0-89116-730-7.

(d) Same. Softbound. (for CODATA review only.)

(e) The ten volumes in this series translated from Russian (additional volumes covering hydrogen, propane, and n-hexane are in preparation for 1988) present tabular data for technologically and environmentally important fluids. The analytical work that led to the development of generalized and smoothed equations of state covers a wide range of experimental studies, many of which have not been known to English-speaking scientists. This research has been carried out and validated by the National Standard Reference Data Service, an arm of the State Committee for Standards of the Council of Ministers of the USSR. Part 1 of each volume deals with necessary analysis and experimental data interpolation and analysis; Part 2 with the fundamental constants, symbols with units, and tables of data. Contents include experimental data on thermodynamic properties of individual gases, methods of deriving the equation of state and calculating thermodynamic tables, the equation of state and evaluation of computed thermodynamic functions relative to experimental data, and tables of the thermodynamic properties of gases. NSRDS Series Set. Book code #66-55724. \$1,230. Hemisphere Publishing Corporation, A Subsidiary of Harper & Row, Publishers, Inc., 79 Madison Avenue, New York, N.Y., 10016-7892. U.S.A. ISBN 0-89116-667-X.

(f) Reliable data are provided over a wide range of conditions-vital to helium extraction from natural gases as well as to the design of cryogenic apparatus. Spanning temperatures between the  $\lambda$ -line and 1500 K, the tables list thermodynamic properties of He for pressures up to 100 MPa. ca. 320 pp. January, 1987. Book code #66-55211. \$120. ISBN 0-89116-613-0.

(g) Thermodynamic properties are provided of gaseous and liquid nitrogen for temperatures between the triple point and 1500 K, and pressures from 0.01 to 100 MPa. ca. 352 pp. January, 1987. Book code #66-55237. \$120. ISBN 0-89116-615-7.

(h) This book based on extensively verified material provides a unified equation of state calculated tables of properties and presents error of calculated relative to experimental methane properties. The temperature range spans the triple point to 1000 K, and the pressures extend from 0.1 to 100 MPa. Moreover, it presents a range of parameters of state and scope of tabulated quantities far in excess of data offered in most other sources. ca. 350 pp. January, 1987. Book code #66-55229. \$120. ISBN 0-89116-614-5.

(i) Detailed tables present thermodynamic properties of ethane from the triple point to 700 K, and at pressures from 0.1 to 80 MPa. Properties along the liquid-vapor and liquid-crystal coexistence curves are also included. ca. 300 pp. March, 1987. Book code #66-55195. \$120. ISBN 0-89116-611-4.

(j) This volume incorporates new information about density and isochoric specific heat into a reliable set of tables. Temperatures and pressures covered range from the triple point to 1500 K and 0.1 to 100 MPa, for both liquid and gaseous phases. ca. 300 pp. March, 1987. Book code #66-55245. \$120. ISBN 0-89116-616-5.

(k) Reliable tables of the thermodynamic properties of gaseous and liquid air-for temperatures from 70 to 1500 K, and pressures from 0.01 to 100 MPa. The new method used to compile these tables not only assures accuracy, but permits evaluation of the maximum possible errors in the form of tolerances. ca. 275 pages. March, 1987. Book code #66-55187. \$120. ISBN 0-89116-610-6.

(l) Focusing on ethylene, this work presents methods for calculating tables of thermodynamic properties based on results of a critical analysis of the most reliable PVT data published to date by developing an averaged equation of state. Data are provided for both gaseous and liquid ethylene for the temperature range 110-600 K, and pressures from 0.1 to 300 MPa including properties at the saturation and solidification curves. ca. 280 pages. March, 1987. Book code #66-55203. \$120. ISBN 0-89116-612-2.

(m) Addressing Freons of the methane series, the tables in this work systematize and evaluate a reliable set of data about fundamental thermophysical properties of the series Freon-20 through Freon-23. As do the other books in this series, this volume offers calculations spanning a broad range of temperatures (normal boiling point to 473 K) and pressures (0.1 to 20 MPa) for these industrially important fluids. ca. 232 pp. March, 1987. Book code #66-55260. \$120. ISBN 0-89116-600-9.

