

25 CODATA / NEWSLETTER

April 1983

CODATA ELECTS NEW EXECUTIVE COMMITTEE -

PLANS 'FUTURES' WORKSHOP IN JUNE

Dr. W. W. Hutchison, presently the Assistant Deputy Minister for Earth Sciences at the Canadian Ministry of Energy, Mines and Resources, was unanimously elected President of CODATA for the period 1982-1986 at the last CODATA General Assembly in October 1982 in Poland. Dr. Hutchison, a geologist, former Secretary General of the International Union of Geological Sciences, has been long associated with CODATA as IUGS delegate and later as member of the CODATA Executive Committee.

Dr. David R. Lide, Jr., Chief, Office of Standard Reference Data of the National Bureau of Standards, Washington, D.C. and outstanding molecular spectroscopist, was elected Secretary-General for the same period. The composition of the new Executive Committee is as follows:

President:	Dr. W. W. Hutchison (Canada)
Past President:	Prof. Masao Kotani (Japan)
Vice-President:	Prof. Jacques-Emile Dubois (France)
Secretary General:	Dr. David R. Lide, Jr. (USA)
Treasurer:	Dr. David G. Watson (U.K.)
Members:	Prof. Alain Bussard (IUIS)
	Prof. Andrzej Bylicki (Poland)
	Dr. E. Richard Cohen (IUPAP)
	Dr. Harald Haendler (IUNS)
	Prof. C.N.R. Rao (India)
	Prof. Wolfgang Schirmer (G.D.R.)
	Prof. V.V. Sytchev (U.S.S.R.)
	Prof. E.F. Westrum, Jr. (IUPAC)



W.W. Hutchison



D.R. Lide, Jr.

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

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

One of the new President's first actions was to call for a Workshop to review the past activities of CODATA and to discuss how it can best serve the needs of science in the next 15 years. The Workshop is scheduled to be held in La Gaillarde, France on 26-28 June 1983 and will be immediately followed by a meeting of the new Executive Committee.

At the same General Assembly, the following Task Groups and Working Groups were approved for the period 1982-1984:

- Accessibility and Dissemination of Data (Chairman, Mme A. David, France)
- Biothermodynamic Data (Chairman, Prof. H. J. Hinz, F.R.G.)
- Chemical Thermodynamic Tables (Chairman, Dr. Howard White, U.S.A.)
- Computerized Data Handling (Chairman, Prof. Jacques-Emile Dubois, France)
- Critically Evaluated Phase Equilibrium Data (Chairman, Prof. A. Bylicki, Poland)
- Data for the Chemical Industry (Chairman, Dr. Calvin Spencer, U.S.A.)
- Data for Environmental Needs (Chairman, Prof. Nikolai Rambidi, U.S.S.R.)
- Fundamental Constants (Chairman, Dr. E. Richard Cohen, USA)
- Gas Phase Chemical Kinetics (Chairman, Dr. Alistair Kerr, U.K.)
- Hybridoma & Monoclonal Antibodies Data Bank (Chairman, Prof. Alain Bussard, France)
- Multisatellite Thematic Mapping (Chairman, Dr. J.P. Monget, France)
- Property Data on High Pressure Phases (Chairman, Prof. J. Osugi, Japan)
- Standardization of NMR & Photoelectron Spectroscopy (Prof. C.N.R. Rao, India)
- Data for Surveillance of Active Volcanoes (Chairman, Prof. M. Carapezza, Italy)
- Thermophysical Properties of Solids (Chairman, Dr. Merrill Minges, U.S.A.)

CODATA TASK GROUP ON THERMOPHYSICAL PROPERTIES OF SOLIDS

This Task Group, under the chairmanship of Dr. Merrill Mingos (USA), is nearing completion of two major projects awaited with considerable anticipation in the international thermophysics community. One project focuses on increasing the accuracy of newly generated information through the development and improvement of standard reference materials (SRM's). The second is concerned with the critical analysis of key data existing in the current literature.

