

# International Council of Scientific Unions Committee on Data for Science and Technology

Number 69 CODATA / NEWSLETTER

DECEMBER 1994

## HIGHLIGHTS

1. CODATA on W.W.W.
2. CODATA's General Assembly
3. Books and/or Databases
4. Thermodata Europe
5. Computerization and Networking of Materials Property Data
6. CODATA Calendar

## CODATA Explores the WWW "Web"

The Internet World Wide Web (Web or WWW) is providing explosively expanding means of access to information around the world. CODATA, with one of its objectives being to improve accessibility to scientific and technical data, MUST exploit-and adapt quickly to-this changing world. As a first step, we have formed a Working Group to assist in the development of a Web site for CODATA. The National Research Council of Canada has offered to host our site on a machine in Ottawa.

The Web address (URL) is -

*<http://www.cisti.nrc.ca/codata/welcome.html>*

We plan to use the site to publicize the work of CODATA and encourage participation by a wider group of scientists. Furthermore it will provide more current and rapid access to the activities, the people, the Task Groups, the Members (National, Union and Affiliate), the Supporting Organizations and the administration of CODATA. A direct mail input to the site will be established shortly. In the meantime, please contact either Jim Crease ([jimc@delocn.udel.edu](mailto:jimc@delocn.udel.edu)) or John Rodgers ([rodgers@snd.cisti.nrc.ca](mailto:rodgers@snd.cisti.nrc.ca)) if you want to contribute to the development of our Web pages.

*--James Crease*

---

The impact of Internet's WWW ("Web") linking computers and scientists in a hypermedia universe capable of communicating research results, dissemination of information and data as well as online conferences adds new dimensions to the electronic conferencing format. It can be a client/server system that enables sharing a unique copy of a file rather than having many copies in multiple locations. For example, the last CODATA Newsletter.

already displayed at the above address has colored photographs which can readily be accessed by a browser (e.g., "Mosaic") to maneuver through the Web and to download.

CODATA's General Assembly Meets in Chambéry



*Most of the General Assembly delegates in session on Sept. 24, 1994.*

## **UNION DELEGATES TO CODATA\***

- I. Astronomical Union (IAU), *Prof. A. Heck*
- I. U. of Geodesy and Geophysics (IUGG), *Prof. C. C. Tscherning*
- I. U. of Pure and Applied Chemistry (IUPAC), *Dr. K. N. Marsh*
- I. U. of Pure and Applied Physics (IUPAP), *Dr. E. R. Cohen*
- I. U. of Biological Sciences (IUBS), *Dr. F. A. Bisby*
- I. Geographical Union (IGU), *Dr. R. F. Tomlinson*
- I. U. of Crystallography (IUCr), *Dr. J. R. Rodgers*
- I. U. of Theoretical and Applied Mechanics (IUTAM), *Prof. D. C. Drucker*
- I. U. of Biochemistry and Molecular Biology (IUBMB), *Prof. Ralph Bradshaw*
- I. U. of Geological Sciences (IUGS), *Prof. R. Sinding-Larsen*
- I. U. of Psychological Science (IUPsyS), *Prof. L.-G. Nilsson*
- I. U. of Pure and Applied Biophysics (IUPAB), *Prof. L. C. M. De Maeyer*
- I. U. of Nutritional Sciences (IUNS), *Dr. John Klensin*
- I. U. of Pharmacology (IUPHAR), *Dr. G. J. Cosmides.*
- I. U. of Immunological Societies (IUIS)
- I. U. of Microbiological Sciences (IUMS), *Prof. R. R. Colwell*

---

\* I=International; U=Union

## **CO-OPTED DELEGATES**

- ICSU Panel on World Data Centers, *Dr. M. A. Chinnery*
- Federation of Astronomical and Geophysical Services, *Prof. P. Melchior*
- I. Council of Scientific and Technical Information, (To be named)
- I. Society of Soil Scientists, *Dr. M. F. Baumgardner*
- World Federation for Culture Collections, *Dr. Hideaki Sugawara*

## **AFFILIATE DELEGATE**

Commission of the European Communities (Directorate-General for Science, Research and Development), *Prof. P. Fasella.*

