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

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HIGHLIGHTS

CODATA Task Group on Thermodynamic Data for Key Chemical Substances

The CODATA Task Group on Thermodynamic Data for Key Chemical Substances met in Paris at the CODATA Headquarters on 26-27 October 1995. The purpose of the meeting was three fold: (1) develop a long range generic plan to continue the work started by Professor Lev Gurvich, (2) implement a short term program to critically evaluate, recommend, and publish thermodynamic values for key chemical substances in a reasonable and effective time scale, and (3) clearly state the rationale for each study conducted by the participating parties. Those Task Group Members in attendance included Imo Ansara, Mal Chase, Erik Cordfunke, Rudy Konings, Philip Spencer, and Volodya Yungman, as well as Phyllis Glaeser and CODATA President Jacques-Emile Dubois. After a minute of silence in memory and honor of Lev Gurvich, and a tribute to him by Dr. Yungman, the meeting began with a presentation of each attendee stating the role which they thought was appropriate for their home organizations.

[PICTURE HERE] L to R.: I. Ansara, P. J. Spencer, E. H. P. Cordfunke, M. Chase, V. Youngman, R. Konings

After a lengthy discussion as to possible avenues of activity for the group, technical discussion ensued in which the group analyzed a preliminary interpretation of the thermodynamic data for Sr (cr, l, g) and SrO (cr, l) as a function of temperature, and Sr2+ (aq), as prepared by the staff at the Institute of High Temperatures in Moscow. Similarly, they discussed a preliminary interpretation of the thermodynamic data for Ba (cr, l, g) and BaO (cr, l) as a function of the Research Foundation in Petten. Plans were developed to improve this preliminary analysis, to exchange pertinent information for the possible inclusion of the thermodynamic properties of SrCl2 (cr, l) and BaCl2 (cr, l). In addition, plans were made to extend the program to the analysis of other elemental systems, e.g., indium, lanthanum, platinum, ruthenium, and tellurium, together with data on an oxide, halide, and aqueous ion, and perhaps a halide. The choice of the particular species is to be determined by the organization performing the initial study. The intent is to prepare recommended (or in some cases only best or preferred) values and publish them in a CODATA Special Report. After further review, the results would be collected together into a CODATA Monograph. This Task Group has set as its goal the steady addition of evaluated data to the book, - CODATA Key Values for Thermodynamics+ by Cox, Wagman, and Medvedev, by adding temperature dependent information as well as confirming that the data in the book are still valid. As part of the evaluation, the Task Group will provide insight into the need for experimental or theoretical data

significantly improving the quality of the recommended, as well as the experimental difficulties which might be encountered. Dr. Malcolm Chase was selected to replace Professor Gurvich as Chairman.

ELDATA: Int. J. Physico-Chem. Data

Henry V. Kehiaian, honored in CODATA Newsletter No. 71 with a "Kudo" and in Domas de Maria, Sardinia with a banquet, has pushed back the publishing frontiers once again with an innovative scheme that will benefit physico-chemical data generally and thermophysical/thermochemical data particularly. ELDATA now publishes: Ñ Bibliographic Database on Vapor-Liquid Equilibrium in Mixtures and Solutions Ñ Journal (alias ELDATA: The International Electronic Journal of Physico-Chemical Data) while in preparation are: Ñ Bibliographic Database on Heats of Mixing and Solution Ñ Numerical Database on the Properties of Pure Gases and Mixtures from the Virial Equation of State. All the publications appear (or will appear) in both a printed version (book) and in an electronic version (diskette). The common feature of all the ELDATA Publications is that each one may be used separately or in association with any of their other Publications (Integrated Databases). This is possible by the application of consistent nomenclature and codification rules for Physico-Chemical Properties, Chemical Systems, and References, in the bibliographic information, and in the Standardized Data File Formats used for the numerical information. All the Databases can be accessed with the same search program. [PICTURE HERE] Dr. Henry Kehiaian demonstrating ELDATA on Sardinia. Each Bibliographic Database covers a given Group of Physico-Chemical Properties and contains References to the experimental data published in the literature. The printed version of the Database provides the most convenient means of locating References, if any, for a well-defined Chemical system when all the components are specified. The electronic version allows the user to Retrieve or View on the computer screen, Print, or Save as an external ASCII File, the required bibliographic information in a variety of ways. The Bibliographic Databases are updated yearly and distributed in the cumulative electronic version and also in the accompanying printed Supplement. Cumulative printed versions will be published at intervals of several years. The ELDATA Journal publishes papers reporting essentially original physico-chemical property data obtained by experiment. Original compilations of selected and assessed, good quality, literature data, as well as recommended data obtained by careful analysis of the experimental data, if available, and/or by using well established predictive methods are accepted for publication. Dr. Kehiaian thanks the Institute of Topology and System Dynamics of the University of Paris 7 - CNRS and its former Director, Prof. J. E. Dubois (President of CODATA), as well as its present Director, Prof. P. C. Lacaze, for continued support and encouragement. He also acknowledges the assistance of his wife, Dr. C. Kehiaian, for her invaluable contributions to his editorial activities for several decades.

