International Council Of Scientific Unions Committee On Data For Science And Technology

Number 70 Codata Newlsetter

February 1995

HIGHLIGHTS

21st Century Data Challenges

An Inter-Association Workshop, sponsored by the International Association of Seismology and Physics of the EarthUs Interior (IASPEI), and co-sponsored by the International Association of Geodesy (IAG), the International Association of Geomagnetism and Aeronomy (IAGA), the ICSU Committee on Data for Science and Technology (CODATA), and the ICSU Panel on World Data Centers will be held all day on Thursday, July 13, 1995, and will consist of invited and contributed oral papers, and a poster session during the International Union of Geodesy and Geophysics General Assembly, Boulder, Colorado, U.S.A., July 3-14, 1995.

This Workshop will focus on the changing requirements of the research community for access to scientific data in the next century. Important aspects of these requirements are likely to involve high band-width networks, distributed data archive and dissemination facilities, sophisticated network search and retrieval systems, parallel processor computing facilities, and innovative ways to provide data to non-technical users. These will be accompanied by software developments such as hierarchical data systems, artificial intelligence, and neural networks, the use of geographic information systems, and advances in optical character recognition methods. This Workshop will provide a forum for interactions between research geophysicists concerned about data availability and the computer scientists who will design the data systems of the future.

Abstracts are to be submitted to the American Geophysical Union by February 1, 1995 and copies to the Principal Convenor. For more information, contact any of the Convenors.

Principal Convener: Dr. Michael A. Chinnery, National Geophysical Data Center, 325 Broadway, Boulder, Colorado 80303, U.S.A. Telephone: +1-303-497-6215; Fax: +1-303-497-6513; E-mail: mchinnery@ngdc.noaa.gov

Co-Convener: Prof. G. A. Sobolev, Institute of Physics of the Earth, Molodezhnaya 3, Moscow 117296, RUSSIA. Telephone: +7-095-930-0546; Fax: +7-095-930-5509; E-mail: sgc@adonis.iasnet.com

Co-Convenor: Prof. C. C. Tscherning, Geophysical Department, University of Copenhagen, Haraldsgade 6, DK2200 Copenhagen N., DENMARK. Telephone: +45-35-320582; Fax: +45-35-822565

Issues in the Transborder Flow of Data

The U.S. National Committee for CODATA is undertaking a major international study to identify important issues and trends in the transborder flow of scientific and technical (S&T) data, particularly on electronic

networks. The study will characterize the technical, legal, economic, and policy issues that have an influenceQwhether favorable or negativeQon access by the scientific community to S&T data. Special attention will be given to the specific conditions inherent in the transborder transfers of electronic S&T data among the academic, governmental, and private sectors. The study will then identify and describe those barriers that have the most adverse impact in discipline areas within CODATA's purviewQthe physical, astronomical, biological, and geological sciencesQand across those disciplines, using representative examples. Finally, it will identify trends likely to have significant discipline-specific and interdisciplinary influence on the use of S&T data, particularly in electronic forms, and, where appropriate, suggest approaches that could help overcome barriers to access in the international context. The study is being conducted between July 1, 1994 and June 30, 1995. Its goal is to help improve data access and services internationally.

This study follows up on a similar survey and report done by CODATA and the International Council for Scientific and Technical Information (ICSTI) in 1990. If you have information on significant issues (e.g., restrictions on data, cost recovery policies, academic scientists' needs, protection of intellectual property, effect on economically developing countries, technical barriers, Internet, etc.), regarding the dissemination of and access to numerical data in the natural sciences from the legal, policy, economic, and technical perspectives, *please send your response and any related documentation you are able to provide to*: Paul F. Uhlir, Director, usnc/codata, National Research Council, 2101 Constitution Avenue, N.W., Washington, DC 20418, U.S.A. Telephone (202) 334-3061; Fax: (202) 334-2154; Internet: puhlir@nas.edu.

Materials Database Management TG

The Task Group met in Chambéry September 14, 1994, and has begun to prepare a 3rd Edition of the International Register of Materials Database Managers to be available late in 1995 and possibly to be included on CODATA's WWW Internet array. Prior Editions: 1990 and 1993. It will continue to focus on personnel, but provide e-mail addresses and more detailed description of the nature, scope, purpose and utilization of the databases enumerated.

Further cost/benefit studies by the Task Group are contemplated. These studies will distinguish between public and private databases, and between online, PC, and CD-Rom and include anecdotal accounts where appropriate.

Decision about the next meeting site and date was deferred.