## **NATIONAL DELEGATES TO CODATA**

- Australia, *Mr. Clyde Garrow*
- Brazil, *Mr. A. L. C. de Miranda*
- Canada, *Prof. H. W. King*
- China, Academy located

in Beijing, *Prof. Xu Zhihong*  
in Taipei, *Dr. Jen Leih Wu*

France, *Prof. J.-L. Delcroix* Germany, *Prof. E. Fluck*  
Hungary, *Prof. László Keviczky*  
India, *Prof. J. C. Ahluwalia*  
Israel, *Prof. Avi Degani*  
Italy, *Prof. Antonio Sgamellotti*  
Japan, *Prof. Akira Tsugita*  
Korea, *Dr. Ki Soo Sung*  
Poland, *Prof. Andrzej Bylicki*  
Republic of South Africa, *Dr. S. F. Rossouw*  
Sweden, *Dr. Göran Falkenberg*  
Russia, *Prof. Fedor A. Kuznetsov*  
United Kingdom, *Dr. G. B. R. Feilden*  
U.S.A., *Dr. Jack H. Westbrook*

A main function of the biennial General Assembly is to receive progress reports from the Commissions, Task Groups (TG) and Working Groups, which do the scientific work of CODATA, as well as applications for new ones, and then to decide which units should be approved for the next biennium. The General Assembly typically meets biennially near the site of the International Conferences described in [CODATA Newsletter No. 68](#).

. Among the prime CODATA goals are the promotion of the evaluation and-in general-the quality control of data as well as the improvement of the methods by which data are acquired, managed, analyzed, and disseminated. To this end the Fundamental Constants TG reviews existing data and plans to complete and publish the next readjustment of fundamental constants by end of 1995. In the area of data that are important to global change, geology, and industry, the Geothermodynamic Data TG continued evaluations and assessments of data relating to sulphides, oxides, and silicates and have a book waiting for publication. The very active Survey of Data Sources in Asian-Oceanic Countries TG is undertaking the establishment of a database on animal viruses as well as surveys of databases dealing with microbes, fish, and environmental protection endeavors in that part of the world.

Means of reducing costs and duplication of effort in data collection, data publishing, database development, and data dissemination are being pursued according to their respective concerns by the Distributed Data Depository Network for Experimental Thermophysical Property Data TG and Electronic Information Transfer Working Group. Following an editorial tour de force, the Commission on Data for Global Change published the proceedings of their workshop on Crop Modeling.

The facilitation of cooperation among those collecting, organizing and using data also involves several TGs. Continuing its record of solid achievement, the Biological Macromolecules TG convened a colloquium (cf. [CODATA Newsletter No. 68](#)).

) bringing together representatives from all the major international genome sequencing projects and provided an active forum for information exchange among the international bioscience databases. Similarly, the Commission on Standardized Terminology for Access to Biological Data worked with groups as diverse as the Federation of Scientific Editors and the IUBS Commission on Plant Taxonomic Databases to encourage policies that will result in more uniform use of terminology and hence easier development of comprehensive taxonomic data networks.

In areas related to health, important gains were made by this Commission as they raised funds for, and collaborated with, the International Committee on the Taxonomy of Viruses and the International Leishmaniasis Network in developing standardized descriptors for viral characteristics and setting up pilot databases respectively.

Scientists from every country in the region with significant scientific activity were brought together at a highly successful meeting (cf. CNL #67) convened by the Survey of Data Sources in Asian-Oceanic Countries TG. Workers from a wide variety of disciplines, who otherwise might never have met, assembled to discuss data issues of common concern and to formulate new, innovative projects. As another example of the cross-fertilization fostered by CODATA-engineers, industrialists, academics, and economists gathered at a workshop on the role of data in decision making in science and technology which was organized by the Artificial Intelligence TG and Computer Graphics TG.



