

45 CODATA / NEWSLETTER

JULY 1988

CODATA Symposium at Toronto

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A full-day symposium on CODATA concerns was hosted by the ACS Chemical Information Division at the North American Chemical Congress, June 14 in Toronto, Canada, potentially providing an expose to the 12,000 participants--but the "competition" was great enough to reduce the participation to nearer the one percent level.

Concise presentations on CODATA goals and structure (D.R. Lide), on thermodynamic data evaluation (D. Itkin), on biology and biotechnology (L. D. Blaine), on materials property databases and networks (J.G. Kaufman), on environmental data (J.L. Clark), on CODATA's referral database (B.B. Molino), on the Canadian scientific database service (G.H. Wood), on thermophysical properties AICHE/DIPPR (T.B. Selover), on databases for analytical chemistry (S.G. Lias), on molecular biology databases (M. Zuker), and on chemical structure search systems (C. Jochum).



J.G. Kaufman, B.B. Molino, and G.H. Wood (l to r) expound CODATA concerns at Toronto's North American Chemical Congress.

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.

Highlights of a session were the presentation of the Herman Skolnik award to CODATA's president, David R. Lide, Jr. (elsewhere in this issue), as well as the recipient's award address.

A supplementary session on computerized dissemination of numerical data for chemists provided further development of relevant techniques.

Finding the Future

The National Governors' Association (NGA) Center for Policy Research, together with a number of the major federal statistical agencies and various organizations, including the U.S. National Committee for CODATA, is convening the second annual conference on integrating data for decisionmaking. The conference will be held 12-14 December 1988 at the OMNI Shoreham Hotel in Washington, D.C.

The theme of the conference, called "Finding the Future," is forecasting. A three pronged examination of forecast applications and development, targeted to decisionmakers and managers, will focus on:

- decisions about tomorrow that decisionmakers are asking today; applications to socio-demographic, economic/fiscal and natural resource decisionmaking, at global, national, and state and local levels;
- best organizational practices and where they can be found; organizational strategies in using and developing forecast data and integrated information systems; plus
- common methodologies that cut across diverse applications.

Aspects of particular interest to CODATA-related decision-making are:

- improving effective forecast and integrated data use, determining the best model, techniques and data sources for the user's specific decisionmaking needs, issues of adequacy of data for the application at hand, issues of access and dissemination, determining costs, preserving data for future use, etc.,

as well as

- developing integrated model approaches; improving forecast accuracy through quality control procedures; uncertainty and error treatment; error propagation; statistical information, and database development issues.

The three-day conference program will explore the full range of issues to be considered during the information life cycle; the request to develop information; identifying available data sources; accessibility, data integration and sharing; the role of information in formulating policy; and the policy's ultimate effect on delivering future services and products. The appropriateness of forecast data and integrated information systems at different geographic levels of decisionmaking will be discussed.

A unique audience--generally not found elsewhere--will represent a multi-discipline mix of governmental, industrial, and academic decisionmakers and managers, who will participate from various public policy areas, science and technology, and information specialty fields.

The agenda features extensive information exchange opportunities through plenary and concurrent sessions, ancillary short courses and an exhibit area. Exhibit booths will showcase state-of-the-art information systems, software and hardware

products and services from private-sector firms, public agencies, and non-profit organizations.

The highly successful 1987 initiatory conference has been described in CODATA Newsletter 41 and proceedings are available.

For program information, contact Lorraine Amico at NGA, (202) 624-5346. For registration and hotel information, contact Jan Dunlavey at NGA, (202) 624-5347. The NGA address is: National Governors' Association, 444 North Capital Street NW, Washington, D.C. 20001; telephone: (202) 624-5346/5334.

Computerization of Materials Property Data

A one-day tutorial seminar by Drs. H. Mindlin of Battelle Memorial Institute and J. H. Westbrook of Sci-Tech Knowledge Systems was presented in Tel Aviv, Israel, on 16 May 1988 under the auspices of the Israeli Committee for CODATA, the Israel Academy of Sciences and Humanities, and the Israeli Military Industries Co. The intent was to acquaint managers, scientists and engineers from both industry and academia with the present state-of-the-art in the computerization of materials property data.