Korea

The Korea CODATA Committee is made up of the following people:

Honorary National Delegate: Ki Soo Sung [President, Dong Myong Information Technology University]

Chairman: Mu Shik Jhon [Professor, Korea Advanced Institute of Science and Technology];

National Delegate: Jin Hyung Kim [President, Korea Research & Development Information Center];

Vice-Chairman: Young Kyu Yang [Director, Artificial Intelligence Division, Systems Engineering Research Institute, KIST];

Secretary: Yeon Dae Chung [Senior Research Scientist, Software Engineering Division, System Engineering Research Institute, KIST];

Members; Moon Hi Han [Senior Research Fellow, Korea Research Institute of Bio Science and Bio Technology] Sung-Kee Chung [Professor, Chemistry Department, Pohang University of Science &

Technology] Sin Chul Bae [Professor, Mechanical Engineering Department, Dan Kook University]

Education for Internet Use in China

When China registered on the Internet in May 1994, only two leased lines of 64 Kbps linked with it: one from the National Computing and Networking Facility of China (NCFC), another from the Institute of High Energy Physics (IHEP). Both are institutes of the Chinese Academy of Sciences (CAS). The NCFC is the largest computer network in China, set up in 1990 in Zhongguancun area of Beijing with financial support of 70 million yuan ($8.2 million) from the World Bank loans and the State Planning Commission. It is composed of a backbone network of 100 Mbps and three campus networks (CASnet, PUnet and TUnet) linking more than 30 institutes of CAS, Tsinghua University, and Peking University in this area, including 700 minicomputers and work stations, and more than 2,000 PCs. (The WWW server of CODATA-China is located on the NCFC.)

In 1995 China added another four leased lines linking Internet. People have shown great enthusiasm for the primary form of information highway, especially in scientific and educational circles. Many information networks are under development, e.g., the economic information networks and China Education and Research Net (CERNet). To help a large number of scientists and educators to rapidly master the use of Internet, CODATA-China is organizing a training program under the support of the High-Technology Research and Development Center of the State Science and Technology Commission. The Laboratory of Computer Chemistry (LCC) of CAS, in cooperation with the IHEP, will operate the training program starting in mid-December, 1995. Moreover a book, Internet System and Its Resources, written by the scientists of the LCC, will be published (in Chinese) soon. Hu Yaruo (Beijing)

Environmental Protection

Regularly organized each year since 1984 by the Technical Committee on CSEP of the German Computer Society, the International Symposium on Computer Science for Environmental Protection was co-organized in cooperation with ICSU-CODATA in 1995 after the contact initiated by Horst Kremers during the 1994 CODATA International Conference in ChambÄry. More than 390 authors and/or co-authors contributed to the Proceedings on Space and Time in Environmental Information Systems [see Books]. The Symposium, conducted both in German (56 papers) and in English (43 papers) was held at the Technical University of Berlin. The participants and co-authors were mainly from Germany (300), other Western European countries (58), Russia (26), the American continent (4), and Africa (2).

