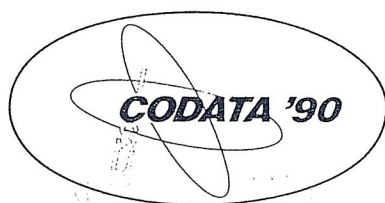


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CODATA / NEWSLETTER

MAY 1989



HIGHLIGHTS

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

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

12th International CODATA Conference

"Data for Discovery"

15-19 July, 1990--Columbus, Ohio, U.S.A.

Announcement/Invitation

The Columbus Local Organizing Committee, *CODATA '90*, in cooperation with the National Academy of Sciences, will host "*Data for Discovery*."

The Conference will be organized around sessions in the area of scientific and technical data for discovery. It will emphasize the importance of collection, organization, and analysis of large data sets which can lead to new insights into scientific phenomena. In particular, the management aspects of the ICSU Global Change Program will be highlighted, as well as exploratory molecular manipulation. It will provide an appropriate framework for discussion on the following major themes:

- Prediction of Global Change
- Spatial Databases
- Materials Data Systems
- Expert Systems and Other Knowledge Tools
- Trends in Integration of Information Across Biology
- Impact of New Technology on Data Handling

CODATA, is concerned with all types of quantitative data resulting from experimental measurements or observations in the physical, biological, geological, and astronomical sciences. Particular emphasis is given to data management problems common to different scientific disciplines and to data used outside the field in which they are generated.

Call for Papers

All major themes of the Conference will be covered by invited papers. In addition, contributed papers will be presented, either in oral or poster form. Specialists in the fields of data collection, analysis, evaluation, and organization of data sets and data systems applications are invited to submit contributions on

(cont'd. on p. 2)

"Data for Discovery" (cont'd.)

subjects within the scope of the Conference. To facilitate discussion and interchange of ideas, workshops will be organized from the poster sessions in which groups of related posters will be discussed with an appointed chairman after the poster sessions.

A title and abstract of about 500 words should be submitted as soon as possible to the Program Committee Chairman: Dr. Margaret E. Courain, 420 Harding Drive, South Orange, New Jersey 07079, U.S.A. Electronic mail may be sent on DIALCOM142: CDT0355.

Abstracts will be required by 31 August, 1989. Authors will be notified before 15 October, 1989, about the acceptance of their contribution and will receive instructions on providing the full text at that time.

Who Should Attend CODATA '90

Practitioners in all scientific disciplines, especially those in the physical, biological, geological, and astronomical sciences concerned with the management of quantitative data resulting from experimental measurements or observations, will find this Conference of benefit.

Exhibits and Database Demonstrations

Display space will be available for organizations which would like to inform the participants about their equipment, services, and books relevant to CODATA's interests.

Ample space will be available for scientific and technical database producers and developers to conduct demonstrations of their equipment and/or services.

Social and Cultural Activities

Social and cultural activities planned for participants and their accompanying guests attending CODATA '90 include:

- Opening Reception • All-Conference Reception and Banquet and • Reception at the Center of Science and Industry, one of only 22 science technology centers in the world with four floors of interactive exhibits, programs, and demonstrations.

- Tours of Columbus' unique neighborhoods such as German Village, a 19th century German community containing beautifully restored homes, shops, and restaurants.

- Visits to the world-renowned Columbus Zoo and to the Ohio Historical Center/Ohio village, one of America's premier historical museums, featuring a recreated 19th-century town with costumed artisans.

- A trip to the United States Air Force Museum in Dayton.

- Conference attendees and their guests may also discover Columbus at their leisure, independently of the organized events.

Columbus Local Organizing Committee, CODATA '90

- Dr. G. O. Platau, Chairman, *Chemical Abstracts Service*
- Mr. G. M. Minot, Business Agent, *AITRC*
- Mr. H. Mindlin, *Batelle Memorial Institute*
- Dr. M. Muller, *The Ohio State University*
- Mr. J. Price, *Ashland Chemical Company*
- Mr. J. Rue, *CompuServe*
- Mr. D. L. Trotter, *OCLC Online Computer Library Center*



ACTION!

Don't delay!

Xerox card below (or send appropriate requested information) to:

12th International CODATA Conference
Applied Information Technologies Institute
1880 Mackenzie Drive, Suite 111
Columbus, Ohio 43220, U.S.A.

I am interested in the 12th International CODATA Conference entitled "Data for Discovery" to be held in Columbus, Ohio, U.S.A., from 15-19 July, 1990.

- ☐ Please send the preliminary program when available.
☐ I intend to contribute a paper ☐ orally ☐ at a poster session.
Theme (see Invitation): _____
Title: _____

Titles and abstracts of ca. 500 words shall be sent to the Program Committee Chairman as soon as possible. See Call for Papers for address.

