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

Number 72 Codata Newlsetter

August 1995

HIGHLIGHTS

CODATA Working Group on Data Access

CODATA's Working Group on Data Access was established to examine problems, policies, and possible solutions to the issue of international access and exchange of data for scientific research. To begin, and in order to keep the work of the Group focussed, the study concentrated on those problems associated with global change research. The Group held its first meeting at ICSU headquarters in Paris on 8 and 9 March. From left to right: Martine Feissel, Nicole Petit-Marie, Domingo Antonio Gagliardini, David Abir (ex-officio), Bruno Rudolf, Ferris Webster, David Lide, Ichtiaque Rasool, Peter Adeniyi, Michael Chinnery (not in photo: Fedor Kuznetsov) ICSU/CODATA policies on freedom of data exchange, constraints on data access, and datasets critical for scientific research occupied the Group's attention. These issues are particularly important for global change research, where worldwide sharing of environmental data is critical. While endorsing the concept of full and open data access for scientific research, the Group noted that complete access to everything was unlikely to come to pass. There (continued from page 1) are likely always to be constraints on data access for a variety of reasons. At least, it was felt, the scientific community needs to define why access to data is needed. In particular, why does global change science need open access to data in order to progress more rapidly? In a lively and far-ranging discussion, the group discussed the case for and against full and open access to scientific data. A number of points were made that could become elements of an eventual CODATA policy:

- The policy should encourage all levels to make scientific data available.
- No scientist is self-sufficient, but requires data from peers. We reduce cost by sharing.
- Climate does not know national boundaries. Its study requires data from all over the world and will benefit all nations.
- Scientists supported by public money should make their data available without delay after publication. In some cases, the investigator should hold the data until the quality is assured.
- "Full and open" means that not only is there no discrimination in data access, but that the cost is within the reach of scientists in all countries.

In discussing the case for restricting access to data the following points were made:

- Certain types of data may not be appropriate for exchange, for example, high-resolution topographic and bathymetric surveys. On the other hand, such a statement does not take into account the importance of scale: local thunderstorms can have regional impact. Global modelers sometimes want data on a local scale.
- There are commercial and national security restraints against full and open data access.

- Many scientists feel that if they collect a dataset, they have rights over it and often want proprietary rights to data for a period of time.

This final point occasioned considerable discussion. Some Group members argued that it was inconsistent to urge full and open access and yet establish a policy whereby scientists can have proprietary rights for a period of time.

On the second day of the meeting, the Working Group considered Draft Resolution 11.4 (CG-XII) of the World Meteorological Organization entitled "WMO policy and new practice for the exchange of meteorological and related data and products including guidelines on relationships in commercial meteorological activities." This proposed resolution would establish a two-tiered WMO data-access policy and establish constraints on data access for commercial purposes. The Working Group prepared a draft statement to be considered by the ICSU Executive as a basis for an ICSU position at the WMO Congress. In addition, Ferris Webster, the Working Group Chairman, agreed to attend the WMO Congress to present the ICSU position.

Finally, the Group began work on an ICSU statement regarding open access to scientific data and information. The Group, though constituted to look at global change data issues, agreed to develop the first draft of such a statement. It was noted that most aspects of the data access issue are general, and not particular to any discipline. The final version of an ICSU statement should be reviewed to assure its applicability to the many scientific areas represented by ICSU Unions and associations. The goal is a statement that can be disseminated by ICSU on behalf of all scientists.

Members of the Working Group are: Peter Adeniyi (Nigeria), Michael Chinnery (CODATA Executive Committee liaison), David Lide (USA), Martine Feissel (France), Antonio Gagliardini (Argentina), Fedor Kuznetsov (Russian Federation), Nicole Petit-Marie (France), Ichtiaque Rasool (France), Bruno Rudolf (Germany), Ferris Webster (USA, Chairman), and Phyllis Glaeser (CODATA Secretariat). The initial membership of the Working Group was chosen to reflect expertise in global change and the environment. At the same time, problems of scientific data access go well beyond issues in global change. Issues in other scientific fields would probably best be addressed by a rotating Working Group membership that could examine the questions of data access in a series of scientific areas.