*David R. Lide, Jr. presides over Strategic Planning Meeting in Chambéry.*

An ongoing problem encountered by those associated with any type of data-related data to a given goal is having a means of quantifying the value of data to that endeavor. Towards that end, the Materials Database Management TG completed a cost/benefit survey and a preliminary analysis of the results. In service to ICSU, the Commission on Standardized Terminology for Access to Biological Data continued its important work in raising the awareness level within the bioscience unions and other international scientific organizations of the need for standardized terminology and nomenclature for data collection and management of biological inventories and surveys. Finally, the Industrial Data Commission and the Distributed Data Depository Network for Experimental Thermophysical Property Data TG both hosted workshops aimed at making their respective communities more conscious of data activities and their relevance.

In summary, it was made evident in the discussion that these working units generally enjoyed a productive biennium. Since CODATA is an organization operating primarily through volunteers and suasion such results are to be applauded. In addition, some pride may be taken in that the aggregate leveraged value of activities is estimated to be about ten times the actual amount expended from CODATA's budget.



*J. Crease Treasurer, President D. Abir, and G. H. Wood Secretary General manage the General Assembly in Chambéry.*

Delegates representing the Scientific Union, National, Co-opted, and Affiliate Members of CODATA approved those Commissions and Task Groups which had requested renewal along with two new Task Groups-Global Plant Checklist Network and Thermodynamic Data for Key Chemical Substances. In addition, the establishment of the Working Group on Data Access, initiated previously by the Executive Committee, was formally ratified thus bringing to eleven the number of Task Groups and Commissions for 1995-96 as reported in detail in CODATA Newsletter No. 68.

The work of the General Assembly is sometimes done, in specialized committees as the meeting of the Strategic Planning Group at Chambéry. Their program was described in [CODATA Newsletter No. 68](#).

## Books and/or Databases

*Trends '93: A Compendium of Data on Global Change*, T. A. Boden, D. P. Kaiser, R. J. Sepanski, and F. W. Stoss, eds.

This large format ca. 1000 page volume (ORNL/CDIAC-65) provides synopses of frequently used global-change data. This third issue of the Trends series presents historical and modern records of atmospheric concentrations of carbon dioxide, methane, nitrous oxide, two chlorofluorocarbons (CFC-11 and CFC-12), a hydrochlorofluorocarbon (HCFC-22), and two halon (H-1301 and H-1211) from an expanded number of globally distributed data sets. Additional trace gas data presented in Trends '93 include historical atmospheric CO<sub>2</sub>, CH<sub>4</sub>, and N<sub>2</sub>O records derived from ice cores. Trends '93 also includes revised and updated estimates through 1991 for global, regional, and national CO<sub>2</sub> emissions produced from the burning of fossil fuels, gas flaring, and the production of cement.

In addition, *Trends '93* updates and expands the presentation of long-term temperature records, whose spatial coverage ranges from an individual Antarctic (ice core) site to the entire globe and from the Earth's surface to the lower stratosphere. New subject matter appearing in Trends '93 includes a chapter for long-term regional precipitation records, several time-series records for atmospheric aerosols, and isotopic <sup>14</sup>C measurements for atmospheric CO<sub>2</sub> from several sites.

All data appearing in *Trends '93* are available on digital media from the Carbon Dioxide Information Analysis Center (CDIAC). This report and all other electronic versions of the data contained in the report are available from CDIAC at no cost.

For further information: World Data Center-A for Atmospheric Trace Gases, Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, P. O. Box 2008, Oak Ridge, Tennessee 37831-6335.

*Intelligent Information Retrieval: The Case of Astronomy and Related Space Sciences*, A. Heck and F. Murtagh, eds.

Intelligent Information Retrieval comprehensively surveys scientific information retrieval, which is characterized by growing convergence of information expressed in varying complementary forms of data/textual, numerical, image, and graphics; by the fundamental transformation which the scientific library is currently being subjected to; and by computer networking which has become an essential element of the research fabric. Intelligent Information Retrieval addresses enabling technologies, so-called 'wide area network resource discovery tools', and the state of the art in Astronomy and other sciences. 1993, 220 pp., hardbound, US\$89.50, ISBN 0-7923-2295-9.

*Three Views of the Internet*, A. M. Cunningham and W. Wicks, eds.