- ☐ Please send information on exhibits of ☐ equipment/services ☐ books.
☐ Please send information on database demonstrations.
☐ I shall probably be accompanied by _____ persons.

My address is (please print):

Name: _____ Title: _____
Affiliation: _____
Street Address: _____ City: _____
State/Province: _____ ZIP/Postal Code: _____
Country: _____ Tel. No.: _____

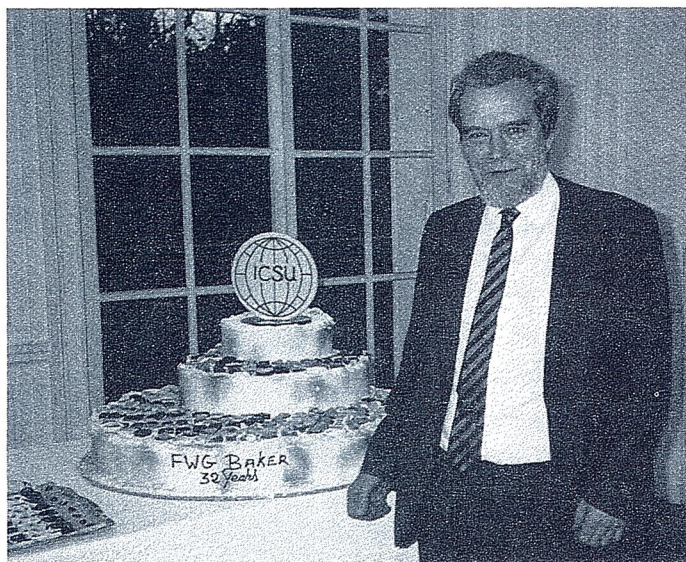
ICSU's Executive Secretary Retires After 24 Years

"Mike" (F.W.G.) Baker, Executive Secretary of the International Council of Scientific Unions (ICSU) for 24 years has weathered a total of 32 years with them.

As Tennyson wrote:

*"The old order changeth, yielding place to new
And God fulfills Himself in many ways,
Lest one good custom should corrupt the world...."*

Julia Marton-Lefèvre is the new Executive Secretary of ICSU.



"Mike" (F.W.G.) Baker

Mike has proven to be an initiator of scientific activity, an educator of many officers, an unrivalled storehouse of relevant knowledge and experience, and an Executive Secretary of great distinction.

Although he retired from this activity at the end of March, he may still need to be heard from time to time.

Mike has been honored by *Science International's* March 1989 issue which is indeed a *Mike Baker Festschrift* in which nearly fifty individuals have expressed their compliments, congratulations, and memories of Mike's three decades (plus) of service to international science.

CODATA Key Values for Thermodynamics

The Final Report of the CODATA Task Group has been awaited for years despite the publication of 13 interim reports and/or *Bulletin* issues of (*Tentative*) *Key Values*.

The particulars of the book are described on page 5 (*CODATA Publications*). Because thermodynamics--with its breadth of utility in technology, chemistry, physics, and geosciences--spans a wide range of scientific disciplines, it is particularly embraced within the CODATA mandate of "improving the quality, reliability,

(cont'd. on page 5)

CODATA Calendar

1989

March

4-8 Materials Database Management Task Group, Novosibirsk, U.S.S.R.

December

CODATA Officers Meeting, Paris, France

1990

March

22-24 CODATA Executive Committee, Paris, France

July

15-21 12th International CODATA Conference, "Data for Discovery," Columbus, Ohio, U.S.A.

22-23 CODATA General Assembly, Columbus, Ohio, U.S.A.

CODATA Personalities in the News

R. Norman Jones, CODATA's former Vice-President and Director of the epoch making CODATA Freiburg Symposium on Data Handling. Although officially retired from the National Research Council Sussex Drive facility's internationally famed spectroscopy laboratory which he had established in 1977, he had been honored by the Spectroscopy Society of Canada's Herzberg Prize in 1979.

The 1988 Volume 5, No. 33 issue of the *Canadian Journal of Spectroscopy* has been dedicated to him on the occasion of his 75th birthday anniversary. Dr. Jones has been a long-standing supporter of Canadian science--as well as CODATA--and through a distinguished research career has made a worldwide impact on the field of molecular spectroscopy. Some of his earlier friends and collaborators have contributed articles to the dedicated issue in recognition of his ability and dedication to his chosen field. As Ian Butler, Senior Editor, comments, "It is their way and that of the Spectroscopy Society of Canada of saying thank you to a great scientist."

CODATA, too, honors him for his many significant contributions to CODATA's endeavors and hopes that he enjoys continued success in his career.