The SRM project includes another important goal, the intercomparison, on an international basis, of the best experimental measurement methods used in leading laboratories. Thirty-seven data sets were generated from 22 laboratories covering the temperature range from 5K to 3000K. Although thermal conductivity was of principal interest, important ancillary data on heat capacity and electrical transport properties were obtained because such information is important in correlation and consistency assessment. Reflecting on developments in the field in recent years, a number of thermal diffusivity data sets were also obtained since this property is now commonly measured at both scientific and engineering laboratories around the world.

A number of rather surprising disagreements among the measurement results developed and received considerable attention before being successfully resolved. Highlights from the SRM phase of the program include a revision in the **austenitic stainless steel** certification based on new data. The program also provided new results to confirm the certification below room temperature where the original data base had been marginal. For high purity metallic materials such as the **electrolytic iron** and **tungsten** SRM's, impurity and grain boundary scattering are dominant influences on the transport properties and can cause large changes with seemingly minor differences in physical/chemical state especially at low temperatures. Methods were developed to quantify these relationships and were verified experimentally for both iron and tungsten SRM's thus confirming and broadening the certification. This project is rounded out with evaluations of **polycrystalline graphite** as a potential SRM; this material has important practical features and is of interest in the industrial engineering community, for example, nuclear power. Recent results on the graphite were reported at the international thermophysics symposium (1981) where a full session was

devoted to this material.

The objective of the critical analysis project has been to produce internationally accepted recommendations for the principal thermophysical properties of several key materials. The property/material matrix of the project is as follows:

Thermal conductivity	Cu, Fe, W, Pt
Electrical resistivity	Cu, Fe, W, Pt
Thermal diffusivity	Cu, Fe, W
Thermal expansion	Cu, Fe, W, Pt, Si, Al ₂ O ₃
Thermoelectric power	Cu, Pt, Pb
Heat capacity	Al ₂ O ₃ (Single crystal)

The criteria applied in establishing the matrix included: 1) scientific importance, 2) practical engineering importance, 3) existence of a sufficiently broad data base to make critical evaluation feasible. Analyst/reviewer teams were established for each property/material topic. Principal duties for the project were shared by 15 individuals from several countries. Special attention was focused on presentation format and on a precise, thorough and uniform critical analysis methodology for the entire project. Reporting the details of the evaluation rationale in each case was established as an important general feature of this project since previous efforts in this area had often omitted such vital information. The overall project has been closely coordinated with related programs particularly the CINDAS (Purdue University) evaluations under NBS Office of Standard Reference Data sponsorship and the Landolt-Bornstein New Data Series which is to be published shortly.

Other activities of the Task Group include extension of the SRM/Methods program into the lower thermal conductivity area which includes rocks and minerals of special interest for geosciences applications and also includes the field of thermal insulations, which has broad scientific and engineering interest. Workshop and education projects are being planned covering key areas where CODATA lead activities in thermophysical properties will be brought to a broader international community. Specific workshop topics being considered are: measurement methods from cryogenic to ultra high temperatures, standard reference materials available internationally, summaries of and accessibility to thermophysical property data compilations and critical analysis techniques.

SYMPOSIUM ON GEOCHEMICAL SURVEILLANCE OF VOLCANIC AND SEISMIC ACTIVITIES

CODATA's Working Group on Data for the Surveillance of Active Volcanoes will be one of the sponsors of an Italian-Soviet Symposium on the Geochemical Surveillance of Volcanic and Seismic Activities scheduled to be held in Palermo and the Eolian Islands in Sicily from 4-12 May 1983. The symposium will cover comparison of data throughout the world on the following topics: 1) chemical, physical-chemical and physical parameters of the gases and waters coming out of different high-risk volcanic and seismic areas; 2) the relationship between the variations of the forementioned parameters and any volcanic and seismic activity; 3)

the scientific and technical possibility of organizing a geochemical monitoring of volcanic and seismic areas; 4) the present state of knowledge related to some fundamental phenomena such as heat and mass transport processes in mantle and crust; and 5) mutual exchange of information from some scientific fields such as the monitoring of active geothermal fields or high environmental risk areas.