(n) The second volume devoted to this group of halogenated hydrocarbons features thermophysical properties of Freon-10 through Freon-14. Tables offer data on temperatures from the normal boiling point to 473 K, and pressures from 0.1 to 20 MPa for Freon-10 (CCl<sub>2</sub>F<sub>2</sub>), Freon-11 (CF<sub>3</sub>Cl), Freon-12 (CF<sub>2</sub>Cl<sub>2</sub>), Freon-13 (CF<sub>3</sub>Br), and Freon-14 (CF<sub>3</sub>I). ca. 264 pp. Book code #66-55278. \$120. ISBN 0-89116-601-7.

(o) Thermophysical properties of the rare gas elements-neon, argon, krypton, and xenon-this work offers new research and uniform data covering properties of crystalline, liquid, and gaseous states, spanning a temperature range of 0-1300 K, and for pressures up to 100 MPa. ca. 635 pp. Book code #66-55765. \$120. ISBN 0-89116-673-0.

(p) This new translated quarterly reports only officially approved property data, selected and correlated by the Soviet State Committee on Standards. This research includes information from physics of atoms, nuclei, and molecules, thermodynamic and transport properties of liquids and gases, electrophysical properties, mechanical, thermophysical, electrical, and magnetic properties as well as optical properties of solids and materials. Volume 1, 1987 (4 issues per volume). Subscription rates \$369.00 per year. Hemisphere Publishing Corporation, New York, N.Y. 10016-7892. ISSN: 0888-6903. CODEN: NSRUEC.

(q) This large (29" x 40") two-color chart spans up to 30,000 bar, and -60 to 1400°C. It comes folded in a clear, sturdy plastic envelope, ready for mounting. Included are instructions for use, complete explanatory text, and nomenclature. 1976. chart. Book code #66-50691. \$13.95. Hemisphere Publishing Corporation, New York, N.Y. 10016-7892. ISBN 0-89116-625-6.

(r) The permanent gases, alkali metals, and organic compounds are included. Experimental binary gas diffusion coefficients at one atmosphere are tabulated as are thermal diffusion data. Some mixture viscosities and thermal conductivities are also given. 738 pp. 1975. Book code #66-53687. Hemisphere Publishing Corporation, New York, N.Y. 10016-7892. ISBN 0-89116-356-5.

(s) The handbook covers a wide range of substances including organic substances, inorganic substances, engineering materials, architectural materials, fuels, refrigerants, foodstuffs, metals, alloys, etc. A section includes conversion factors and comparison of a wide variety of useful units and measures. 392 pp. 1976. Book code #66-52887. \$74.50. Hemisphere Publishing Corporation, New York, N.Y. 10016-7892. ISBN 0-89116-370-1.

(t) The Pascal database-soon to be available through the American host Dialog-currently contains six million bibliographic references available online. Dialog users can easily pass into Pascal from their usual files. Additional information from Madame Laure Hugnet-Pouchetel, Centre

de Documentation Scientifique et Technique du CN 26, rue Boyer, 75971 Paris, France.

(u) Sadler's Standard university package of digital infrared spectra for the IBM PC is now available. The package of 200 digital spectra is designed to be used by colleges and universities on the IBM PC for instructional purposes. It consists of selected standard spectra, and includes peak location, peak intensity, name file and name search capabilities. For further information, contact Sadler Research Laboratories, 3316 Spring Garden Street, Philadelphia, PA 19104, USA.

(v) MS library. Teknivent now offers the complete Wiley/NBS mass spectral library on a 60 Megabyte tape cartridge for its VectorOne and Model 1050 GC-MS data systems. The library can be searched in less than 15 seconds for easy identification of unknowns. Further details are available from Teknivent, 10774 Trenton Avenue, St. Louis, Missouri 63132, USA.

(w) Harwell's chemical hazard evaluation database, Chemdata, is now available in the US through Aqua-tech of Port Washington, Wisconsin. Harwell's National Chemical Emergency Centre provides overseas Chemdata subscribers with a master data set, six-monthly intervals. The database contains chemical product information and emergency action advice, together with sources of specialist advice. Further information from Bob Cumberland, National Chemical Emergency Centre, Harwell Laboratory, Didcot, Oxfordshire U.K., OX11 0RA, telephone 0235 24141, ext. 3110.

