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COMMITTEE ON DATA FOR SCIENCE AND TECHNOLOGY
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26 CODATA NEWSLETTER

August 1983

CODATA HOLDS PLANNING CONFERENCE

The CODATA Executive Committee held a Conference on the Future of CODATA at La Gaillarde, France, on 29-30 June 1983. In addition to the Executive Committee, the following outside guests participated in the sessions: **C.B. Alcock,** (Canada, Professor of Metallurgy and Materials Science, University of Toronto); **Stein Bie,** (Norway, Norsk Regnesentral, Specialist of computer handling of geoscience data); **Carlos E. Brockmann,** (Ecuador, Former Director Remote Sensing Institute, Bolivia); **Margaret Courain,** (USA, Deputy Asst. Director, NESDIS); **M. Hashizume,** (Unesco - Earth Sciences Division); **Nicholas Kurti,** (U.K., Emeritus Professor of Physics, Oxford University, former Treasurer of CODATA); **Thomas Malone,** (USA, Treasurer of ICSU, Director of Holcomb Institute, former Foreign Secretary of the US National Academy of Sciences); **Lennart Philipson,** (F.R.G., Director, European Molecular Biology Laboratory, Heidelberg); **John Rose,** (Unesco Program of General Information); **Jacques Rosselin,** (France, Mission Internministérielle de l'Information Scientifique et Technique); **Richard Sinding-Larsen,** (Norway, Chairman, COGEODATA; Chairman, CODATA Committee on the Geosciences); **Lucien Sobel,** (France, Research Advisor to Produits Chimiques Ugine Kuhlman, member of the CODATA Task Group on Data for the Chemical Industry); **Jacques Vigneron,** (France, Director, European Summer School on the Environment; Scientific Advisor to the French Minister of the Environment; Professor of the Environment, Université Paris VII); **Jack Westbrook,** (USA, Materials Information at General Electric, Chairman, CODATA Committee on Data for Industry); **R.L. Wigington,** (USA, Director of Research, Chemical Abstracts, Computers and telecommunications).

From left to right: W.W. Hutchison, M. Courain, A. Bussard, E.R. Cohen, L. Sobel, S. Bie, D.G. Watson, C.N.R. Rao, T. Malone, J.H. Westbrook, C.B. Alcock, M. Hashizume, W. Schirmer, J.E. Dubois, J. Rose, M. Kotani, J. Vigneron, R. Wigington, H. Haendler, D.R. Lide, Jr., A. Bylicki, N. Kurti, E.F. Westrum, Jr., R. Sinding-Larsen, (Missing from photo: C. Brockmann, L. Philipson, J. Rosselin)

The objective of the conference was to assess CODATA accomplishments in the 17 years since its founding, discuss future challenges, and set directions for CODATA for the next decade. The five major topics addressed during the conference were: critical evaluation and improvement of data quality; accessibility and dissemination of data; structure and format of data files; computers and telecommunications in data dissemination; and propagation of CODATA's outputs to the scientific and technical community. In addition, the relation of CODATA to the unions, other ICSU bodies, and Unesco received much discussion.

The group reached consensus on the growing importance of computers and telecommunication systems for the storage, retrieval and dissemination of scientific and technical data. Opportunities for CODATA action include setting guidelines for structuring data files so as to achieve maximum compatibility, advising on data base management techniques, and coordinating related activities by different unions or countries. An increased role in providing information on sources of data, especially in computer-readable form, was recommended. (See further the Letter from the President on page 2).

The full report of the conference will be available from the Secretariat in early October.

he Committee on ata for Science and echnology (CODATA) as established in 1966 y the International ouncil of Scientific nions.

orking on an inter- ational, interdiscipli- ary basis, CODATA eeks to improve the uality, reliability and ccessibility of data of nportance to science nd technology.

LETTER FROM THE PRESIDENT

CODATA'S FUTURE

CODATA can make significant global contributions to the development of science and technology and to our rapidly evolving technological society. This was the overriding message that came out of the "Futures" Workshop on CODATA, convened in La Gaillarde, France in June. And if some members of CODATA's Executive Committee had harbored any thoughts about possibly dissolving the Committee, they quickly disappeared in the face of the opportunities and challenges for data management highlighted during the Workshop.

The challenges stem from recent important changes in science and technology, many of which have already had direct impact on the scope of CODATA's work. Specifically:

The development of a better understanding of the microstructure of matter and its relation to macroscopic properties and behavior, thus making possible the prediction of complex phenomena such as the effect of pollutants on the environment.