For further information on the symposium, contact Professor Marcello Carapezza, C.N.R. - Istituto di Geochimica dei Fluidi, Via Archirafi 36, 90123 Palermo, Italy, Telex UNIVPA 910170.

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Ninth International CODATA Conference

The Ninth International CODATA Conference, under the auspices of the Israel Academy of Sciences and Humanities, will be held 24-28 June 1984 in Jerusalem, Israel.

The scientific program is built along two avenues: Sessions and Symposia. The six Sessions:

- Methodology of Scientific Consolidation and Processing of Data
- Computerized Databases, Technology and Management
- Computer Techniques in Data and Systems Analysis
- Numerical Information Systems in Materials Science, Technology and Engineering
- Numerical Information Processing in Biosciences
- Numerical Data Processing in Geosciences

deal with broad interdisciplinary and disciplinary topics. Each session consists of an invited paper and oral/poster contributed papers.

Symposia, organized by individual experts deal with specific, well defined and framed numerical data topics within a given discipline or subdiscipline. All Symposia are grouped into four broad areas of

- Bio- and pre-clinical medical sciences
- Geosciences, oceanography and environmental sciences
- Chemistry, chemical engineering and materials science
- Physics, metallurgy and energy-related topics

For further information please return the slip below to Professor A.S. Kertes, Institute of Chemistry, The Hebrew University, Jerusalem 91904, Israel (Telephone: +972 2 585354; Telex: 25391 HU IL).

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Please send me further information on the Ninth International CODATA Conference

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Position/Title -----

Mailing address -----

Date-----

Signature

MATERIALS USERS WORKSHOP CALLS FOR COMPUTERIZED MATERIALS DATA SYSTEMS

Computer applications in engineering are revolutionizing engineering methods and generating increased needs for computer accessible data. With an awareness of these changes, a workshop of materials users has recently enthusiastically endorsed the concept of a comprehensive system of computerized materials data bases to meet the needs of materials selectors, designers, and manufacturers in industry and government in the 1980's. They proposed large-scale distributed materials data systems which would include information on a wide variety of materials including metals, alloys, ceramics, polymers, and composites. In addition, the workshop strongly recommended that such systems be developed by close cooperation among individual materials data base producers, technical societies, industry, publishers and government.

The meeting, through intensive discussions, identified the four principal ingredients for success of computerized materials data systems as 1) a gateway structure to allow access to independent data bases on specific properties and materials; 2) close cooperation between industrial users, data base builders, and system developers; 3) data on engineering properties of commercial materials plus statistical, graphical and other user friendly capabilities; and 4) international input and cooperation.

Further, the participants recommended that a pilot materials data system be started as soon as possible. The aim of the project would be to develop experience in linking together engineering data bases and to define user interface and support. It was felt that the pilot system would require initial investment from groups such as the technical societies and government, but that the operations should be supported by the users. Royalties would be paid to producers of the participating data bases which might include data centers, trade associations and technical data publishers.

A parallel phase to the pilot project would be additional systems definition to specify the parties that would be involved in larger, more comprehensive systems and to outline the systems

operations, specifications, finances and cooperation. It is proposed that this work be done under the auspices of groups such as the Metals Properties Council and the U.S. National Academy of Engineering in conjunction with similar groups in Europe.

The Materials Data Workshop was held at Fairfield Glade, Tennessee, on 7-11 November 1982. The meeting featured small task groups which examined the key issues involved in building computerized materials data systems. The topics included non-technical barriers, the economics of building and operating data systems and legal/societal problems. Also vigorously discussed were technical issues such as the minimum size of the data system, user interfaces, specification of the data, data validations, and data applications. A summary report of the Workshop findings will be issued in early 1983.

The 75 participants who attended came from many sectors of private industry including aerospace, airframe, automotive, machine tools and electronics plus several smaller industries and engineering consulting firms. Also represented were the publishing industry, national laboratories, government, universities and technical societies. Nations represented were the USA, Federal Republic of Germany, Sweden, the Netherlands, the U.K., Canada and Japan.