The seminar began with an extensive introduction to the subject covering--among other matters--the special problems posed by materials data because of the large number of independent variables affecting properties, the diversity of terminology, and lack of standardization of materials designations, units, test methods, etc. These and other complexities have made materials database building expensive and time-consuming with the result that available machine-readable materials databases are often of limited scope--and consequently of limited utility.

Westbrook reviewed international activities in the field, the need to share expertise and funding costs and to reduce redundant efforts, and also the need to effect as much international standardization as possible. Particular activities included were: CODATA, VAMAS, Chemical Abstracts' STN, the European Economic Community materials data network demonstrator program, NATO's AGARD Lecture Series, the Schluchsee Workshop and the 1st Int'l. Symposium held at Philadelphia, November 1987.

Mindlin summarized current activities in the U.S.A. (by the Federal government, by professional scientific and engineering societies, and by private companies) and described various individual databases, e.g., ACTIS (tribology), EDEAC (environmentally assisted crack growth) and DIEL (fluid dielectrics). The overall picture is one of a great many, narrowly focussed, separate projects, inadequately funded and with minimal coordination. The one broadly based program, the National Materials Property Data Network (loosely affiliated with CAS-STN), is supported by a consortium of industrial and utility companies. It has progressed to a demonstration program incorporating four metallic materials databases with common access and support facilities.

Integrated numeric data systems for materials or some other subject field comprise several individual components: data

(cont'd. on p. 6)

CODATA's President Receives Herman Skolnik Award

Dr. David Reynolds Lide, Jr. received the Herman Skolnik Award of the American Chemical Society's Division of Chemical Information in a ceremony during the Third Chemical Congress of North America at Toronto, Canada, 7 June 1988. The award was based on his outstanding contributions to the field of chemical information. After the presentation by Arlene N. Somerville, Dr. Lide presented the award lecture, "Assuring Reliable Data for Science and Technology."

As current President of CODATA, a scientific committee of the International Council of Scientific Unions, Dr. Lide is active in the coordination of data programs and database development in physical, biological, and geosciences. He is a Fellow of the American Physical Society and has served in a number of capacities in the American Physical Society, American Chemical Society, and other professional groups.

Dr. Lide is the author of over 100 papers on molecular structure and spectroscopy, free radicals, molecular lasers, and various aspects of scientific information. He is Editor of the *Journal of Physical and Chemical Reference Data*, which he founded in 1972, and has served on several other editorial boards including that of the *Journal of Chemical Information and Computer Science*. He has been Chairman of the Commission on Symbols, Terminology, and Units of the International Union of Pure and Applied Chemistry, as well as President of the IUPAC Physical Chemistry Division.

He joined the National Bureau of Standards in 1954 to establish a laboratory for research in microwave spectroscopy and molecular structure. From 1963 to 1968 he headed the Molecular Spectroscopy Section at NBS, which included research groups in ultra-violet, infrared, and microwave spectroscopy. Since 1969 he has been Director of the Standard Reference Data Program at NBS. In this capacity he oversees a national effort to develop reliable databases of physical, chemical, and materials properties, which includes a major publication program, as well as the recently established NBS Standard Reference Database Series.

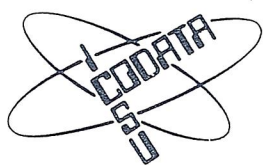
Dr. Lide was born in Gainesville, Georgia and raised in Columbia, South Carolina. He was educated at Carnegie Institute of Technology (B.S., 1949, in chemistry) and Harvard University (M.A., 1951, in physics and Ph.D., 1952, in chemical physics). He subsequently studied at Oxford University under a Fulbright grant. In 1959 - 1960 and again

in 1967-1968, he held NSF Senior Postdoctoral Fellowships for advanced study and research at London, Copenhagen, and Bologna Universities.



David R. Lide, Jr.