Postscript: The resolution on data access adopted by the WMO Congress in June was considerably modified from the draft version seen by the Working Group at its meeting in March. The two-tier categorization of data was eliminated and the resolution urges WMO Members to provide free and unrestricted access to all data and products exchanged under the auspices of WMO to the research and education communities for their non-commercial activities. Moreover, CODATA is preparing Special Report 15 to provide further details on this very important issue.

Materials Database Management

The CODATA *Task Group on Materials Database Management* met at the CODATA Headquarters in Paris on May 9 and 10. It discussed plans to update the *Register of Materials Database Managers* and issue a new edition in June 1996. Initial work on a "Cost-Benefit" study of materials databases was unable to provide the "quantitative" results hoped for so a "bibliography of benefits" from database activities will be compiled in its stead. First row: Dipl.-Ing. A. Brandstätter, Dr. S. Nishijima, Dr. J.-P. Caliste. Back rows: Mr. J.G. Kaufman, Prof. J.-E. Dubois, Mr. H. Kröckel, Mr. W.G. Jackson, Mr. Norman Swindells, Mr. Keith Reynard

The former "Eco-Materials" Project has been renamed "Environmental Interactions of Engineering Materials." The Task Group agreed to look at the ISO Draft on Environmental Management - Life Cycle Assessment (LCA) - "Principals and Guidelines" to determine if it could contribute to the data management aspect, and a position paper is being drafted to look at the possible role of the CODATA Task Group in the matter of LCA data inventory building and maintenance. There is a rapidly emerging focus on life-cycle assessment (LCA) methodology in Europe and the USA. The CODATA Bulletin 69 on Guidelines for Materials Database Management will be examined in view of applying the guidelines to life-cycle assessment inventories.

Concerning quality issues, including those related to Internet quality distribution of data, an updated Code of Practice has been published by the European Union and a joint publication prepared by the EU and CODATA on general data guidelines will be considered. As for STEP (Standard for the Exchange of Product Data) activities, the STEP materials model going into Part 45 of ISO 3030 is nearing completion.

The Task Group reviewed the regional reports submitted by the members. Of particular interest were the EU programs built around the "Information Superhighway," INFO2000 project, part of the Fourth Framework of EU's program "Telematics" which focuses on information engineering. Additionally, the EU is exploring the legal protection of data and databases. RAPRA's RUBBERCAMS database and software, including environmental, health and safety data and a "technology foresight" program (investments needed in the materials industry) are developing in the U.K. A French database directory has been updated by AFNOR and the latest AFNOR book on French data sources may be ordered as ISBN 212380 021 X. The Task Group noted that CODATA now has a home page on the WorldWideWeb. Several NIST databases will soon be available via CODATA as well as on the NIST pages via the Web. An updated list of designations systems by Reynard is underway as well as a joint activity between VAMAS WG10 and WG14 on ceramics.

Lev V. Gurvich, 1927-1995

On August 23, the world of science lost an outstanding member of its community, and CODATA, a cultivated, warm, and sensitive friend, when Prof. L. V. Gurvich, Vice President of CODATA, died of a heart attack at the age of 68.

Born in Baku on March 22, 1927, Prof. Gurvich graduated from the Department of Chemistry of Moscow State University in June 1951, where he obtained his Diploma with work on construction and testing of the first Russian unit for electron diffraction, studying the structure of molecules in high temperature vapors. From 1951 to 1963 he worked at the Institute of Combustible Minerals in the USSR Academy of Sciences. His studies were connected with the investigation of the dissociation energies of simple molecules using flame spectrophotometric techniques. Using the results of this research, in 1957 he presented his PhD thesis to the Science Council of the Chemical Department of Moscow University. In parallel, in 1952, Gurvich began critical analyses of molecular and thermochemical data, as well as calculations of the thermodynamic properties of substances at high temperatures. The results of this work were used for the selection of rocket fuels, and in 1957 when the first Sputnik became operational, L. Gurvich received high honors for this work.