Among the opening keynote lectures, Prof. J.-E. Dubois presented the ICSU-CODATA missions and activities. CSEP'95 focused on various problems related to the environment, modeling, retrieval systems, databases, and networks. The main fields discussed during the Meeting were:

- Space and Time in Environmental Information Systems (18 papers) Ñ
- Environmental Impact Analysis (3 papers) Ñ
- Soil and Agro information (5 papers) Ñ
- Atmosphere (8 papers) Ñ
- Simulation and Modeling (9 papers)
- Meta Information (8 papers)
- Computer-Based Environmental Education (5 papers)
- Municipal Environmental Information Systems (13 papers)
- Data Highways and Networks (4 papers)
- Visualization (3 papers)
- Neural Networks (3 papers)
- Fuzzy Logic (6 papers)
- Production Processes (10 papers)
- Environment, Health and Information (3 papers)

The Poster Session embraced:

- Central and Eastern European Atlas of "Avoidable Death" CEEAAD
- Gilbert Projection and Gilbert Globe
- Wind Energy Utilization in Estonia
- Computer Aided Mapping of Landscape by Geoinformatics: Caucasus Case study
- Vegetation Survey using GIS in Greenland
- Water and Air Quality Maps from the Berlin Environmental Atlas

This clearly shows that this year a relative lower priority was given other important environmental topics such as water resources and pollution, domestic and industrial wastes, soil remediation, and legislation. The Symposium also showed the wide utilization of GIS systems together with overlapping maps to present data. These maps appear to be a natural media support to visualize and display computerized data. Several new insights were suggested and discussed and various needs were expressed for future developments. Another observed trend shown at this meeting was that GIS and commercial database software do not presently cover all user needs, especially when using the Internet World Wide Web network. New conceptual developments and realizations are being developed to make advanced information systems more efficient. Most user tools are developed using high level programming languages or systems such as NEXT, object oriented procedures, HTML, Oracle or Arc Infostructures.

There were extensive discussions on metadata structures and concepts concerning text analysis and data. This approach shows that much progress on meta information for information system structure, accessibility, and on the +meaning+ as well as the quality of information is needed for the future. The plenary lectures on data diffusion and special considerations were focused on needs for developing easy user interfaces on the Internet Web Network. Both presentation and computer dissemination were considered in research results of worldwide coverage in health science and epidemiology. The French CODATA delegation presented a methodological matrix based approach for accessing valuable information and URL (Uniform Resource Locators) on the Internet Web Network. Examples were presented of environmental studies and GIS systems. Several CODATA members participated in CSEP'95: E. Fluck, C. Bardinet, J.J. Royer, and J.-E. Dubois.

Information Systems available on the Internet

Several environmental information systems developed by European Agencies or Universities are now accessible on the Internet through various URL, including the following:

- USGS-Reston (Dr. J. A. Kelmelis) http://edcwww.cr.usgs.gov/sast-home.html
- Informatic frei.univ.Berlin (Dr. Agnes Voisard) http://www.inf.fu-berlin.de/voisard
- SEPAN Bremerhaven http://www.awi-bremerhaven.de/
- The CSEP Technical Committee: http://miserv1.kfk.de/Fachgruppe/GI/
- Thomas Blaschke http://www.llnl.gov/liv_comp/metadata
- Claude Bardinet: GIS system of the French Ecole Normale Superieur http://mercator.ens.fr
- Philippe Tarroux: Bio informatic research group on neural network, vision, and animal behavior http://www.ens.fr/bioinfo/www/index.html
- The European Climate Support Network (ECSN) has developed a Working Group on Data Exchange and Management accessible through: http://www.dkrz.de/ecsn/docs/ecsn.wg.html

Fundamental Constants - CODATA

While the Key Values Task Group prepares their next report, some interim reports that may be useful are listed below.