Advances in the understanding of genetic coding and the subsequent establishment of the complex discipline of biotechnology, opening new vistas for data capture and management, as witnessed in the current pilot project setting up an international Hybridoma and Monoclonal Antibodies Data Bank..

Continuous acquisition of vastly increased volumes of data emanating from satellite sensing and seismic exploration, straining our conventional capacities to store and analyze information.. and

The rapid evolution of computing devices (such as the powerful, rugged and versatile mini-computer) which has facilitated scientists' ability to manage and process data and which has accelerated computer literacy in general.

Growing worldwide societal concerns about critical issues such as the environment, energy sources and supply, and biotechnology have created new demands for systematic, authoritative information as a basis for decision-making and regulation. These too have underscored the need for an international authority to address and refine the art of data processing and management, particularly on a multidisciplinary basis, for an information-intensive society.

If CODATA is to maintain and enhance its reputation in the future as the authoritative, international, non-governmental advisory body on the acquisition, management and use of scientific and technical data, it will have to target its programs strategically in support of the opportunities presented by these scientific and technological advances. And it will have to meet the expanding needs of society, increasingly more sophisticated and cognizant of the technoogical revolution underway in information processing.

CODATA's traditional interests - quality control of data, international standards or key values, methodologies for data handling, storage and retrieval - have been pursued for the past seventeen years. They will continue as the baseline of all our undertakings. The emphasis in our future programs, however, is likely to shift away from key values toward data structures and management, data bases in different disciplines, and the application of modern computer technology and telecommunications.

CODATA can contribute to an improved understanding of the "data flow" or use of data in science and technology - crucial to decisions on requirements for data and selection of appropriate data for archiving. Consequently, CODATA's activities in the use of data will probably increase, especially in the development of various descriptive, genetic, predictive models, as well as in engineering design. The extent to which key data in a discipline are of restricted or multidisciplinary interest is already of concern to CODATA, and more attention is likely to be given in the future to the nature of the data that are collected and their attributes. An even greater emphasis on methodologies of data handling is anticipated if CODATA is to achieve more effective interaction across disciplines.

There are a number of opportunities for Committee initiative in establishing policies for more effective dissemination of data. For example, CODATA can provide input to developing international guidelines on copyright protection for data banks that will be publicly available.

Clearly, CODATA's "Futures" Workshop pointed to the need for the Committee to establish a framework from which we can, in an organized and deliberate way, recognize the opportunities before us and mobilize our policies and activities to ensure that these opportunities do not pass us by. More purposeful debate is required, along with careful long-term planning and improved communication of our achievements and outputs. Our "Futures" Workshop was a reassuring and promising first step in that direction.

W.W. Hutchison
President, CODATA

CODATA Secretariat,
51 Boulevard de Montmorency, 75016 Paris, France
Tel: 525.04.96 - Telex: 630553 F ICSU

Editor and directeur de la publication: Phyllis Glaeser, Executive Secretary
Associate Editors: David R. Lide, Jr. and Edgar F. Westrum, Jr.

NINTH INTERNATIONAL CODATA CONFERENCE

There is still time to send in proposals for contributed papers to the Ninth International CODATA Conference scheduled to be held in Jerusalem on 24-28 June 1984. Contributed papers may be submitted for one of the following scheduled sessions:

A. Methodology of Scientific Consolidation and Processing of Data

Data description, presentation, standardization and normalization. Compilation, evaluation of data. Critical analysis and recommended data. Scientific indexing and coding.

B. Computerized Data Bases, Technology and Management

Data banks and centers. Search and storage. Input, monitoring and updating. Retrieval and dissemination. Communication languages and protocols. Large data networks. Users' feedback. Economics and marketing. Legal aspects.

C. Computer Techniques in Data and Systems Analysis

Computer-assisted conceptions and design systems. Simulation, estimation and prediction of complex natural systems. Mathematical modeling..

D. Numerical Information Systems in Materials Science Technology and Engineering

Properties of substances and mixtures. Standards and reference materials. Phase diagrams. Structure theories. Atomic and nuclear data. Composite materials data. Combustion and energy conversion data.

E. Numerical Information Processing in Biosciences

Coding. Pattern recognition. Drug data. Genetic engineering. Evolutional heritage Human physiological and population data. Toxicological information systems. Plant breeding.

F. Numerical Data Processing in Geosciences

Geoscience field data capture. Remotely sensed data in geology, oceanography and meteorology. Environmental information systems and automatic cartography. Artificial satellites.

The following plenary lectures are planned which follow roughly the above-listed sessions:

The Oceans and the World Climate Research Program, **James Crease** (Institute of Oceanographic Sciences, Surrey, U.K.