(x) 420 pp. 1985. This second issue of the Quantitative Data File for ore minerals (QDF) of the Commission on Ore Microscopy, International Mineralogical Association (COM-IMA), consists of 420 sets of data (cards), 327 for individual species and 93 for compositional and structural variants. The common ore minerals are represented, as are many less common and rare species. Most of the data are previously unpublished and were obtained specifically for the QDF. Data listed include: spectral reflectance, color values calculated from these data, chemical composition, X-ray data, and microhardness (VHN). 420 pp. 1985. Published by the British Museum (Natural History), \$89.50. Available from Brookfield Publishers, Old Post Rd., Brookfield, VT 05036. USA. ISBN 0-565-00997-4.

(y) 201 pp. 1987. \$9.95 for AIAA members. \$14.95 others. Published by The American Institute of Aeronautics and Astronautics, 555 West 57th St., New York, NY 10019, U.S.A. ISBN 0-930403-26-6.

(z) IUPAC Thermodynamic Tables Project Centre, Department of Chemical Engineering and Chemical Technology, Imperial College of Science and Technology, London. Tables of the equilibrium thermodynamic properties of ethylene for both the gas and liquid phases and along the saturation and the melting curves cover 104-320 K for pressures up to 270 MPa and 320 K to 350 K for pressures up to 40 MPa. The properties listed are volume, entropy, enthalpy, isobaric heat capacity, compression factor, fugacity-pressure ratio, Joule-Thomson coefficient, ratio of heat capacities and speed of sound as functions of pressure and temperature, and pressure entropy, internal energy and isochoric heat capacity as functions of density and temperature. This monograph gives a critical assessment of the accuracy of all the available experimental data and comparisons of the tables with the experimental data. About 270 pp. Early 1987. Mainly tables, 20 illustrations. Cloth about £32.00. Blackwell Scientific Publications Ltd., Osney Mead, Oxford, OX2 0EL, U.K. ISBN 0-520-01709-0.

(aa) Guide to the selection of computer software for the management and analysis of molecular sequences. The Software Directory for Molecular Biologists provides an introduction to computers and computing from the point of view of the scientist who wants to get the best out of his computing system. The comprehensive catalogue of specialist software for molecular sequence and data analysis is indexed. Paperback. 412 pp. 1986. Stockton Press, 15 East 28th Street, New York, NY 10010. U.S. \$90. ISBN 0-843818-37-0.

(bb) This book describes and reviews the more important information sources in biotechnology. It outlines the basic science and business structure of biotechnology and then describes and analyzes the trade and research literature, patents, market surveys, online databases, company directories, conferences and organizations. Paperback. 403 pp. October 1986. Stockton Press, 15 East 28th Street, New York, NY 10010. U.S. \$100. ISBN 0-333-39290-6. ISBN 0267-4998.



## New CODATA Publications

**Computer Handling and Dissemination of Data.** Bulletin 64. December 1986. (a)

**Coding Microbiological Data for Computers.** By M. Rogosa, M.I. Krichevsky, and R.R. Colwell. (b)

**CODATA Thermodynamics Tables.** Selections for some compounds of calcium and related mixtures. (A prototype set of Tables). By D. Garvin, V.B. Parker, H.J. White, Jr. (c,d)

## Books for the Bookshelf .....

**National Standard Reference Data Service of the USSR: A Series of Property Tables.** Edited by T.B. Selover, Jr. (e)

**Thermodynamic Properties of Helium (Volume 1).** By V.V. Sychev, A.A. Vasserman, A.D. Kozlov, G.A. Spiridonov, and V.A. Tsymarny. (e,f)

**Thermodynamic Properties of Nitrogen (Volume 2).** By V.V. Sychev, A.A. Vasserman, A.D. Kozlov, G.A. Spiridonov, and V.A. Tsymarny. (e,g)

**Thermodynamic Properties of Methane (Volume 3).** By V.V. Sychev, A.A. Vasserman, V.A. Zogoruchenko, A.D. Kozlov, G.A. Spiridonov, and V.A. Tsymarny. (e,h)

**Thermodynamic Properties of Ethane (Volume 4).** By V.V. Sychev, A.A. Vasserman, V.A. Zagoruchenko, A.D. Kozlov, G.A. Spiridonov, and V.A. Tsymarny. (e,i)

