

54 CODATA / NEWSLETTER

NOVEMBER 1990

HIGHLIGHTS

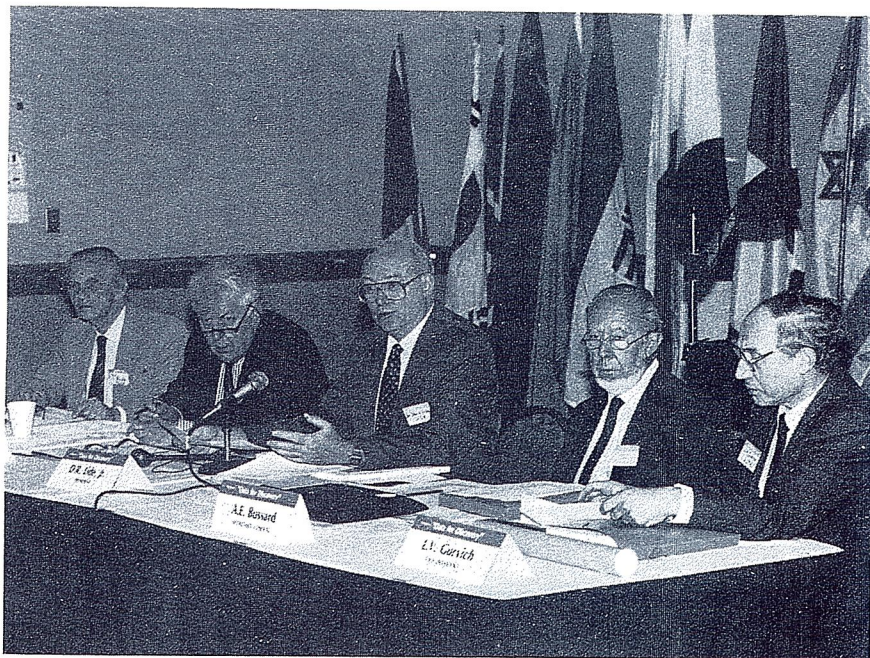
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The Committee on Data for Science and Technology (CODATA) was established in 1966 by the International Council of Scientific Unions.

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

Major Decisions of CODATA 17th General Assembly

The major decisions of a hard-working General Assembly (GA) produced many important and useful directions for CODATA's near future at their two-day meeting in Columbus, Ohio, July 20-21, 1990.



The head table at the 17th General Assembly (l to r): Prof. A. Bylicki (Vice-President); Mr. J. Crease (Treasurer); Dr. D. R. Lide, Jr. (President); Prof. A. E. Bussard (Secretary General); Prof. L. V. Gurvich (Vice-President).

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Materials Data for Computer Aided Engineering

A CEC-CODATA Joint Workshop on Materials Data for Computer Aided Engineering co-sponsored also by the International Federation for Information Processing and by the Society of Manufacturing Engineers is to be held at Petten, The Netherlands, 19-22 March 1991.

Design for manufacturability and materials optimization is gaining an increasing acceptance as an economic and technical incentive for the integration of computerized engineering processes. However, developments for achieving the integration of information on engineering materials into this system have not kept pace with the automation of the other engineering disciplines, to their disadvantage. Materials information has neither been computerized to the same level as the other engineering systems, nor has it been adequately interfaced with them.

The principal objectives of this workshop, therefore, are to define the actions needed for a more effective integration of materials information into Computer Aided Engineering (CAE) systems and to identify those individuals and organizations most capable of contributing toward those actions. More specifically the aims of this workshop are:

- to bring together experts in CAE and materials data to discuss and analyze the reasons for the existing situation and to propose solutions to change it;
- to identify the materials data which are needed to fully meet the various engineering requirements such as: analysis, design, process planning, production scheduling, etc.;
- to identify methods and techniques which provide solutions to the integration of industrial functions which require common access to materials data;
- to identify the organizations which should continue to ensure progress towards the full integration of materials data with the other computerized engineering methods.

The potential and capacity of computerized engineering systems can only be fully exploited when digitized information for design, production and material properties can be totally integrated.

The first day consists of plenary lectures and tutorials from world experts in the relevant fields in order to ensure adequate preparation for the discussions. The second part will analyze the situation and its transformation in a highly participatory mode, involving each member of the workshop. Proposals and strategies for the future will be derived using small expert working groups followed by reports and discussion in plenary sessions.

Participation in this Workshop is by invitation only, but interested persons are cordially invited to outline their experience, expertise and interest to qualify for such an invitation. Participation is especially sought from members of the design and manufacturing engineering communities. The working language of the Workshop will be English and

proceedings will be published. The cost of participation in the Workshop is \$300, exclusive of travel, accommodation, and subsistence.