- "Changes in the Fundamental Constants-Past and Future," E. Richard Cohen, IEEE Trans. Instrumen. & Meas. 38(2), 167-171 (1989)
- "Recommended Values of the Fundamental Physical Constants: A Status Report," Barry N. Taylor, J. Res. Natl. Inst. Stand. Technol. 95, 497-523 (1990)

- "How Accurate are the Josephson and Quantum Hall Effects and QED?" Barry N. Taylor and E. Richard Cohen, Phys. Lett. A 153(6,7), 308-311 (1991)
- "The Status of the Fundamental Constants-1992," E. Richard Cohen and Barry N. Taylor, Inst. Phys. Conf. Ser. No. 132, Section 9, pp. 969-977 (1992) [6th Int. Conf. on Nuclei Far From Stability and 9th Int. Conf. on Atomic Masses and Fundamental Constants, Bernkastel-Kues]

International Property Rights

A large part of the one-day technical session of the 1995 General Assembly of ICSTI was devoted to the contentious question of intellectual property rights in the context of the emerging Global Information Infrastructure-the information superhighways. The relevant presentation by Dr. Harold Schoolman, of the U.S. National Library of Medicine, on the U.S. working group in charge of examining the intellectual property implications of the National Information Infrastructure and the impact on the U.S. Copyright Law, aroused considerable interest. This can be read in the ICSTI FORUM 21, September 1995, pp. 3-7 (ISSN-1018-9580).

ICSTI Elects New Boards

At its 1995 General Assembly held at the European Patent Office, Rijswijk, the Netherlands, the International Council for Scientific and Technical Information (ICSTI) made the following elections to its Executive Board for the period 1995-1998: President, David RUSSON, the British Library, UK; Vice-President, Ben FOUCHâ, CSIR, South Africa; General Secretary, Claude PATOU, INIST, France; and Treasurer, John REGAZZI, Engineering Information, USA.

The other elected members of the Executive Board are: CODATA (to be represented by David R. LIDE, Jr., USA and by Keith REYNARD, UK); The Royal Society of Chemistry, UK; BIOSIS, USA; Chemical Abstracts Service; Canada Institute for Scientific and Technical Information (CISTI); Elsevier Science; European Patent Office; and U.S. Department of Energy.

Questel-Orbit, France, has been coopted. Bob BARâ of the European Patent Office was reappointed Chairman of the Technical Activities Coordinating Committee. ICSTI, affiliated with the International Council of Scientific Unions, is dedicated to increasing awareness of and accessibility to scientific and technical information.

Books and Databases

- Space and Time in Environmental Information Systems. Horst Kremers and Wener Pillman, eds. [a]
- Multilingual Thesaurus of Geosciences, 2nd edition. J. Gravesteijn, C. Kortman, R. Potenza, and G. N. Rassam, eds. [b]
- ProCite in Libraries. Applications in Bibliographic Database Management. Deb ReneÄ Biggs, ed. [c]
- Key Guide to Electronic Resources: Engineering. Melissa McBurney, ed. [d]
- Vapor-Liquid Equilibrium in Mixtures and Solutions Bibliographic Database, 3rd edition. I. Wichterle, J. Linek, Z. Wagner, and H. V. Kehiaian, eds. [e]
- ELDATA: The International Electronic Journal of Physico-Chemical Data. H. V. Kehiaian, editor-in-chief. [f]

CODATA Books

Data Access. CODATA Special Report Series, Number 15. [g]

Footnotes

[a] Two volumes totalling 880 pp, distributed during the 1995 CSEP Symposium in Berlin [see page 5] (about evenly split between German and English language texts). ISBN 3-89518-061-0. 118 DM plus postage and handling. Metropolis-Verlag GmbH, Postfach 1748, D-35007 Marburg, Germany.

[b] This new, expanded version of the Multilingual Thesaurus contains 5,847 key terms expressed as descriptors or non-descriptors in six language versions (English, French, German, Russian, Spanish, and Italian). The terms are classed in 37 groups or fields, 20 of which correspond to major subdivisions of geoscience such as structural geology and geochemistry; 11 concern the systematic parts of classification domains such as stratigraphic units and fossil groups; and 5 distinct fields describe concepts such as methods and properties, common to all geoscience subfields. A new special field containing 1,076 terms is devoted to geography. Additions and deletions in this new edition (first edition 1988) were based on term frequency and usage analysis in existing bibliographic databases. A total of 624 key terms covering general and non-systematic geoscience concepts were deleted, and 575 new key terms were accepted for the new edition. Additionally, many new terms were introduced in specific "systematic" fields related to mineralogy, paleontology, petrology , extraterrestrial geology, stratigraphy, and soil science, as well as in chemistry and economic geology. Sponsored by the International Council for Scientific and Technical Information (ICSTI) and International Union of Geological Sciences (IUGS).