The recent excitement generated by the particular networking marvel known as the Internet prompted the National Federation of Abstracting and Information Services (NFAIS) to prepare a report on the implications of this growing network phenomenon for the information community. NFAIS took the lead in addressing the perceived impacts of this high-capacity network on database publishers, distributors, and networkers by organizing a compelling Internet program at its 1993 Annual Conference and publishing this timely report, which includes Internet resources, user interface, acceptable use policy, data security, privacy, intellectual property rights, pricing, public policy frameworks, licensing, and standards, both the contributors' position papers on networking issues and the conference proceedings and discussion. 1993, ISBN 0-942308-42-5.

*Thermodynamics of Organic Compounds in the Gas State*, by M. Frenkel, G. J. Kabo, K. N. Marsh, G. N. Roganov, and R. C. Wilhoit.

Complete and comprehensive book on the thermodynamic properties of organic compounds in the ideal gas-phase state. The introductory chapter discusses theoretical considerations of the problem concerned with statistical-mechanical calculations of thermodynamic functions for organic substances, including

- Contributions resulting from different molecular motions (translational, vibrational, external rotational, internal rotational)
- Conformational composition and its effect on thermodynamic properties
- Tautomeric composition and its effect on thermodynamic properties
- Error analysis

Some other related problems considered are additive methods of calculation and methods of thermodynamic analysis of complex chemical equilibria.

The book contains about 1200 tables of thermodynamic values as functions of temperature for the ideal gas state. They include only values obtained by statistical or additive-statistical methods. Comments to the tables contain information on the spectral data used, related experimental results, previous calculations, etc.

Data for more than 200 compounds (800 of which were obtained by correlation methods) are fitted by the methods developed by the authors to give the best possible polynomial and non-linear function of temperature. The coefficients of the polynomials are conveniently summarized, allowing their incorporation into different databanks and simulation packages. The coefficients are also provided in an IBM PC diskette distributed with the book.

The Scientific Group Thermodata Europe Group, SGTE

The Scientific Group Thermodata Europe, SGTE, was established under French law in 1979 as a consortium engaged in the development of high quality thermodynamic databases for inorganic and metallurgical systems of all types and in the application of those data to a wide range of problems in materials technology. SGTE members have unique experience and expertise in the modelling and thermodynamic evaluation of solution phases and the SGTE solution databases are regularly being used by the metallurgical industry to guide such processes as alloying, casting, slag-metal refining, heat-treatment, etc. for multicomponent systems.

The SGTE Pure Substances Database contains evaluated thermodynamic data for over 4000 condensed and gaseous substances. The data for all substances are stored as the enthalpy of formation and standard entropy at 298 K together with heat capacities and transformation enthalpies for higher temperature ranges. Integration of these values yields the Gibbs energy function.

The SGTE Solution Database contains evaluated thermodynamic data for over 150 binary, some 70 ternary, and about 20 higher-order systems. The phases of the different alloy-, oxide-, salt-, etc. systems concerned have generally been modelled in such a way as to realistically represent the atomic structure involved. This often implies use of the sub-lattice model, in which the occupation of the different lattices by atoms (or ions) and vacancies as a function of composition and temperature is reproduced by the thermodynamic description.

SGTE members carry out joint research contracts using the databases in conjunction with their own software, and generally with the specific aim of further developing the databases to allow thermodynamic calculations to be made for specific areas of materials technology. Thus, for example, SGTE data and SGTE members have played an important role in projects concerned with providing a thermodynamic basis for the production of high-temperature oxide superconductors, the development of light metal alloys, in investigating the possibility of using substitute elements in alloys, in developing a thermodynamic software interface for process simulation, and in simulating selected materials processes, etc.

SGTE databases are available world-wide via the members or their agents both online and in the form of packages for use with mainframe or PC computers. At the same time, SGTE is cooperating in a broader international effort, including CODATA activities, to unify thermodynamic data and assessment methods.

A book, in which practical case studies treated by SGTE members using thermodynamic calculation techniques in association with SGTE databases are presented, will shortly be published as an illustration of the power of computational thermochemistry in investigating materials problems of many different types.

The member organisations of SGTE are:

**France:** Institut National Polytechnique (LTPCM), Grenoble, and Association THERMODATA, Grenoble; IRSID, Maizières-les-Metz.