Further inquiries: **Europe**—Tel: +31-2246-5224 (Norman Swindells), +31-2246-5230 (Hermann Kröckel); FAX: +31-2246-1917. **USA**—Tel: 518-399-2827 (Jack H. Westbrook); FAX: 518-399-6621.

NASA Master Directory

The NASA Master Directory (MD) to Earth and space science data is one mode of an interconnected directory system spanning the world with nodes in Japan (1), USA (3), Europe (2), with seven additional nodes (including Bangkok, Nairobi, and Ottawa) expected to be in operation by summer 1991.

In the U.S. the federal agencies have been working together to create a directory to data global change under the auspices of the Interagency Working Group on Data Management for Global Change (IWGDMGC). This Global Change Master Directory (GCMD) is managed by the National Space Science Data Center (NSSDC). Other federally-related directories such as the NOAA Earth Science Data Directory and the NCAR/NOAA/NASA STORM data management project will pass data information to the GCMD. Other agencies simply create DIF files describing their data holding and submit them to the GCMD for entry. Staff at the NSSDC are responsible for reviewing the entries for technical content and overall consistency with other entries.

Even those countries not having a directory node are participating by supplying information on their data in the DIF form. The World Data Center system is advocating this approach. Recent discussions with the Soviet Geophysical Committee/World Data Center A in Moscow have resulted in an agreement to do this. Plans are well underway to provide access for the Soviet Interkosmos Institute (IKI) to a separate copy of the directory at NSSDC in exchange for information about IKI data holdings.

ENTVAPOR Now Available

A new database based on computations from *Enthalpies of Vaporisation of Organic Compounds, Critical Review and Data Compilation* by V. Majer and V. Svoboda, an International Union of Pure and Applied Chemistry publication, is now available from Blackwell Scientific Publications.

This database called ENTVAPOR gives reliable temperature extrapolation of enthalpy and entropy of vaporization beyond the range of experimental values for over 600 organic compounds.

As a result, even for compounds where experimental values were reported at only one temperature, a calculation over a wide temperature range can be performed quickly and easily.

ENTVAPOR is available from Blackwell Scientific Publications LTD., P. O. Box 88, Oxford, U.K. The U.S. Office is c/o PBS, P.O. Box 447, Brookline Village, MA 02147 (Tel: 617-524-7678).

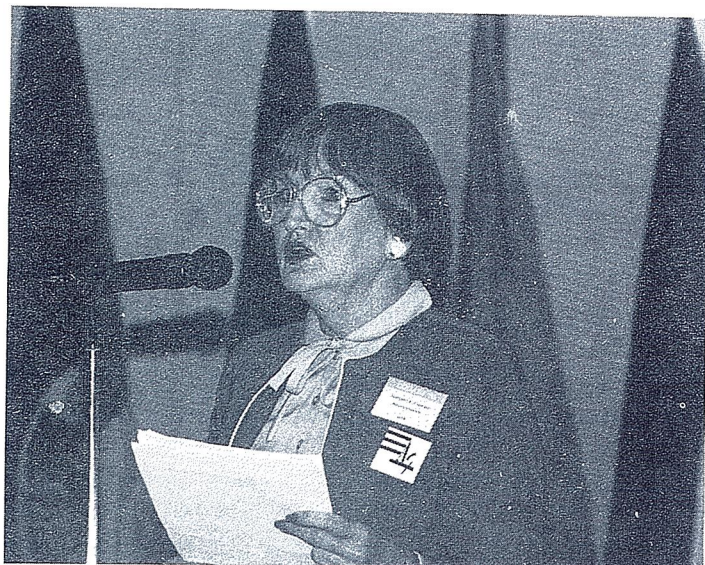
CODATA General Assembly

(continued from page 1)

The Task Groups and Commissions approved for the biennium 1991-92 are:

Materials Database Management
Fundamental Constants
Referral Database
Biological Macromolecules
Commission on Data for the International Geosphere
Biosphere Program
Chemical Thermodynamic Tables
Commission on Standardized Terminology for Access to
Biological Data
Artificial Intelligence and Computer Graphics
Industrial Data Commission
Geothermodynamic Data
Survey of Data Sources in East-Asian Countries
Critically Evaluated Phase Equilibrium Data
Hybridoma Data Bank
Microbial Strain Data Network
Systematic Nomenclature for Foods in Numerical Data
Banks

Prof. J. E. Dubois (*France*)
Dr. R. Eckermann* (*Germany*)
Academician F. A. Kuznetsov* (*U.S.S.R.*)
Prof. R. Simpson (*Australia*)
Prof. R. Sinding-Larsen (*Norway*)
Prof. A. Tsugita (*Japan*)
Dr. J. H. Westbrook* (*U.S.A.*)



Dr. M. Courain, Program Chairman for the International CODATA Conference at Columbus, reports to the General Assembly.