1995, 645 pp, hardcover, ISBN: 1-57387-009-9, $99.00, Information Today, Inc. (formerly Learned Information, Inc.), founded in 1979, 143 Old Marlton Pike, Medford, NJ 08055-8750, USA. Tel: +1-609-654-6266; FAX: +1-609-654-4309.

[c] ProCite uses data-entry templates based on the format of the cited work. Hence, there is a template for monographic citations, one for serial citations, one for musical scores, one for maps, and so forth. Among the standard data elements available in a template are strictly librarian-type fields such as ISBN, ISSN, and call number. ProCite, from Personal Bibliographic Software of Ann Arbor, Michigan is the only software developer of this type of program that has designed software to download citations from an integrated online library system. 1995, 221 pp, hdbd., ISBN: 0-938734-90-3, $39.50. Information Today, Inc. (see [b]). [d] This volume, part of the ongoing topic-related series of reference guides, is an evaluative directory of electronic reference sources in engineering. Each chapter provides details on where and how to access these sources. Topics covered in the directory are divided into specific chapter headings as follows: Online Databases, CD-ROMs, Locally Loaded Databases, Library OPACs, Bulletin Board Systems, and Electronic Journals.

1995, 196 pp, softbound, ISBN: 1-57387-008-0, $39.50. Information Today, Inc., (see [b]).

[e] The most recent and the most complete Vapor-Liquid Equilibrium bibliographic reference work with accompanying (gratis) cumulative diskette, 1900-1994. Full price (1900-1991 Volume and 1992-1994 Supplement) 2750.00 FF; Educational institution (10% discount) 2475.00 FF. Further details on licensing, delivery, charges, etc. may be obtained from ELDATA, 81-83, Rue Michelet, 93100 Montreuil, France. FAX: +33-(1)-49-88-30-45.

[f] Editorial Office: Institut de Topologie et de Dynamique des SystÅmes, UniversitÄ Paris VII - CNRS, 1 rue Guy de la Brosse, 75005 Paris, France. Published and distributed by ELDATA SARL, 81-83 rue Michelet, 93100 Montreuil, France. (A list of commercial prices as well as academic discounts are available from the Editorial Office.) [See also page 2 this newsletter.] [g] Summary of Initial Meeting of the CODATA Working Group on Data Access. Published Sept. 18, 1995. 20+8 pp (No ISSN number). (In short supply; contact Secretariat).

CODATA Calendar

1996 January

24-25 CODATA Task Group on Materials Database Management. Paris, France

March

- 17 CODATA Officer's Meeting. Paris, France
- 17 CODATA Publication Advisory Board Meeting. Paris, France
- 18-19 CODATA Executive Committee Meeting.Paris, France

September

Prior to CODATA Task Group on the Survey of Data Conference

Sources in Oceanic Countries. Tokyo Conference University Sanjo-Kaikan, Tokyo, Japan [Contact person: Prof. M. Tasumi (tasumi@tansei.cc.u-tokyo.ac.jp) Fax +81-3-38142627]

- 28-29 CODATA Task Group on Biological Macromolecules. Tokyo University Sanjo-Kaikan, Tokyo, Japan [Contact person: Dr. T. Kunisawa (kunisawa@jpnsut31.bitnet) Fax +81- 475-221544]
- 29 -Oct. 3 International CODATA Conference. Tsukuba, Japan

October

- 1 CODATA Working Group on Electronic Information Transfer (1000 to 1600), organized by Prof. E. Fluck & Dr. J. R. Rodgers. Tsukuba, Japan [Contact person: Prof. S. Iwata (iwata@race.u-tokyo.ac.jp) Fax +81-3-34670648
- 3 CODATA Commission of Standardized Terminology for Access to Biological Data Banks (1300-1800), organized by Dr. F.A. Bisby. Tsukuba, Japan [Contact person: H. Sugawara (sugawara@viola.riken.go.jp) Fax +81-484-624618]

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