**Germany:** Rheinisch-Westfälische Technische Hochschule (LTH), Aachen; MPI für Metalloforschung (PML), Stuttgart.

**Sweden:** Royal Institute of Technology (Materials Science), Stockholm United Kingdom: National Physical Laboratory (MTDATA), Teddington and AEA Technology, Harwell.

The SGTE can be contacted through its Chairman, Philip J. Spencer, Institut für Theoretische Huttenkunde, Rheinisch Westfälische Technische Hochschule Aachen, D-5100 Aachen, Germany. Tel.: +49 241 805971/84. Fax: +49 241 8888295.

--*Philip Spencer (Chairman)*

1994 CODATA Books

#### CODATA MONOGRAPH SERIES

Vol. 2 CODATA Directory of Data Sources in Asian-Oceanic Countries Y. Hu and E. F. Westrum, Jr. - Editors  
208 pp. Softbd. \$33

#### CODATA PROCEEDINGS SERIES

Vol. 1 Data Sources in Asian-Oceanic Countries; DSAO, Taipei, 1994 J-L. Wu, Y. Hu, and E. F. Westrum, Jr. - Editors 318 pp. Softbd. \$39; Hardbd. \$72

Vol. 3 Database Developments in Asian-Oceanic Countries; DSAO, Beijing, 1992 Y. Hu and E. F. Westrum, Jr. - Editors 176 pp. Softbd. \$33

Prices in US\$ and are postage prepaid. Order from CODATA Paris Secretariat or Ann Arbor "Outpost". Address and contact numbers at end of newsletter.

#### Computerization and Networking of Materials Property Data

The Fifth International Symposium on Computerization and Networking of Materials Property Data, cosponsored by ASTM Committee E49 on Computerization of Material and Chemical Property Data and the National Research Institute for Metals (NRIM) will be held November 6-8, 1995 at NRIM in Tsukuba Science City, Japan.

Since its formation in 1986 the ASTM Committee E49 has been working extensively, in concert with the other international groups such as CODATA and VAMAS, on the development and dissemination of computerized materials information. Much work has focused on the computerization and networking of materials property data; quite a number of databases and data systems for materials have been built worldwide.

The quantity and quality of such data resources are evoking drastic changes not only to utilization of materials information for research and development but also to decision making based on the shared information in a global and dynamic society. More serious evaluation of compiled information is now taking place through dynamic interactions between large databases and robust knowledge implementations. Increased transparency of the software to the complexities of materials would lead to greater reliability of data as well as meaningful utilization of materials.

Papers on global sharing of materials information for research, development, and decision making on the following topics are to be featured:

- 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
- economic impact of computerized materials information systems
- possibility of hypermedia to describe the complexity of materials and their behavior
- specialized materials information toward perfect engineering
- role of materials data systems in the interplay between computation and experiment.

More information is available from Symposium Chairmen

1. Dr. Satoshi Nishijima, National Research Institute for Metals (NRIM), 1-2-1 Sengen, Tukuba 305, Japan, Tel: +81-298-53-1000, FAX: +81-298-53-1005, Email: nishijima@nrim.go.jp.
2. Professor Shuichi Iwata, Prof. of Life Cycle Engineering, 4-6-1 Komaba, Meguro-ku, Tokyo 153-8904, Japan RACE, the University of Tokyo, (Ph.:+81-3-5453-5884/+81-3-5841-6985, Fax:+81-3-3467-0648/+81-3-5841-8621, Email: iwata@race.u-tokyo.ac.jp)

## CODATA Calendar

1995

March

- |     |   |
|-----|---|
| 5   | Publications Committee. Paris, France       |
| 6-7 | CODATA Executive Committee. Paris, France   |
| 8-9 | Working Group on Data Access. Paris, France |

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 |
|-----|---|

Editor:

Edgar F. Westrum, Jr.,  
 Department of Chemistry,  
 University of Michigan,  
 Ann Arbor, MI 48109-1055.

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

Published four times per year (February, May, August, November). Assistance in dissemination provided by National Committees.

---