The officers of CODATA are now (individuals newly elected to their offices are indicated by an asterisk):

President: Prof. D. Abir* (*Israel*)
Past President: Dr. D. R. Lide (*U.S.A.*)
Vice-President: Prof. L. V. Gurvich (*U.S.S.R.*)
Secretary General: Dr. G. H. Wood* (*Canada*)
Treasurer: Mr. J. Crease (*U.K.*)

The eight elected members of the Executive Committee are (newly elected individuals are indicated with an asterisk):

Dr. G. C. Carter* (*U.S.A.*)



Dr. B. B. Lide presents the CRD (CODATA Referral Database) to the General Assembly.

The new dues structure program was also adopted by the National Delegates to CODATA.

CODATA Columbus Conference

The Columbus Conference was judged to be a success in participation, intellectually, socially, and in many other respects. A final registration of 365 persons involved attendees representing 29 countries—more than CODATA's 26 member countries. A truly stellar program ensured that 250 people were on hand even for the closing session. M. E. Courain, Program Chairman, and Gerard Platau, who headed the Local Arrangements Committee, deserve high praise for the work of their group.

Topics which were explored included global change, spatial data, error propagation and tracking, as well as human factors in the design, fabrication, and integration of data. Three significant trends in biology were well covered: the human genome project, interaction between databases, and nomenclature and terminology.

At CODATA90, the original charge always given to any ISCU committee to be inter- and cross-disciplinary is truly being achieved and pervaded the sessions and the CODATA activities.

CODATA Personalities in the News

Charlotte M. Sitterly Dies at 91

Charlotte M. Sitterly was an astrophysicist who supervised compilation of the multivolume tables of atomic energy levels, as derived from optical spectra, that became a standard reference in laboratories around the world. She was the first International Astronomical Union Delegate to CODATA and a speaker at the first CODATA Conference (1968). She had devoted much of her career to the study of the sun's spectrum, including wavelengths that could not penetrate the atmosphere and were therefore observed from rockets. She demonstrated that the radioactively unstable element technetium occurs in nature by the analysis of sunlight.

Her principal affiliations were at Princeton University (after 1916), Mount Wilson Observatory (after 1925), a doctorate at Berkeley (1931), Princeton University (after 1931), and then at the National Bureau of Standards (1945).

Her interest in data compilation and evaluation may have been inspired by work with Henry Norris Russell whose classifications of stars by spectral type and brightness has become the global standard.

New NIST Databases

THERM/EST, an estimation algorithm which calculates thermodynamic properties at 298.15 K and has a database with experimental and estimated values for 379 hydrocarbon compounds, has been released. The thermodynamic properties have been developed for the gas, liquid, and solid phases. The hydrocarbon compounds and their properties are divided as follows:

- straight-chain aliphatic
- branched aliphatic/tertiary carbon branching
- branched aliphatic/quaternary carbon branching
- straight-chain alkene
- substituted alkene
- alkyne
- aromatic
- alicyclic

The NIST Mass Spectral Database of Common Compounds, which contains spectra of 10,215 common chemical substances extracted from the primary database, includes those that are commercially available, as well as those of environmental or pharmaceutical interest. (A major asset of this database is that it requires only a fraction of the disk space needed for the larger version.)

The NIST/CARB Biological Macromolecule Crystallization Database is heralded as the first NIST database on biotechnology and brings together for the first time all published data on the crystallization of proteins and nucleic acids. It contains crystal data and crystallization conditions for more than 1,000 crystal forms of 600 biological macromolecules. This database is already proving to be a boon to biochemical

researchers in the pharmaceutical industry and in the academic community.

X-ray Photoelectron Spectroscopy Database is a best-selling database which gives easy access to critically evaluated photoelectron and Auger spectral data on more than 13,000 measurements and allows for searches on photoelectron and Auger lines, as well as chemical shifts by element, line energy, and other variables. (A major update to this database is currently underway.)

All NIST databases were demonstrated at the 12th International CODATA Conference in Columbus, Ohio—"Data for Discovery." For ordering information on these and other SRD databases: Joan Sauerwein, Standard Reference Data, National Institute of Standards and Technology, 221/A323, Gaithersburg, MD 20899. Tel: 301-975-2208; FAX: 301-926-0416.