New Edition of CODATA Glossary

The 1991 first edition of the Glossary produced primarily by Jack H. Westbrook was a resounding success. An updated and expanded edition to be created by a Working Group of about seven people representing particular areas is already underway. Five of them have already accepted the invitation. Proposed Membership:

J. E. Dubois, Chemistry (France)
H. Bestougeff, Information Science (France)
L. Blaine, Biology (USA)
J. H. Westbrook, Materials (USA)
T. V. Gulashvili, Atomic Energy (Russia)
I Fujiwara, Information Science (Japan)
A. Heck, Astronomy (France)

Working and collaborating by mail, e-mail, and telefax, they hope by late 1996 to produce a better product. The scope of their endeavor will include: substitution of standard for ad hoc definitions, improvement of ad hoc definitions; deletion of un-needed, deprecated, or controversial terms; introduction of new terms and definitions; addition and improvement of thesaurus relationships; and possibly to identify term equivalents in other languages.

The new initiative is also being directed by Jack H. Westbrook. Those wishing to help criticize, enhance, or expand the present document are welcome to send their suggestions directly to Dr. Jack H. Westbrook,

Brookline Technologies, 5 Brookline Road, Ballston Spa, NY 12020, USA; Tel/FAX: 1-518-885-8840; or to communicate with other members of the Working Group.

New Books

CODATA Books

CODATA Monograph Series Volume 3. International Geothermodynamic Tables. Editors: I. L. Khodakovsky, E. F. Westrum, Jr., Bruce H. Hemingway. *Forthcoming* (*ca*. June 1995).

> **Geothermodynamic Tables** is a prototype volume on geothermodynamic data produced by the Task Group on Geothermodynamic Data Tables. *Expected ca*. June 1995. Approximately 300 pp. From CODATA Secretariat, 51 Blvd. de Montmorency, 75016 Paris, France, or Edgar F. Westrum, Jr., Department of Chemistry, University of Michigan, Ann Arbor, MI 48109-1055 USA.

Other Books and/or Databases

CRC Handbook of Thermophysical and Thermochemical Data, Editors: D. R. Lide, H. V. Kehiaian. [c,d]

> **Thermochemical Data** - The CRC Handbook of Thermophysical and Thermochemical Data is an interactive software and handbook package that provides an invaluable source of reliable data embracing a wide range of properties of chemical substances, mixtures, and reacting systems. The handbook and software together quickly and easily generate property values at any desired temperature, pressure, or mixture composition.
>
> The software program -CRCTHERM - contains algorithms for calculating properties and values based on parameters tabulated in the handbook. To create your own customized tables, simply take the compounds you need from the book, enter them into your computer, and specify the temperature, pressure, or composition range. Coefficients in the equations used to express the dependence for a given property are stored on disk for each property or mixture at a single value of the variable or over a range, printing the results or saving them to disk. The default units are SI, but all other common units have been included.
>
> For each group of properties, data are given for representative substances of different chemical classes, emphasizing the compounds of the greatest industrial and laboratory importance. Those properties that are functions of temperature, pressure, or composition are presented as equations with tabulated coefficients. Properties presented in the handbook include:
>
> - Physical constants, thermodynamic properties of pure substances
> - Enthalpy and Gibbs energy of formation, phase transition properties, vapor-liquid, liquid-liquid, and solid-liquid equilibrium properties of binary mixtures
> - Surface tension
> - Azeotropic data
> - Viscosity
> - Thermal conductivity
> - Diffusion coefficients, etc.
>
> All data are derived from evaluated sources and presented in SI units. All properties are defined, thermodynamic relationships are explained, and extensive references to other compilations and databases of thermodynamic and transport properties are included.
>
> Catalog no. 197MZL (Lide). 1994, 528 pp., 5.25" diskette. ISBN: 0-8493-0197-1. U.S. $149.95/Outside U.S. $180.00. CRC Press, Inc., 2000 Corporate Blvd., N.W., Boca Raton, Florida 33431-9868.

Numerica® Logkow Database.

LogKow Database - A new database providing more than 22,000 experimentally measured log KOW values for 14,650 chemical compounds is now available. The partition coefficient for a chemical in a specific solvent systemQoctanol and waterQknown as log KOW, has become the standard value for predicting biological activity in many applications, notably as the standard of the U.S. Environmental Protection Agency. It claims to provide critically evaluated values for chemicals of interest because of their environmental, pharmaceutical, or health and safety effects. Included are organic compounds such as steroidal and non-steroidal drugs, other pharmaceuticals, poisons, toxins, amino acids, peptides, herbicides, pesticides, fungicides, insecticides, dyes, etc. Searches can be done by CAS Registry number, full or truncated molecular formula, chemical name, or the user may enter upper and lower value limits to retrieve all substances with log KOW values within a specified range. References from a full bibliography of over 1,500 references in CAS style can be viewed at a keystroke.