In honor of the first recipient (in 1976), the Division of Chemical Information of the American Chemical Society established the Herman Skolnik Award to recognize outstanding contributions to and achievements in the theory and practice of chemical information science. By this Award, the Division of Chemical Information hopes to provide role models that scientists may emulate in the continuing advancement of chemical information science, in areas such as: production and dissemination of chemical information; editorial innovations; design of new and unique indexing, classification and notation systems; design of new and unique computerized information systems; chemical nomenclature; structure-activity relationships; and data correlations.



Task Group on Materials Database Management

Materials Database Newsletter

July 1988, Number 4

Members of the CODATA Task Group on Materials Database Management held their third meeting at the Institute of Metals, London, on 12th and 13th May, 1988. Two Corresponding Members, Dr. Lu Yunwen of Tsinghua University, Beijing, and Mr. Dan Phelan of Chisholm Institute of Technology, Victoria, also took part in the meeting. Expert visitors, from the fields of economic analysis and science policy evaluation, assisted the Group during an in-depth discussion of the assessment of the benefits of materials property databases and of the economic consequences in the national and commercial settings. A report on the conclusions which were reached and which will specify actions aimed at quantifying benefits will be prepared. The Task Group approved the final draft of its Guide to Material Property Database Management, edited by J. G. Kaufman, which will be issued in the CODATA Bulletin series. Progress was made on other projects; these included the Group's international register of materials database managers and the updating of reports of national and regional materials database activities.

STANDARDS

The Second International Symposium on Computerized Materials Databases will be held in Orlando, Florida, USA, on December 7-9, 1989 (see CALENDAR listing). The meeting will be sponsored by ASTM Committee E49 on Computerized Material Property Data, J. R. Rumble, Chairman. The Symposium Chairman is J. G. (Gil) Kaufman. The theme of the meeting is expected to be "Issues in Data Exchange", with particular focus in areas including data exchange protocols, interface formats and interactions with computer-aided engineering/design/manufacturing.

DATABASES

The Royal Institute of Technology, Stockholm, has developed MATEDS, an educational database system covering the mechanical and physical properties, formability, corrosion, joining, surface treatment, etc., of aluminum alloys. The aims of the system are to illustrate characteristic properties and the effects of composition thereon, and to demonstrate different approaches to materials selection. The development of the system has been financed by Skan Aluminum, and the package will be distributed to technical universities in Scandinavia in August 1988. FURTHER INFORMATION: Rolf Sandstrom, Department of Materials Technology, Royal Institute of Technology, S-100 44, Stockholm, Sweden.

The European Aluminum Association, a collaborative organization representing the European aluminum industry, has initiated the development of a common property database. Property data for 25 wrought aluminum alloys are being assessed and harmonized. Some 70 properties will be covered. The technical work is being carried out at the Royal Institute of Technology, Stockholm, and is expected to be completed by the end of 1989. There will be a publicly available version of the harmonized property values. FURTHER INFORMATION: Rolf Sandstrom, Department of Materials Technology, Royal Institute of Technology, S-100 44 Stockholm, Sweden; OR J. P. Roullier, European Aluminum Association, Konigs Allee 30, PO Box 1207, Dusseldorf 1, Federal Republic of Germany.

The IMMAMAT materials selection program is available from The Institute of Metals and Materials Australasia. The system is supplied with data on 312 copper and aluminum alloys and steels, but is not limited to these. The user may add, delete or edit single items; this allows for the addition of new alloys or local in-house specifications. The system is designed for IBM PC, XT, AT or truly compatible computers. FURTHER INFORMATION: The Institute of Metals and Materials Australasia, Suite 215, 191 Royal Parade, Parkville, VIC 3052, Australia.

The JANAF Database (Joint Army-Navy-Air Force) of information corresponding to the JANAF Thermochemical Tables, providing critically evaluated chemical thermodynamic properties of inorganic and certain organic substances, has recently become available online on STN International. Properties available include heat capacity, entropy, Gibbs energy function, enthalpy, enthalpy of formation, Gibbs energy of formation, and log of the equilibrium constant for about 1800 substances. The database is produced by the U. S. National Bureau of Standards.