Standard Reference Data now has a comprehensive, convenient catalog of all electronic databases and best-selling, classic data compilations in hard-copy. For a free copy, send a self-addressed label to: Standard Reference Data, National Institute of Standards and Technology, 221/A323, Gaithersburg, MD 20899.

CODATA Calendar

1991

January/February

31/2 CODATA Task Group Meeting on Survey of Asian and Oceanic Databases. Seoul, Korea

March

11-13 CODATA Task Group on Biological Macromolecules. Washington, D.C., U.S.A.

19-22 CODATA/CEC Joint Workshop on Materials Data for CAE. Petten, The Netherlands

21-22 CODATA Scientific Program Committee (for '92 Conference). Paris, France

23-24 CODATA Materials Database Steering Committee for Moscow Meeting. Paris, France

25-27 CODATA Executive Committee. Paris, France

28-29 CODATA Referral Data Task Group. Paris, France (Tentative)

July

----- CODATA Materials Database Management Task Group. Trondheim, Norway

1992

April

----- Materials Database Experiences. Moscow, U.S.S.R.

August

17-20 International CODATA Conference. Beijing, P.R. China

21-22 CODATA General Assembly, Beijing, P.R. China

Research Policies and Quality Assurance

The 2nd International Conference on Research Policies and Quality Assurance will be held on May 6-7, 1991, at the Hotel Columbus, Rome, Italy. It is concerned with the societal implications of data integrity, the quality assurance of research data, and related data and ethical problems of scientific research. The proceedings will be published in "Accountability in Research: Policies and Quality Assurance."

For registration materials, contact: Dr. Adil E. Shamoo, Department of Biological Chemistry, University of Maryland School of Medicine, 660 West Redwood Street, Baltimore, MD 21201 (USA); Tel: 301-328-3327; FAX: 301-328-8297.

Comparative Study of Data between the Natural and Social Sciences

In the Social Sciences much data and many data collections are apparently not used for a variety of reasons (e.g., unsuitable methods of data collection, lack of proper description and definition of the collected data, questionable relevancy of the data to the specific research needs, etc.).

Solution of data problems is, of course, the main theme of the CODATA organization—but even in the exact sciences various aspects of data problems have recently undergone basic and significant changes. Much of such data are today obtained by expensive research projects and installations utilizing billions of dollars in hardware, software, maintenance, and the employment of highly qualified manpower. Particle accelerators in physics, the "Hubble" telescope in astronomy, NASA's Earth Observation System (EOS), the Landsat earth surveillance program, the Human Genome project are only some examples. In spite of enormous and careful preparations their suitability and success is by no means assured—see the initial (?) problems of the "Hubble" telescope—on the other hand, some of them produce such an enormous amount of data that it may take years to analyze and apply them (e.g., the accumulated Landsat data, which have not yet been evaluated). All these problems seem to

make it imperative that in the natural and exact sciences, too, the approach to—and the methods of—data collection and treatment should be carefully reinvestigated and analyzed.

Dr. Eliahu Hoffmann, the Secretary of the Israel National CODATA Committee was invited by the "Wissenschaftszentrum Berlin für Sozialforschung" to be a guest scientist during the months of mid-1990 to develop the outline of a research project which would compare and evaluate the production and collection of data in the natural and social sciences. This topic was suggested by the Head of the Social Sciences Department of the German Ministry of Research and Technology [Bundesministerium für Forschung und Technology (BMFT)].

Dr. Hoffmann presented a proposal for a three-year research project to the BMFT. This proposal is presently being processed and approval is expected by the end of 1990.

Those having relevant data bearing on these problems may wish to share them with Dr. Hoffmann (address: Center of Scientific & Technological Information, P. O. Box 43074, Tel-Aviv, ISRAEL 61430). --Ed.

Special Memorial Issue for Jiro Osugi

In memory of Jiro Osugi, the last editor-in-chief of the *Review of Physical Chemistry of Japan*, the Physico-Chemical Society of Japan has decided to publish a memorial volume composed of original papers on pressure related problems contributed specially by the scientists brought up and influenced by Jiro Osugi, Emeritus Professor of Kyoto University, throughout his life. He died of pancreatic cancer on 12 August, 1989, at the age of 69. His sudden—and too early—demise was a great loss to the high pressure research community. All research workers formerly under his guidance met together at Takaragaike—a scenic spot which he most loved and where he held the fourth International High Pressure (AIRAPT) Conference—to celebrate his 70th birthday in October, 1989. Those deeply grieved over his passing wrote papers sacred to his memory. The Physico-Chemical Society of Japan

accepted this project as a special issue of the *Review* in view of his outstanding contribution to make this journal popular all over the world.