The workshop was supported by the U.S. National Bureau of Standards, Fachinformationszentrum of the Federal Republic of Germany, the Committee on Data for Science and Technology (CODATA), and the Oak Ridge National Laboratory (USA).

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SYMPOSIUM ON CRITICAL EVALUATION AND PREDICTION OF PHASE EQUILIBRIA IN MULTICOMPONENT SYSTEMS

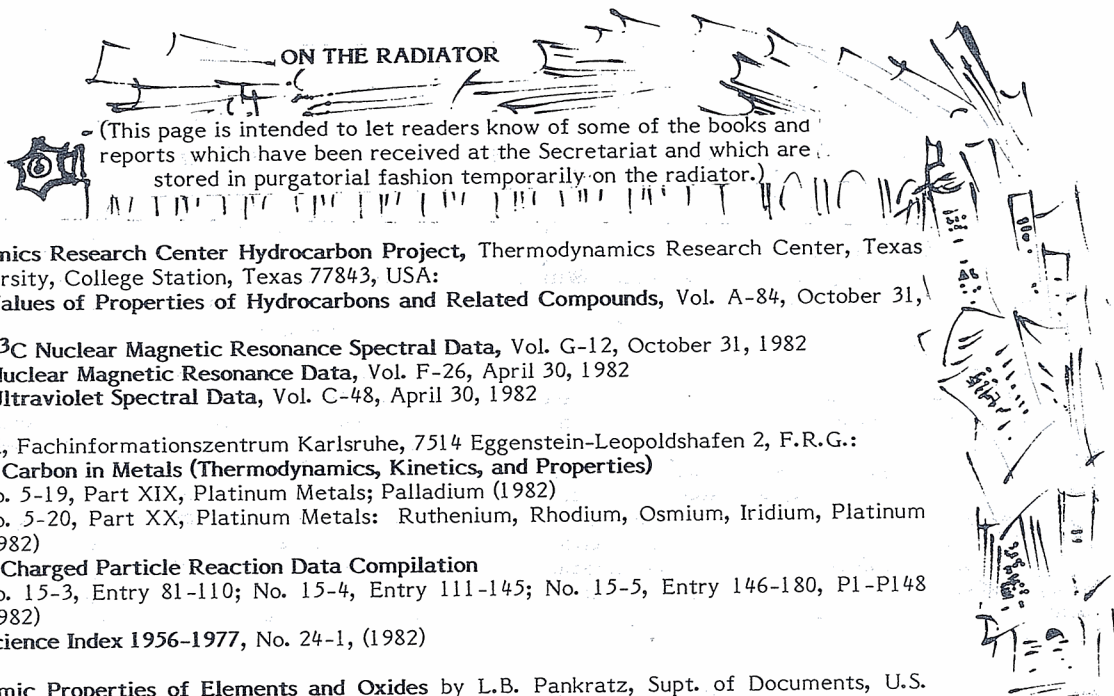
The CODATA Task Group on Critically Evaluated Phase Equilibria in Mixtures and the Institute of Physical Chemistry of the Polish Academy of Sciences is organizing a Symposium on Critical Evaluation and Prediction of Phase Equilibria in Multicomponent Systems on 9-12 May 1984 in Warsaw. The Symposium is to serve the exchange of experience, discussion of recent research methods of critical evaluation and prediction of vapor-liquid, liquid-liquid and solid-liquid equilibrium data in multicomponent systems of organic compounds, plus organic compounds and water at moderate pressures.

The Symposium will cover 1) statistical and numerical fundamentals of the correlation of thermodynamic data; 2) estimation of experimental errors; 3) simultaneous correlations of various

thermodynamic data; and 4) comparison of various methods of prediction and correlation of phase equilibria in multicomponent systems.

For the discussion and comparison of methods of critical evaluation and prediction of VLE and LLE data, the selected data will be prepared as a computer printout for use by the participants.