From Technical Database Services, Inc., 135 West 50th Street, Suite 1170, New York, NY 10020-1021, USA. Telephone: (212) 245-0044. Fax: (212) 247-0587.

DECHEMA Chemistry Data Series, Vol. XII, Electrolyte Data Collection; Part 1a, Conductivities, Transference Numbers, Limiting Ionic Conductivities of Ethanol Solutions; Authors: J. Bartel, R. Neueder; Editors: R. Eckermann, G. Kreysa.

Electrolyte Data XII, 1a - *Electrolyte Data* is a volume of the *DECHEMA Chemistry Data Series* providing scientists and engineers with reliable data. The collection of data on thermodynamic, transport, dielectric and spectroscopic data for electrolyte solutions and their solvents began in 1976 within the framework of the DECHEMA study "Forschung und Entwicklung zur Sicherung de Rohstoffversorgung" and was the reason for the development of the database ELDAR (ELectrolyte DAta Regensburg) at the University of Regensburg. Up to now, approximately 500,000 measured data of electrolyte solutions from 16,000 publications have been stored in ELDAR. "Electrolyte Data" and the database ELDAR have complementary functions. The data books give a clear arrangement of critically selected recommended data for each property of an electrolyte solution. The electrolyte solutions are classified by their solvents and solvent mixtures. The electrolytes are arranged in alphabetical order according to their molecular formulas, which are also written in the alphabetical order of their chemical elements. Indices of the formulas names and Chemical Abstracts Service (CAS) Registry Numbers facilitate searching. Smoothed data from the literature are not included in the tables. They already have been subjected to special adjustment procedures by the authors with the help of a variety of fitting equations and different solvent parameters, and therefore are unsuited as the basic data for the calculation of recommended values. The volume *Electrolyte Data* was guided by the rules of the Commission 1.2, Thermodynamics, of the Physical Chemistry Division of IUPAC.

1993. 638 pp. ISBN 3-926959-39-8. From DECHEMA Deutsche Gesellschaft für Chemisches Apparatewesen, Chemische Technik und Biotechnologie e.V., Postfach 150104, D-60061 Frankfurt am Main, Germany.

DECHEMA Chemistry Data Series, Vol. XII, Electrolyte Data Collection; Part 1b, Conductivities, Transference Numbers, and Limiting Ionic Conductivities of Solutions of Propanol, Butanol, and Higher Alcohols. Authors: J. Bartel, R. Neueder, P. Schröder; Editor: G. Kreysa.

Electrolyte Data XII, 1b - This volume continues the critical evaluation for solutions in butanol and higher alcohols. In this volume the third part of a very comprehensive collection of properties of electrolyte solutions is presented. These include values of solvent properties and distance parameters, conductivities of dilute and concentrated solutions, transference numbers and limiting ionic conductivities in C3 and higher alcohols. The data are preceded by a detailed introduction, showing various correlation methods and giving the theoretical basis for the interpretation of the data.

1993. 258 pp. ISBN 3-926959-41-X. From DECHEMA Deutsche Gesellschaft für Chemisches Apparatewesen, Chemische Technik und Biotechnologie e.V., Postfach 150104, D-60061 Frankfurt am Main, Germany.

Thermodynamics of Organic Compounds in the Gas State (Volumes I and II). Authors: M. Frenkel, G. J. Kabo, K. N. Marsh, G. N. Roganov, R. C. Wilhoit. PC Diskette (IBM) incorporated.

Thermodynamics of Organic Compounds - More than a quarter century has elapsed since Stull, Westrum, and Sinke published their comprehensive monograph on the thermodynamic properties of organic compounds, and a database providing a comprehensive summary of recent advances in statistical thermodynamic calculation methods, as well as the systematic collection of thermodynamic data or organic compounds, is long overdue. The present publication is a result of almost three years of collaboration between the Thermodynamics Research Center (TRC) at the Texas A&M University System and the Laboratory of Thermodynamics of Organic Compounds (LTOC) at the Byelorussian State University (Minsk). Volume I contains a description of the methods of statistical mechanics as applied to thermodynamic properties of organic compounds as well as information on the methods of determination of molecular data, peculiarities of practical calculations, and estimates of the uncertainties obtained. Volume II also contains a review of the existing empirical functions used to express the temperature dependence of the thermodynamic properties of the ideal gas, their comparisons, and test results required to make a judgment about the most reliable functional form.