In 1963 Gurvich, with a group of his co-workers, moved to another Institute of the USSR Academy of Sciences--the Institute of High Temperatures--where he continued his work connected with calculations of thermodynamic properties at high temperatures. He developed more accurate methods for calculating the properties of gases based on molecular constants and studied electron spectra of diatomic molecules to obtain these constants. The results of this work were included in the Thesis for the Degree of Doctor of Science presented in 1965 at the Chemical Department of Moscow State University.

In 1966 Gurvich created the Department of Chemical Thermodynamics at the Institute of High Temperatures, with four experimental laboratories (spectra, mass-spectra, electron diffraction, and calorimetry) as well as a laboratory devoted to the calculation of the thermodynamic properties of substances and the preparation of reference books. He was head of this Department from 1966 to 1984 when the Department was renamed the Data Center of the Academy of Sciences on the Thermodynamic Properties of Substances under the leadership of L. Gurvich. The Department and the Data Center fulfilled a number of important studies in the fields of high temperature chemistry, chemical thermodynamics, and molecular structure. The results of these studies were presented by the staff members of this unit at numerous international and national conferences and published in journals. L. V. Gurvich is the author of more than 160 papers and books, including the well known reference book, Thermodynamic Properties of Individual Substances, whose fourth edition was published by CRC Press (in 1984 he, together with co-authors, received the State Prize for this set of 5 books), CODATA books on Key Values for Thermodynamics and on properties of Calcium and its Compounds, books published by IAEA and IUPAC. Under his guidance four databases on thermodynamic properties were created. One of them was presented at the CODATA Conferences in Karlsruhe and in Columbus and is distributed by NIST and CRC Press; two others are included in the program of the Conference in Beijing; and the fourth one at the Chambéry Conference September 1994.

Since 1968 Lev Gurvich has been a Professor at the Moscow Physical Technical University where he lectured on Physical Chemistry of High Temperature Processes. He is a member of the Scientific Council in Physical Chemistry of the Chemical Department of Moscow State University, a member of the Editorial Boards of High Temperature Science, the Journal of Chemical Thermodynamics, Mendeleev Communications, and the Russian Journal of Physical Chemistry.

Prof. Gurvich participated in many national and international scientific activities. From 1965 to 1977, he was a member of the IUPAC Commission I.2 (Thermodynamics), from 1979 to 1987 a titular member of the IUPAC Commission 2.3 (High Temperature and Solid State Chemistry). Prof. Gurvich was consecutively titular member of three CODATA Task Groups, including Chairmanship of that on Key Values for Chemical Thermodynamic Data, a member of the Executive Committee from 1986 to 1988, and CODATA Vice-president since 1988.

Professor Gurvich always said it took at least seven years to train a scientist in critical data evaluation and quietly shared his wisdom with all those he encountered. CODATA extends its sincere condolences to his wife, Lena, and his daughters, Natasha and Olga.

Professor Masao Kotani Memorial Fund

Professor Masao Kotani was an expert in mathematical physics. His earliest paper was on the Rayleigh disk and in the late 1930's he worked on distorted wave calculations of some electron-atom collision cross sections.

With his colleagues he did systematic numerical computation of molecular integrals in the 1940's, before electronic computers were available in chemical physics. They also studied electronic structure and properties of some simple molecules (including H2, Li2, O2, etc.). Then he studied electronic structure in metallic complex where he applied field theory elegantly. Through this research he turned to the studies of hemoproteins. Subsequently, his research activity was focused on biophysical problems.

He established the Biophysical Society of Japan and was nominated as the first President of this Society in 1962. Moreover, he was interested in problems of handling scientific data. The Committee on Data for Science and Technology (CODATA) is said to be one of his children. The famous report on "Accessibility and Dissemination of Scientific Data" prepared under his chairmanship has served as a model for decades.

Professor M. Kotani as born in January 1906 in Kyoto and passed away on 6 June 1993 in Tokyo.