Spatial Analysis in the Earth Sciences, **F. P. Agterberg** (Geological Survey of Canada, Ottawa, Canada)

Peculiarities and Problems of Materials Engineering Data, **G. Dathe,** (Betribsforschungsinstitut, Dusseldorf, F.R.G.)

Optimal Classification of Files and Situations, **A. Lerner,** Academy of Sciences of the U.S.S.R., Moscow, U.S.S.R.

Immunoglobulins Sequence Data - The Generation of Diversity and Its Genetic Control, **Elvin A. Kabat,** Columbia University, U.S.A.

In addition to the Sessions the following Symposia have been organized to take place during the Conference:

Toward a Human Protein Map; Nucleic Acid and Protein Sequence Analysis and Evaluation; X-Ray Structure, Storage and Retrieval, and Correlation of Protein Nucleic Acid Structural Data; Data Needs for Genetic Engineering/Biotechnology; Antibody Diversity Reconsidered in the Light of Recent Structural Data; Efforts and Progress in Evaluation and Compilation of Phase Diagrams; Phase Equilibria: Data Banks and Process Calculations; Phase Equilibria: Correlations and Predictions; Compilations in Elementary Particle Physics; Numerical Data for Energy Conversion Projects; Management and Analysis of Numerical Data in Geochemical Exploration; Selection of Physicochemical Data of Actinide Compounds; Solid-Seawater Equilibrium Data; Data on Actual Chemical Concentrations in the Oceans; Environmental, Chemical and Toxicological Data Bases; Numerical Data for Energy Systems; Numerical Data for Nuclear Energy; Geostatistics in Mining and Petroleum Industries; Numerical Data Retrieval in Science and Technology; Automatic Information Retrieval in the Sciences; Industrially Oriented Process and Thermodynamic Data Projects in the U.S.A.

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).

Professor A.S. Kertes
Institute of Chemistry
The Hebrew University
Jerusalem 91904, Israel

Please send me further information on the Ninth International CODATA Conference

Last name----------First name----------

Position/Title----------

Mailing address----------

LOIS BLAINE NAMED MANAGER OF HYBRIDOMA DATA BANK

Lois D. Blaine has been engaged as Data Base Manager for the CODATA Hybridoma and Monoclonal Antibodies Data Bank. Ms. Blaine was previously Scientific Manager at Tracor Jitco, Inc. and Project Manager for the design and development of two toxicology data banks: AQUIRE - Aquatic Toxicity and Dermal Absorption/Toxicity.

Ms. Blaine comes to the CODATA Data Bank with a vast experience in immunology from the time when she was employed at the National Library of Medicine (NLM). At NLM she was the designated specialist for analysis of the immunology literature, a position which involved monitoring developments in the field of immunology and clarifying complex issues for NLM indexers.

Ms. Blaine will meet with the CODATA Task Group to discuss the results of her first three months' work at a meeting of the Group to take place in Kyoto on 21 August 1983 at the International Congress of the International Union of Immunological Societies.

TASK GROUP ON GAS PHASE CHEMICAL KINETICS

The CODATA Task Group on Gas Phase Chemical Kinetics met on 29 May-2 June 1983 near Montreux, Switzerland. The Task Group's work in preparing an updated and extended evaluation of kinetic and photochemical reaction rate data for atmospheric chemistry is continuing. Although the kinetic data base for understanding the chemistry of the stratosphere has been considerably improved during the past two or three years, there has been little respite in the flow of laboratory data. More than half of their previous data sheets for 230 photochemical and thermal reactions will require updating. Draft data sheets have been prepared for those reactions for which new data have become available.

In addition to this program of updating, the Task Group will be extending the scope of its efforts to include reactions involving more complex organic species. For instance, they have now prepared data sheets for the reaction, $HO + C_3H_8 \rightarrow H_2O + C_3H_7$ and the subsequent atmospheric reactions of the C_3H_7 radicals. It has also added reactions involving nitriles and CN radicals. The inclusion of these additional reactions, of more complex organic molecules and radicals, means that the Task Group's final evaluation will have a wider range of applicability to atmosphere modelling including regions of the troposphere as well as the stratosphere.

Members present at the meeting were **Dr. J. A. Kerr** (chairman), **Dr. R. F. Hampson, Jr.** (secretary), **Dr. D. L. Baulch, Prof. J. Troe and Dr. R. T. Watson.** A follow-up meeting is scheduled for October 1983 in the U.K.

INFOODS

An international planning conference on the topic "An International Network of Food Data Systems" was held on 30 January-5 February 1983 in Bellagio, Italy to explore the needs for food composition data bases, especially in the international context.