Numerical data on the heat capacity, entropy, enthalpy, and Gibbs energy of compounds and the enthalpy and Gibbs energy of formation is given when available. The tables are accompanied with comments providing information on the original spectral and structural parameters, or at least an indication of the sources of this information. Where possible, comparisons with previous calculations and with experimentally-based third law or equilibrium data are given. Volume I also contains the thermodynamic data for the elements, inorganic compounds and radicals, and organic compounds and radicals C1 to C4.

Volume II contains thermodynamic data for organic compounds and radicals C5 to C36. Volume II is also provided with a diskette for an IBM-PC or compatible computer containing the ASCII file of the coefficients of the temperature dependence of the thermodynamic functions.

Each volume contains only references specific to that volume (about 2000 in Volume I and more than 900 in Volume II). The index contained in each volume covers all the compounds contained in both volumes.

This very relevant *tour de force* is exceptionally excellent in all respects - typography (in TEX), mathematically, alternative searching procedures, as well as with respect to its chemical thermodynamics.

Volume I. Library of Congress Card No. 94-060955. 1994. 815 pp. ISBN 1-883400-03-1. Price: USA $250; other countries $280 (prepaid). Volume II. Library of Congress Card No. 94-060955. 1994. 1010 pp. ISBN 1-883400-04-X. Price: USA $250; other countries $280 (prepaid). Two Volume Set. ISBN 1-883400-05-8.

From TRC, TRC Data Distribution, The Texas A&M University System, College Station, TX 77843-3124, USA. For more information call (409) 845-5981 or FAX (409) 862-2352.

Thermochemical Data and Structures of Organic Compounds. Volume I. Author: J. B. Pedley.

Thermochemical Data of Organic Compounds - This comprehensive, up-to-date compilation covers standard enthalpies of formation of both liquid and gaseous phases at 298.15K of organic compounds obtained from experimental data on 3,000 organic compounds. These are derived from

the literature through the end of 1992. Data are subdivided into more than 300 sets defined by a systematic hierarchy of codes corresponding to the presence of functional groups and/or ring systems.

The tables of data presented in this book are a great advance in comprehensive coverage and in critical evaluation, and supersede previous tables of data. This book is the most important source of thermochemical data for organic compounds now available, and users of these tables will be grateful to the author for the effort and care expended in their production. (A careful search revealed the omission of few data on certain compounds.)

The organization of the data and the use of a new parametric scheme allows extrapolation of data within and between families of structurally related compounds to yield missing values. The bibliography consists of more than 1,400 original publications. Three indexes (net formula, chemical name and Chemical Abstracts Service Registry Number) are included to simplify a search for compounds.

Library of Congress Card No. 93-061806. 1994. 472 pp. ISBN-1-883400-01-5. Price: $250 USA ($280 elsewhere), prepaid.

CODATA Calendar

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      1995

March
  5          Publications Committee.  Paris, France
6-7          CODATA Executive Committee.  Paris, France
8-9          Working Group on Data Access.  Paris, France
9-10         Commission on Standardized Terminology for Access to
             Biological Databanks. Geneva, Switzerland

May
9-10         Materials Database TG.  Paris, France

      1996

September
29-Oct 3  International CODATA Conference. Tsukuba, Japan


October
4-5          CODATA General Assembly.  Tsukuba, Japan
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CODATA Supporting Organizations 1995

Supporting Organizations foster CODATA's activities and objectives in many ways and receive certain perquisites and benefits. They are entitled to choose their category of adherence (and the corresponding dues) and usually designate a "Contact" person and may send an Observer to the General Assembly. [Organizations desiring to become Supporting Organizations should contact the Executive Director or the Secretary General.]

CLASS A

Begell House, Inc., Contact: *Dr. W. Begell*
BIOSIS UK-Zoological Record, Contact: *Mr. Michael N. Dadd*
Defense Technical Information Center, Contact: *Mr. Kurt Molholm*
International Atomic Energy Agency, Contact: *Dr. Charles L. Dunford*
Laboratoire National d'Essais (France), Contact: Dr. J. P. Calis
National Library of Medicine, Contact: *Dr. Donald A. Lindberg*
Science & Technology Information Center (SCITIC), Egypt, Contact: *Mrs. Hoda A. El-Sharawy*