The fund will subsidize young scientists involved in scientific data activities for their expenses to attend the biennial CODATA Conferences as well as to honor the memory of Professor Kotani. The fund was proposed and established by the Japanese National Committee for CODATA with the consent of Professor Kotani's family, and will be operated by a committee composed of the Chairman of the Japanese National Committee for CODATA,

the President of CODATA and the Chairman of the Program Committee for each CODATA Conference. It bears the endorsement of Professor D. Abir (President of CODATA), Dr. G. H. Wood (Secretary General of CODATA), Dr. J. Rodgers (Chairman of Canadian National Committee for CODATA), and Ms. P. S. Glaeser (Executive Director of CODATA).

The fund will aim at a target figure of 15 000 000 yen (about 150,000 U.S. dollars) and will be administered as one of the International Funds in CODATA. Your kind support of the Fund is sought. Such contributions for the fund can be accepted by CODATA Treasurer--James A. Crease, Longdown House, Hindhead Road, Hindhead, Surrey GU26 6BB U.K.--payable to "CODATA". [Alternatively, Japanese donations can be relayed through Professor A. Tsugita, Research Institute for Biosciences, Science University of Tokyo, 2669 Yamazaki, Noda, Chiba 278 Japan.

Japanese National Committee for CODATA
Chairman, Akira Tsugita
(Former Chairman, Kazuo Takayanagi)

Books

Properties of Organic Compounds (Version 4.0) [CD-ROM diskettes plus manual]. D. R. Lide and G. W. A. Milne, editors. [a,b]

Names, Synonyms, and Structures of Organic Compounds. D. R. Lide and G. W. A. Milne, editors.[a,c]

Handbook of Data on Common Organic Compounds. D. R. Lide and G. W. A. Milne, editors. [a,d]

Handbook of Organic Solvents, D. R. Lide, Jr., editor. [a,e] [a,e]

Databases/Software

NIST Standard Reference Database 34, "Lipid Thermotropic Phase Transitions: LIPIDAT2 (Version 2.0)". [f]

Key Guide to Electronic Resources: Agriculture. W. Drew, editor. [g]

Index to Scientific & Technical Proceedings. [h] DASYLab Version 2. [i]

Combined Media

Vapor-Liquid Equilibrium in Mixtures and Solutions Bibliographic Database; Vol. II; EVLM'94. (Supplement to Vapor-Liquid Equilibrium Bibliographic Database, 1993.) I. Wichterle, I. Linek, Z. Wagner, and H. V. Kehiaian, compilers. [j]

Footnotes

[a] CRC Press, Inc., 2000 Corporate Blvd., N.W., Boca Raton, FL 33431-9868 U.S.A. Tel: +1-800-272-7737. FAX: +1-800-374-3401.

[b] This new version for 27,000 of the most commonly sought organic compounds, featuring physical data, spectral data, and structures. Data fields include: CAS Index name and synonym(s), molecular formula, line formula, chemical structure, CAS Registry number, Beilstein reference, molecular weight, melting point, boiling point, density, refractive index, specific rotation, color, solubility, spectral peaks and source references (mass, IR, Raman, UV, and NMR), including data from the NIST Mass Spectral Database.

Catalog no. 446MZL, December 1994, ISBN 0-8493-0446-6. Individual license: $695.00. Includes manual, CD-ROM disk, and installation diskettes.

[c] This reference provides names, synonyms, molecular formulas, and CAS Registry Numbers for 27,500 organic compounds. The compendium contains 135,000 synonyms and 20,000 chemical structures. Compounds are arranged in sequence of CAS Registry Numbers, but they are indexed by Name/Synonym and Molecular Formula.

[d] This reference provides physical property data, spectral data, and chemical structures for approximately 12,000 common organic compounds. These compounds encompass those most commonly used in both industry and laboratories, as well as those found on various lists of regulatory concern. The following information is provided for each compound: general identifiers, physical properties, spectral data (references and major peaks), and threshold limit value. Catalog no. 404 MZK; three-volume set: $995.00; December 1994; c. 2,944 pp.; ISBN 0-8493-0404-0. The Handbook is indexed by CAS Registry Number, Molecular Formula, and Name/Synonym.