Jiro Osugi was born in 1919, graduated from Kyoto University in 1943, and in 1962 became Professor of Physical Chemistry, Department of Chemistry, Faculty of Science, Kyoto University. He had been the editor-in-chief of this journal until he retired from Kyoto University in 1983. We can see how he devoted himself to the continued editing of this journal in his preface for the 50th commemorative volume, 1980. He describes: The dream of a few hundred thousands and million bars would be attractive and the trend of researches is like that of a mountain climber approaching a ridge. Further developments would be needed to pass over a few ridges, and it would be necessary to record the present stage of developments as a "milestone." With this idea in mind he invited many leading high pressure scientists to review "Modern Aspects of Physical Chemistry at High Pressure"—the subtitle of the previous commemorative volume. We hope that the contributors to the present special issue and the readers would pay attention to his perspective on the future of this research field.

We thank all the contributors to this special issue, the editors Tadashi Makita and Masaru Nakahara, together with those who greatly assisted, Mrs. S. Yamaguchi, Mrs. S. Toduda, and Miss C. Shiraiwa, in the Special Issue, *The Review of Physical Chemistry of Japan*, sacred to "The Memory of Jiro Osugi," August, 1990, published by The Physico-Chemical Society of Japan.

Global Runoff Data Centre (GRDC)

A permanent Global Runoff Data Centre (GRDC) was established at the Federal Institute of Hydrology in Koblenz, Germany, on 1 May 1987, under the auspices of the World Meteorological Organization (WMO). It provides a mechanism for the international exchange of data pertaining to river flows and surface water runoff on a continuous long-term basis.

"Reference Data Standard"

As a result of the Omnibus Trade and Competitiveness Act, signed into law on August 23, 1988, the (U.S.) National Bureau of Standards officially became the National Institute of Standards and Technology (NIST). The new institute retains all of the traditional functions and services of NBS and takes on several new assignments designed to boost American industry in the world marketplace.

The *Reference Data Standard* (Joan Sauerwein, Editor) is an informal communication of the National Standard Reference Data System (NSRDS) for the exchange of news and ideas about data centers, publications, meetings and other activities related to data evaluation and dissemination. The National Standard Reference Data System, which operates under the authority given in Public Law 90-396, was established to make critically evaluated data in the physical sciences available to the scientific and technical community. Comments and suggestions on *The Reference Data Standard* should be addressed to: Standard Reference Data, National Institute of Standards and Technology, Bldg. 221/A334, Gaithersburg, MD 20899, USA. Tel: 301-975-2208.

Lester Haar

Lester Haar, an outstanding authority on the thermodynamic properties of water, died June 14, 1990, at the age of 67. His standard reference data publication—"The NBS/NRC Steam Tables," published by Hemisphere Press in 1984, is a landmark book presenting a formulation for the properties of steam over previously unavailable ranges of temperature and pressure. The compilation quickly became the best formulation available for scientific and general engineering use and replaced all previously accepted and developed formulations. This book is the basis for NIST Standard Reference Database 10—NIST Thermophysical Properties of Water.

Mr. Haar also did research on the properties of ammonia and on the thermodynamic temperature scale. A member of the International Association for the Properties of Steam, he received the Ludwig Mond award of the Institute of Mechanical Engineering in 1958, the Commerce Department's Bronze Medal (1980), and its Silver Medal (1983).

Although he retired from NBS in 1986, he continued as a guest scientist until his death and was immensely well-liked and respected by co-workers.

Standardizing Terminology Symposium

A *Symposium on Standardizing Terminology for Better Communication: Practice, Applied Theory, and Results* sponsored by ASTM (Amer. Soc. for Testing Materials) is planned for June 12-14, 1991, at Holiday Inn Lakeside, Cleveland, OH, USA. With a galaxy of invited speakers from Europe, Canada, Greece, and P.R.China, as well as the USA, the role, current trends, activities, coordination, standardizing, indexing problems, representations of terminology, keyword selection, quality control, and foreign language equivalents will be treated. Terminology for special languages and nomenclatures, applications of terminology for social sciences and in computerization and database applications are included. These topics obviously are both relevant and broadly applicable to many CODATA concerns. The presentations will be published as an ASTM-STP (Special Technical Report). Further information may be obtained from the Chairman, Richard A. Strehlow, Oak Ridge National Laboratory, P. O. 2008, Bldg. 4508, Oak Ridge, TN 37831, USA, or the Co-Chairman, Sue Ellen Wright, Institute for Applied Linguistics, Kent State University, Kent, OH 44242, USA.

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