The Conference focussed on the design and scope of an organization to be called INFOODS (International Network of Food Data Systems) which would promote international participation and cooperation in the acquisition and interchange of quality data on the nutrient composition of foods, beverages and their ingredients.

Further information about INFOODS can be obtained from **Dr. Vernon R. Young** or **Dr. William M. Rand,** Department of Nutrition and Food Science, Massachusetts Institute of Technology, Cambridge, MA 02139, USA.

RESEARCH CONCERNING METROLOGY AND FUNDAMENTAL CONSTANTS

The Numerical Data Advisory Board of the U.S. National Research Council has recently issued a report on research concerning metrology and fundamental constants. The purpose of the report is to call attention to the important role of fundamental constants and precision measurements in science and to demonstrate a requirement for increased and continuing support in this field.

Precise knowledge of fundamental constants and techniques for making more accurate and reliable measurements is required to test basic theories, to extend our knowledge of the universe, and for practical applications including reference standards for measurements. The report demonstrates by example that research in this field, aimed in its primary goals at basic understanding, has led to profound advances that have an impact on much of our technology-based society. The report reviews the general scope of the field and makes recommendations for future research and applications.

A copy of the report is available from Dr. **G.C. Carter,** NRC, 2101 Constitution Ave. N.W., Washington, D.C. 20418.

THERMODYNAMIC PROPERTIES OF INDIVIDUAL SUBSTANCES

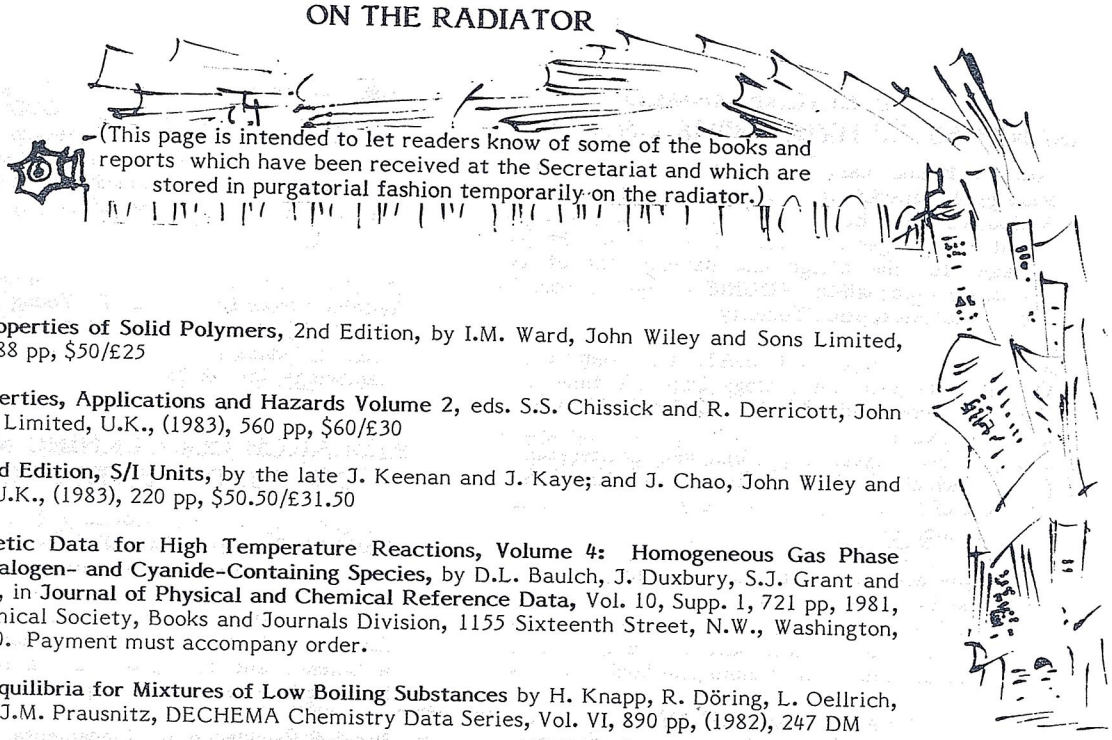
The fourth and final volume of "Thermodynamic Properties of Individual Substances" has just been published. This valuable reference book, edited by **V. P. Glushko, L. V. Gurvich, G. A. Bergman, I. V. Veits, V. A. Medvedev, G. A. Khachkuruzov** and **V. C. Yungman,** consists of four volumes (two books per volume: one containing the data tables with temperatures to 10 000 °K in many instances, the other the references).