Scientists involved in phase equilibrium data and auxiliary data covering vapor pressure, excess enthalpy, second virial coefficients, etc. are kindly invited to cooperate with the organizers in preparing the selected data. Proposals for the data to be treated will be collected until 31 July 1983 and interested scientists are invited to send their proposals to Dr. A. Maczynski, Institute of Physical Chemistry, Polish Academy of Sciences, ul. Kasprzaka 44/52, 01-224 Warsaw, Poland.



Thermodynamics Research Center Hydrocarbon Project, Thermodynamics Research Center, Texas A & M University, College Station, Texas 77843, USA:

Selected Values of Properties of Hydrocarbons and Related Compounds, Vol. A-84, October 31, 1982

Selected ^{13}C Nuclear Magnetic Resonance Spectral Data, Vol. G-12, October 31, 1982

Selected Nuclear Magnetic Resonance Data, Vol. F-26, April 30, 1982

Selected Ultraviolet Spectral Data, Vol. C-48, April 30, 1982

Physics Data, Fachinformationszentrum Karlsruhe, 7514 Eggenstein-Leopoldshafen 2, F.R.G.:

Gases and Carbon in Metals (Thermodynamics, Kinetics, and Properties)

No. 5-19, Part XIX, Platinum Metals; Palladium (1982)

No. 5-20, Part XX, Platinum Metals: Ruthenium, Rhodium, Osmium, Iridium, Platinum (1982)

Karlsruhe Charged Particle Reaction Data Compilation

No. 15-3, Entry 81-110; No. 15-4, Entry 111-145; No. 15-5, Entry 146-180, P1-P148 (1982)

Surface Science Index 1956-1977, No. 24-1, (1982)

Thermodynamic Properties of Elements and Oxides by L.B. Pankratz, Supt. of Documents, U.S. Govt. Printing Office, Washington, D.C. 20402, USA, No. I28.23:672, 509 pp, 1982

USSR Numerical Data Publication Standards, International Atomic Energy Agency, International Nuclear Data Committee, Wagramerstrasse 5, A-1400 Vienna, Austria, Report INDC (CCP)-191/G, 27 pp, 1982

Vapor-Liquid Equilibria for Mixtures of Low Boiling Substances by H. Knapp, R. Döring, L. Oellrich, U. Plöcker and J.M. Prausnitz, DECHEMA Chemistry Data Series, Vol. VI, 890 pp, (1982), 247 DM

Vapor-Liquid Equilibrium Data Collection:

Vol. I, Part 2d, Organic Hydroxy Compounds: Alcohols and Phenols (Supplement 2), 790 pp (1982)

Vol. I, Part 5, Carboxylic Acids, Anhydrides, Esters, 705 pp, (1982)

DECHEMA, 6000 Frankfurt/Main, F.R.G.,

Interactive Fortran Program to Calculate Thermophysical Properties of Six Fluids by B.A. Younglove, Supt. of Documents, U.S. Govt. Printing Office, Washington, D.C. 20402, USA, No. NBS TN-1048, 56 pp, \$4.75

Rate Constants for Reactions of Aliphatic Carbon-Centered Radicals in Aqueous Solution by A.B. Ross and P. Neta, Supt. of Documents, Govt. Printing Office, Washington, D.C. 20402, USA, Publication No. NSRDS-NBS 70, 103 pp, \$5.50

Construction Materials for Coal Conversion, Performance and Properties Data, by H.M. Ondik, B.W. Christ and A. Perloff, Supt. of Documents, U.S. Govt. Printing Office, Washington, D.C. 20402, USA, Publication No. NBS SP 642 (1982), 826 pp

Diatomic Molecules, A Critical Bibliography of Spectroscopic Data, Part IV - 1982, edited by R.F. Barrow, Editions du CNRS, 15 quai Anatole France, 75700 Paris, France, 180 French francs

World Climate Programme, World Meteorological Organization, Case Postale No. 5, Geneva 20, Switzerland

Time Series of Ocean Measurements (Papers presented at the meeting 11-15 May 1981), WCP-21, May 1981