**Thermodynamic Properties of Oxygen (Volume 5).** By V.V. Sychev, A.A. Vasserman, A.D. Kozlov, G.A. Spiridonov, and V.A. Tsymarny. (e,j)

**Thermodynamic Properties of Air (Volume 6).** By V.V. Sychev, A.A. Vasserman, A.D. Kozlov, G.A. Spiridonov, and V.A. Tsymarny. (e,k)

**Thermodynamic Properties of Ethylene (Volume 7).** By V.V. Sychev, A.A. Vasserman, E.A. Golovsky, A.D. Kozlov, G.A. Spiridonov, and V.A. Tsymarny. (e,l)

**Thermophysical Properties of Freons: Methane Series, Part 1 (Volume 8).** V.V. Altunin, V.Z. Geller, E.K. Petrov, D.S. Rasskazov, and G.A. Spiridonov. (e,m)

**Thermophysical Properties of Freons: Methane Series, Part 2 (Volume 9).** By V.V. Altunin, V.Z. Geller, E.A. Kremenevskaya, I.I. Perelshtein, and E.K. Petrov. (e,n)

**Thermophysical Properties of Neon, Argon, Krypton, and Xenon (Volume 10).** By V.A. Rabinovich, A.A. Vasserman, V.I. Nedostup, and L.S. Veksler. (e,o)

**Property Data Update. Official Standards of the National Standard Reference Data Service of the USSR.** Edited by T. B. Selover, Jr. (p)

**Mollier Enthalpy-Entropy Diagram for Water, Steam, and Ice in S.I. Units.** By F. Bosnjakovic, U. Renz, and P. Burow. (q)

**Handbook of Physical Properties of Liquids and Gases. Pure Substances and Mixtures. Second Edition.** By N.B. Vargaftik, with a Foreword by Y. S. Touloukian. (r)

**Handbook of Thermodynamic Tables and Charts.** By Kuzman Raznjevic. (s)

**Pascal Database.** (t)

**Sadtler's Package of Digital IR Spectra.** (u)

**Mass Spectral Library.** (v)

**Chemdata. Hazard Evaluation Database.** (w)

**The Quantitative Data File for Ore Minerals. Second Issue.** Edited by A.J. Criddle and C.J. Stanley. (x)

**Proceedings of the Aerospace Materials Data Workshop.** Edited by J.H. Westbrook and L.R. McCreight. (y)

**Ethylene. International Thermodynamic Tables of the Fluid State, Volume 10.** Edited by K. Marjorie de Reuck. (z)

**Software Directory for Molecular Biologists.** By Christopher J. Rawlings. (aa)

**Information Sources in Biotechnology. Second Edition.** By A. Crafts-Lighty. (bb)

(Further details on content, identification, price, source, etc. for above items--if available at press time--are referenced in footnotes on page four.)

## Thermodynamics of Condensed Phase Organic Compounds

Heat capacities and entropies for approximately 1400 organic compounds, in the liquid and/or crystalline phase, have been compiled--and to some extent--critically evaluated. The survey covers primarily the period 1925-82, with some earlier reports on compounds for which more recent data are lacking. More than 800 references were studied. The values for the enthalpy and entropy increments for phase transitions--solid state, melting, and vaporization (or sublimation)--encountered in the evaluation and tabulation are also incorporated, as well as the empirical formula, compound name(s), physical state, heat capacity, and entropy at 298.15 K, and where available--phase-transition data, Wiswesser Line Notation for the compound formula weight, plus a rating indicating the evaluators' estimated overall quality of the reported data.

The need for such a compilation has been apparent for many years in supplement to Stull, Westrum, and Sinke's treatment primarily of the gaseous organic substances and several National Bureau of Standards' technological publication beamed at incinerator technologists including enthalpies of formation for a comparable number of substances in solid, liquid and gaseous phases. Taken together, the thermophysical and thermochemical data permit the determination of the spontaneity of a chemical reaction under specified constraints and moreover, provide a reference database for estimating and correlating thermodynamic properties for organic substances for which experimental data are lacking.