CLASS B

American Institute of Physics, Contact: *Dr. Marc H. Brodsky*
Beilstein Institut, Contact: *Dr. Clemens Jochum*
Chemical Abstracts Service, Contact: *Dr. Ronald L. Wigington*
CRC Press, Inc., Contact: *Mr. James K. Brody*
CERET, Contact: *Mr. Albert Truyol*
DECHEMA Fachinformationszentrum Chemie, GmbH (FIZCHEMIE), Contact: *Dr. R. Deplanque*
Japan Association for International Chemical Information (JAICI), Contact: *Dr. H. Chihara*
Russian Research Center for Standardization, Information & Certification of Materials (VNITS SMV), Contact:*Prof. A. D. Kozlov*

CLASS C

Boehringer Mannheim K. K., Contact: *Dr. H. Kobatake*
Centre de Documentation de l'Armement, Paris (CEDOCAR), Contact: *Mr. C. Paoli*
Comissao Nacional de Energia Nuclear, Contact: *Eng. Elisabeth Braz Pereira Gomes*
Design Institute for Physical Property Data (DIPPR), Contact: *Ms. Marilyn B. Williams*
Edenglen S. A., Contact: *Mr. Michael Klinger* Engineering Information, Inc., Contact: *Dr. John J. Regazzi*
National Centre for Science Information (N.C.S.I.), Contact: *Dr. T. B. Rajashekar*
Office of Japan Society for CODATA, Japan Society of Information & Knowledge, Contact: *Dr. Kichiya Gosho*
Protein Data Bank, Contact: *Ms. Pamela A. Esposito*
Protein Information Resources (PIR), Contact: *Prof. Akira Tsugita*
Technical Database Services, Inc., Contact: Dr. Mildred R. Green

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Task Group on Materials Database Management

Materials Database Newsletter, March 1995, Number 20

NETWORKS: MPD NETWORK OPERATIONS IN TRANSITION

Effective August 1, 1994, MPD Network as a separate service on STN International was discontinued. STN will continue to offer most of the MPD databases, which can be searched effectively using STN commands, along with a number of other complementary STN databases that contain engineering information. The numeric materials property databases accessible on STN include PLASPEC, IPS, PDLCOM, and PLASNEWS. In addition, AAASD, ALFRAC, ASMDATA, COPPERDATA, and NISTCERAM are accessible but will no longer be updated.

The National Materials Property Data network (NMPDN), Inc. has ceased to operate as a separate entity. Intellectual rights and trademarks of NMPDN have been transferred to the Materials Property Council (MPC), Inc. MPC in cooperation with a team of advisors including J. G. (Gil) Kaufman, former head of NMPDN, Inc. and Dr. John R. Rumble, Acting Manager of Standards Reference Data Program at the National Institute of Standards and Technology, will consider and take appropriate action on future implementation of the MPD Network technology.

THE INTERNET

The use of the Internet for the exchange and dissemination of information has shown rapid growth in recent times. The Editor would welcome information about current and planned proposals that exist for using the Net for materials property information.

FORTH-COMING EVENTS

The Fifth International Symposium on the **Computerization and Networking of Materials Data** will take place 6-8 November 1995 at Tsukuba Science City in Japan. The main theme will be Global Sharing of Materials Information for Research and Development and Decision Making. Topics covered will include: Dissemination and Utilization of Data for Materials Standards, Data Transfer and Exchange; Materials Data Analysis for Quality and Reliability; Role of Materials Information for Global Issues on Resources and Recycling; Calculated and Processed Data Produced by Super-Computing; Legal Liability of Developers and End-Users of Computerized Materials Information; Economic Impact of Computerized Materials Information Systems; Possibility of Hypermedia to Describe the Complexity of Materials and their Behavior; Specialized Materials Information Towards Perfect Engineering; and the Role of Materials Data Systems in the Interplay Between Computation and Experiment.

FURTHER INFORMATION: Dr. Satoshi Nishijima, National Research Institute for Metals (NRIM), 1-2-1 Sengen Tsukuba 305, Japan, Tel: +81-298 53 1000, Fax: +81 298 53 1005

EDITOR: W. G. Jackson, The Institute of Materials, 1 Carlton House Terrace, London SW1Y 5DB, UK: Tel +44 71 839 4071; FAX +44 71 839 2289. There are no restrictions on the reproduction and distribution of the contents of this Newsletter.

Editors:

Editor: Edgar F. Westrum, Jr.
Department of Chemistry, University of Michigan,
Ann Arbor, MI 48109-105
Telephone: (313) 764-7357 / Telex: 8102236056
FAX: +1-313-747-4865

Associate Editor: Phyllis Glaeser
CODATA Secretariat, 51 Blvd. de Montmorency,
75016 Paris, France
Telephone: 33 1 45250496 / Telex: 645554 F
FAX: +33 1 42881466 / Cables: ICSU Paris 016

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