'CAGE' Experiment: A Feasibility Study, WCP-22, May 1982

Optimal Climate Data Utilization: A Climatic Data Acquisition, Archiving, Processing and Dissemination System for Resource Management, WCP-25, September 1982

Climate/Energy Graphics: Climate Data Applications in Architecture, WCP-30, September 1982

Strong Motion Data from Japanese Earthquakes, World Data Center A for Solid Earth Geophysics, NOAA/EDIS/NGSDC, 325 Broadway, Boulder, CO 80303, USA, (1981), 341 pp

Data Base Management: Theory and Applications, Proceedings of the NATO ASI, June 1981, eds. C.W. Holsapple and A.B. Whinston, D. Reidel Publishing Co., Dordrecht, Holland, (1983), 392 pp, \$54.50

Computer Program Synthesis Methodologies, Proceedings of the NATO ASI, September 1981, eds. A.W. Bierman and G. Guiho, D. Reidel Publishing Co., Dordrecht, Holland, (1983), 374 pp, \$52.50

Scientific and Technical Information in the Metals Industry: Report of the Metals Information Review Committee, by L. Jones and J. Vaughan, Publications Section, British Library Lending Division, Boston Spa, Wetherby, West Yorkshire LS237BQ, U.K., BL R&D Report No. 5717, £9.00

Data Management and Computation, Vol. 1: Issues and Recommendations, Space Science Board, 2101 Constitution Avenue, Washington, D.C. 20418 (1982), 167 pp

High Pressure World Directory, available prepaid from AIRAPT-BOURGOGNE, B.P. 90, 71203 Le Creusot, France, 508 pp, 128 French francs

NBS THERMOCHEMICAL TABLES ISSUED

Two decades of intensive effort have come to fruition in the publication of the **NBS Tables of Chemical Thermodynamic Properties: Selections for Inorganic and C₁ and C₂ Organic Substances in SI Units**.

This volume is a modern version of **NBS Circular 500** (published in 1952) and supersedes the eight parts of the **NBS Technical Note 270** series that appeared between 1965 and 1981. It represents the definitive reference source for standard-state thermodynamic properties of inorganic and simple organic compounds.

The tables include standard-state data on enthalpy, entropy, heat capacity, and related properties of over 14 000 substances. The original data on which the tables are based were drawn from 60 000 references. All data have been critically evaluated and checked for consistency with thermodynamic constraints by specially developed computer programs. Thus data taken from these tables may be used in thermodynamic calculations (e.g., to obtain equilibrium constants or heats of reaction) with the assurance that no errors are introduced by thermodynamically incompatible values.

The **NBS Tables** have been published as Supplement 2 to Volume 11 of the **Journal of Physical and Chemical Reference Data**. The book may be ordered for \$40 from: American Chemical Society, Books and Journals Division, 1155 Sixteenth Street, N.W., Washington, D.C. 20036, U.S.A.

CONTRACT SIGNED FOR OPERATION OF HYBRIDOMA AND MONOCLONAL ANTIBODIES DATA BANK

CODATA signed a contract in March 1983 with the American Type Culture Collections in Bethesda, Maryland, for the housing of its data bank on hybridomas and monoclonal antibodies. Staff has been hired and work will begin in early May collecting the available data.

The CODATA Task Group met in Geneva at the World Health Organization headquarters in January 1983 to complete the coding scheme for the data to be collected and to discuss the establishment of satellite banks in Europe and the Far East. Funds for the operation of the bank have been committed by several countries and further participation is expected.

The flow of information regarding hybridomas and monoclonal antibodies is increasing so rapidly that it is estimated that the number of antibodies existing today is certainly in the range of tens of thousands. In view of the importance of these reagents in basic research and diagnosis, not to mention their use in therapeutics, a catalog of these reagents becomes highly desirable. At present, any researcher, clinician, etc. who wants to know if a given hybridoma, monoclonal antibody or cell line exists, if it is available, and if so, where, has almost no way to make a comprehensive search.

It is anticipated that retrieval of data by scientists will be possible in early 1984.

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