The elements and their mixtures contained in each volume are as follows:

Volume I: O, H(D,T), F, Cl, Br, I, He, Ne, Ar, Kr, Xe, Rn, S, P
Volume II: C, Si, Ge, Sn, Pb
Volume III: B, Al, Ga, In, Tl, Be, Mg, Ca, Sr, Ba
Volume IV: Cr, Mo, W, V, Nb, Ta, Ti, Zr, Hf, Sc, Y, La, Th, U, Pu, Li, Na, K, Rb, Cs.

At present the four volumes are available in Russian. The entire set is being translated into English under the editorship of **Professor C. B. Alcock** of the University of Toronto and published by Pergamon Press.

ON THE RADIATOR



(This page is intended to let readers know of some of the books and reports which have been received at the Secretariat and which are stored in purgatorial fashion temporarily on the radiator.)

Mechanical Properties of Solid Polymers, 2nd Edition, by I.M. Ward, John Wiley and Sons Limited, U.K., (1983), 488 pp, $50/£25

Asbestos: Properties, Applications and Hazards Volume 2, eds. S.S. Chissick and R. Derricott, John Wiley and Sons Limited, U.K., (1983), 560 pp, $60/£30

Gas Tables, 2nd Edition, S/I Units, by the late J. Keenan and J. Kaye; and J. Chao, John Wiley and Sons Limited, U.K., (1983), 220 pp, $50.50/£31.50

Evaluated Kinetic Data for High Temperature Reactions, Volume 4: Homogeneous Gas Phase Reactions of Halogen- and Cyanide-Containing Species, by D.L. Baulch, J. Duxbury, S.J. Grant and D.C. Montague, in **Journal of Physical and Chemical Reference Data,** Vol. 10, Supp. 1, 721 pp, 1981, American Chemical Society, Books and Journals Division, 1155 Sixteenth Street, N.W., Washington, D.C. 20036, $80. Payment must accompany order.

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

Thermophysical Properties of Solids, Their Measurements and Theoretical Thermal Analysis, by J. Šesták, Elsevier Scientific Publishing Co., Amsterdam, (1983), 400 pp.

Data Prediction Manual, eds. R.P. Danner and T.E. Daubert, AIChE Publications Sales, Dept. C, 345 E. 47th St., New York, N.Y. 10017, U.S.A., (Chapter 1: General Data, Chapter 2: Critical Properties; Chapter 3: Vapor Pressure; Chapter 4: Density; and Chapter 12: Measures of Environmental Impact, available as of 1 July for $150).

Design and Implementation of Computer-Based Geographic Information Systems, IGU, Commission on Geographical Data Sensing and Processing, c/o Dept. of Geography, State Univ. of NY at Buffalo, Amherst, NY 14260, USA, $16.95 (1983).

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

Regional South East Asian Climate Data Management and User Services (Bangkok, 29 November- 3 December 1982), WCP-32

International Working Group on Data Management for the International Satellite Cloud Climatology Project (ISCCP) (New York City, 13-17 December 1982), WCP-42

The Future Activities of the World Radiation Centre (WRC-Leningrad) (Leningrad, 28 February - 1 March 1983), WCP-48

Computerized Materials Data Systems, eds. J.H. Westbrook and J.R. Rumble, Jr., limited number of copies available from CODATA Secretariat upon request.

Information Services on Research in Progress, A Worldwide Inventory, 2nd Edition, edited by the Smithsonian Science Information Exchange, Inc., Unesco, 7, Place de Fontenoy, 75700 Paris, France, (1982), 320 pp, 75 French francs, Section 10, (1983), 21 pp

Directory of International and Regional Organizations Conducting Standards-Related Activities, ed. M.A. Breitenberg, Supt. of Documents, U.S. Govt. Printing Office, Washington, D.C. 20402, U.S.A., Publication No. NBS SP 649, (1983), 366 pp, $9.50

Directory of Scientific Directories, 3rd Edition, by J. Burkett, Longman Group, U.S.A., 649 pp, (1979), $90

Bulletin of Chemical Thermodynamics, ed. R.D. Freeman, THERMOCHEMISTRY, Dept. of Chemistry, Oklahoma State University, Stillwater, OK 74078, U.S.A., No. 24, (1981), 504 pp, $30

Banques de données du CNRS et de l'Université, CDST, Division Valorisation, Service Promotion-Commercialisation, Ministère de l'Industrie et de la Recherche, 26, rue Boyer, 75971 Paris Cedex 20, France, (1983), 297 pp, 100 French francs

Materials Research Centres (Directory of Organizations and Programmes in Materials Science), eds. E. Mitchell and E. Lines, Longman Group Ltd, U.K., 580 pp, £85.