An interesting feature is the fact that for a given compound, the data from each paper form a separate entry, complete with source identification. For example, for methanol, some 17 sources are cited. Data are presented both in calories and joules; pressures in kilopascals. Indication of the evaluators rating of general quality of the data on a four point scale--A (high) through D (low) depends both on the measurement and the adequacy of the presentation from the evaluators' point of view (cf. CODATA Bulletin 9). Glass transitions, Schottky contributions, metastability, anomalies, and zero-point entropies are noted.

The volume entitled "Heat Capacities and Entropies of Organic Compounds in the Condensed Phase" is authored by Eugene S. Domalski, William H. Evans, and Elizabeth D. Hearing. It is published separately (for the National Bureau of Standards) as a Supplement to the *Journal of Physical and Chemical Reference Data*, edited by David R. Lide, Jr. Further bibliographic details regarding this eminently useful summary table are listed in the Book Section of Newsletter 39. Cloth: U.S. and Canada, \$130. All other countries, \$156. American Chemical Society, Marketing Communications Department, 1155 Sixteenth Street, NW, Washington, DC 20036. ISBN 0-88318-473-7.



## First Latin American Conference on Computers in Geography

The Conference — San Jose, Costa Rica, October 5-9, 1987 — organized by the Commission on Geographical Data Sensing and Processing of the International Geographical Union in cooperation with the International Cartographic Association and local organizations within Costa Rica, provides a medium for communication and exchange of experience among those handling spatial data with computers. Topics include computer-based modeling of spatial processes, digital cartography, remote sensing, and geographic information systems. The languages of the Conference will be Spanish and English.

Proceedings of the Conference will be published in English and Spanish, and will be available at the time of the Conference.

Persons wishing to register should communicate with Dip.-Geogr. Merrill Lyew, Escuela de Geografia, Universidad Nacional, Apartado 86, Heredia 3000, Costa Rica. Registration fees will be US \$50 until July 1st and US \$75 after that date.

I often say that when you can measure what you are speaking about, and express it in numbers, you know something about it; but when you cannot measure it, when you cannot express it in numbers, your knowledge is of a meagre and unsatisfactory kind; it may be the beginning of knowledge, but you have scarcely, in your thoughts, advanced to the stage of science, whatever the matter may be.

*Lord Kelvin, Addresses, 1883*

## Referral Database

(continued from page 1)

dissemination, it is converted to a simpler format which may be searched with either the ISIS software or with a modification of the BIRD software—an extremely user-friendly software developed at Queen's University—for searching. One mode of dissemination planned is the use of floppy disks for searching on personal computers.



*Dr. B.B. Molino, Referral Database TG Secretary*

The Task Group is presently working on finalizing users' manuals, adding several recent Directory Chapters to the database, establishing procedures for maintenance and updating of the database, as well as for distribution and for a pricing structure. A progress report and a target date for having a distributable product will be presented to the Executive Committee at its next meeting.

The Task Group is composed of J.E. Dubois, D.R. Lide, Jr., B.B. Molino (Secretary), F.J. Smith, E.F. Westrum, Jr. (Chairman).

## Microbiological Data

(continued from page 2)

programs, and programming versatility capable of accommodating and handling masses of data. The most compelling argument was that the body of historical data and the rapidly accumulating data were too large, cumbersome, and complicated to be handled conveniently or efficiently by conventional (i.e., non-computerized) methods. Clearly, with passing time and experience, these arguments are even more convincing.

The authors are Morrison Rogosa and Micah I. Krichevsky of the National Institute of Dental Research at Bethesda, Maryland, and Rita R. Colwell of the Department of Microbiology, of the University of Maryland, at College Park, Maryland. Among the many acknowledgements made by the authors are those to Professor V.B.D. Skerman for advice and encouragement and for the truly significant contributions of Elaine J. Krichevsky, for enduring devotion to the maintenance of this document over the years, logical insights, computer knowledge, editing skills, meticulousness, and intelligence contributed greatly to the completion of this book. Other details, including ordering information, are to be found under CODATA Books on page 5.

## Newsnotes.....

Dr. J.D. Cox, CChem, FRSC, has retired from his position as head of the thermal metrology branch at the National Physical Laboratory, Teddington. He has been active in CODATA's Task Group on Key Values for Thermodynamics and is an editor on the forthcoming volume on this subject.

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