BIBLIOGRAPHY

Demaïd A. and Zucker J. A CONCEPTUAL MODEL FOR MATERIALS SELECTION. Metals and Materials, 1988, 4, 291-297.

Sargent, P. M. A MATERIALS DATA INTERCHANGE LANGUAGE. Report No. CUED/C-MATS/Tr.143, April 1988, Cambridge University Engineering Department, Cambridge, UK, CB2 1PZ.

CALENDAR

22-29 Sept 1988: Karlsruhe, FEDERAL REPUBLIC OF GERMANY

11th International CODATA Conference SCIENTIFIC AND TECHNICAL DATA IN A NEW ERA. CONTACT: DECHEMA, Abt. Tagungen, POB 97 01 46, Theodor-Heuss-Allee 25, D-6000, Frankfurt am Main, FRG.

11-14 October 1988: Toronto, ON, CANADA

ASTM Committee E49 on COMPUTERIZATION OF MATERIAL PROPERTY DATA meeting.

15-17 November 1988: Petten, THE NETHERLANDS

VAMAS Workshop on STANDARDS FOR FACTUAL MATERIALS DATABANKS. Participation will be by invitation only. CONTACT: Dr. J. R. Rumble, NBS, A323 Physics Building, Gaithersburg, MD 20899, USA; OR H. Kröcker, CEC-JRC, NL-1755 ZG Petten, The Netherlands.

8-12 December 1988: London, UK

12th International ONLINE INFORMATION Meeting and Exhibition. CONTACT: Learned Information (Europe) Ltd, Woodside, Hinksey Hill, Oxford, UK, OX1 5AU.

27-29 June 1989: St. Louis, MO, USA

ASTM Committee E49 on COMPUTERIZATION OF MATERIAL PROPERTY DATA Meeting.

5-7 December 1989: Orlando, FL, USA

ASTM Committee E49 on COMPUTERIZATION OF MATERIAL PROPERTY DATA Meeting.

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CODATA Calendar

1988

September

— Multisatellite Thematic Mapping, Karlsruhe, F.R.G.

26-29 CODATA Task Group on Materials Database Management, Karlsruhe, F.R.G.

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

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

Oct.1

Materials Property Data

(cont'd. from page 2)

identification, data capture, record organization, data access and manipulation tools, as well as data presentation and application modules. Westbrook discussed the R&D work done by his firm and others in three of these areas: preparation of data source directories, data capture techniques, and indexing and control of metadata.

The U. S. government, particularly the Department of Defense, supports several materials centers which were described by Mindlin. The centers maintain archival files of materials information, both bibliographic and factual, in both print and computerized form, and provide a personalized service by mail and phone to government contractors needing materials information.

American information analysis centers described by Mindlin included the Metals and Ceramics Information Center at Battelle

which offers a very broad coverage of metals and ceramics; the Non-destructive Testing Center at Southwest Research Institute; the High Temperature Materials Information Analysis Center at CINDAS - Purdue University (high temperature properties of structural composites, metals and infrared detector/sensor materials); and the Metal Matrix Composites Information Analysis Center at Kamen-TEMPO in Santa Barbara, California.

To cope with the manifold problems related to all aspects of standardization necessary in building materials property databases, ASTM in 1986 established a new main committee, E-49. The activities of E-49 and its liaison with other organizations having mutual interests were described by Westbrook. E-49 presently conducts its activities through five subcommittees treating, respectively: standards for materials identification, property data reporting, terminology, data structures, and data quality characterization. E-49 was also the sponsor and organizer of the 1st International Symposium on Computerization and Networking of Materials Property Databases held in Philadelphia, November 1987. It is to be succeeded by a second such symposium scheduled for December 1989 in Orlando, Florida.

Computers for the Analysis of Geochemical and Hydrogeochemical Data

The 17th Geochautauqua Tucson to be held at Tucson, Arizona, 7-8 October 1988, is sponsored by the International Association for Mathematical Geology, the Mathematical Geologists of the US, the Arizona Geological Society, and others. For information, contact: Donald E. Myers, General Chairman, Department of Mathematics, University of Arizona, Tucson, Arizona 85721. Telephone: (602) 621-6859.

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