[e] This handbook presents important information on over 500 organic compounds that are used as solvents. Health hazards are discussed. This reference contains many useful data fields, such as: refractive index; solubility; spectral data fields; density; vapor pressures; viscosities; critical temperature and pressure; heat capacity; enthalpies of fusion, formation, combustion, and vaporization; flammability data; surface tension; dissociation constants; dielectric constant; dipole moment; and thermal conductivity. Indices includes name/synonym, molecular formulas, CAS registry numbers, and melting and boiling points for all complexes.

Catalog no. 8930MZL; December 1994; c. 450 pp., ISBN 0-8493-8930-5; U.S. $99.95/Outside U.S. $120.00.

[f] LIPIDAT2 is a convenient, sophisticated and centralized source of data on one of the most diverse and important groups of molecules which is the subject of intensive research. This database provides thermodynamic data on complex polar lipids.

LIPIDAT2 contains thermodynamic data on over 900 lipids--enthalpy increments and transition temperatures; complete literature referencing and list of authors through January 1993; data for partially and fully-hydrated lipids; data on the effects of various other additives, such as proteins, drugs, etc.; complete user manual; and over 15,000 records. Price: $315.00; $50.00 to upgrade. Standard Reference Data Program, National Institute of Standards and Technology, 221/A320, Gaithersburg, MD 20899, U.S.A. Tel: +1-301-975-2208; FAX: +1-301-926-0416. E-mail: SRDATA@ enh.nist.gov.

[g] This is part of an ongoing, topic-related series of reference guides, a comprehensive directory of electronic sources of information about agriculture and agriculture-related sciences. Topics covered in the directory include: online databases, CD-ROMS, magnetic tapes and discs, university library online catalogs, various other sources, such as electronic bulletin boards, Listservs, Almanac Servers, and Gopher Servers. 1995; softcover; 124 pp; 8.5" ¥ 11"; ISBN 1-57387-000-5; $39.50. Learned Information, Inc., 143 Old Marlton Pike, Medford, NJ 08055-8750, U.S.A. Tel: +1-609-654-6266; FAX: +1-609-654-4309.

[h] The Index is a CD-ROM that provides access to five years of bibliographic data from international conference proceedings. It covers about 840,000 full papers from 21,000 conferences. An estimated 45,000 papers and 1,100 conferences are added with each quarterly update. Institute for Scientific Information, $1,650.

[i] This is a Windows-based data acquisition, control, and analysis system. This new version includes fast streaming to disk (at rates of over 200 kHz), more options for setting up experiments, and support for more than 100 data acquisition devices. DASYTEC, $995. [j] Probably the most recent and most complete Vapor-Liquid Equilibrium bibliographic reference work with accompanying cumulative diskette, 1900-1993; 168 pp. Vapor-Liquid Database at the following price: full price (1900-1991 Volume and 1992-1993 Supplement) 2750 FF; educational institution (10% discount), 2475 FF; EVLM'94 Cumulative Diskette (1900-1993) Standard License, gratis. 1994 Supplement and diskette (to purchasers of 1993 edition) 550 FF. ELDATA, 81-83, Rue Michelt, 93100 Montreuil, France. FAX: +33-1-4988 3045.

[j] Probably the most recent and most complete Vapor-Liquid Equilibrium bibliographic reference work with accompanying cumulative diskette, 1900-1993; 168 pp. Vapor-Liquid Database at the following price: full price (1900-1991 Volume and 1992-1993 Supplement) 2750 FF; educational institution (10% discount), 2475 FF;

EVLM'94 Cumulative Diskette (1900-1993) Standard License, gratis. 1994 Supplement and diskette (to purchasers of 1993 edition) 550 FF. ELDATA, 81-83, Rue Michelt, 93100 Montreuil, France. FAX: +33-1-4988 3045. ELDATA, 81-83, Rue Michelt, 93100 Montreuil, France. FAX: +33-1-4988 3045.