Edgar F. Westrum, Jr. has been honored on his 70th birthday for contributions to calorimetry and thermodynamics by a *Thermochimica Acta Festschrift* (Vol. #139, March 1989) edited by H. Suga and Y. Takahashi.

First Canadian Workshop on BioInformatics - 6-7 July, 1989 - Ottawa, Canada

The first Canadian Workshop in BioInformatics to be held in Ottawa, Ontario on 6-7 July, 1989 is sponsored by the national Research Council Canada (NRCC), Federal Department of Industry, Science and Technology Canada (ISTC), Health & Welfare Canada, and the Ottawa Carleton Research Institute.

The goal of this Workshop is to bring together researchers (academic and industry), practitioners, users, and science policy makers to explore the expanding role of data banks and new technologies in present-day biotechnology. A balanced workshop--modular in format and focussing on several inter-related topics--offers presentations on the practical applications of these systems as well as a forum for presenting users' needs and the potential impact of new technologies.

List of Speakers and (Tentative) Titles

New Applications

- **Charles Cantor**, Lawrence Berkeley Laboratory, USA. *Human Genome Project: Problems and Prospects*
- **Richard Feldmann**, National Institutes of Health, USA. *Trends in Molecular Modeling*
- **Christian Burks**, Los Alamos National Laboratory, USA. *Databases Relevant to Molecular Biology: New Directions in Managing and Manipulating Them*
- **Dennis Benson**, National Library of Medicine, USA. *The National Center for Biotechnology Information - Projects and Goals*
- **Lois Blaine**, American Type Culture Collection, USA. *Efforts to Provide Interdisciplinary Access to the Terminology and Nomenclature of Biology*

Sequence and Structural Databanks

- **Chris Sander**, European Molecular Biology Laboratory, Heidelberg, FRG. *Information Systems = Databanks + Networks + Access Software*
- **Arthur Lesk**, EMBL and MRC Laboratory of Molecular Biology, Cambridge, UK. *Vertical and Horizontal Integration of Databases in Molecular Biology*
- **Andrew Coulson**, University of Edinburgh, UK. *Sequence Database Searching Using a Parallel Computer*

- **Martin Bishop**, University of Cambridge, UK. *Computing Needs for Large Scale DNA Sequence Projects and Inference of Sequence Function*
- **Chris Rawlings**, Imperial Cancer Research Fdn., UK. *From Databases to Knowledge-bases for Molecular Biology*
- **Michael Zuker**, National Research Council, Canada. *Protein Comparisons: Sequence Alignment*

Microbiology and Cellular Databanks

- **Alain Bussard**, CODATA, France. *The Exponential Growth of Biological: A Challenge for Science*
- **Micah Krichevsky**, National Institutes of Health, USA. *Global Communication Among Microbiologists: Microbial Strain Data Network with the Microbial Information System (MICRO-IS) as Catalysts for Data Standardization*
- **Arnold Pindar**, Laboratory of the Government Chemist, UK. *The Microbial Culture Information Service: Its Growth and Preservation*

Industrial and Commercial Applications

- **Richard Wakeford**, British Library, European Biotechnology Information Project, UK. *Molecular Data Biological Knowledge - A Wider Field*
- **George Garrity**, Merck Co., USA. *Laboratory Information Management Systems for Large Scale Industrial Screening Programs*
- **Jack Franklin**, ASFRA, Netherlands. *The Commercialization of BioInformatics*
- **Joe Modelevsky**, Digital Equipment Corporation, USA. *Why are Industrial Scientists Interested in BioInformation Technologies*

For information, contact: Dr. John R. Rodgers, National Research Council Canada, M-55, Room-275, Montreal Road, Ottawa, Ontario, CANADA K1A 0S2. Tel: 613-993-3294. BITNET: JRR@NRCVM01. Dialcom: CDT0099. FAX: 613-952-9112. For registration forms, contact: Ottawa Carleton Research Institute, (BioInformatics Workshop), 300 March Road, Suite 204, Kanata, Ontario CANADA K2K 2E2.

THE New CODATA BULLETIN

New Directions!

Note the 1988 titles and the 1989 preview on page 5 (CODATA Books)

Annual Institutional Subscription £6S US\$120.

Single and back issues available also.

Available from:

Subscriptions Department, Hemisphere Publishing Co., 79 Madison Avenue, New York, NY 10016-7892

New Format!

New Publisher!

CODATA Publications

Books

Computational Molecular Biology Sources and Methods for Sequence Analysis. Editor: Arthur M. Lesk. (a)

CODATA Key Values for Thermodynamics. Editors: J. D. Cox, D. D. Wagman, V. A. Medvedev. (b)

1988 Bulletins

Abstracts from the 11th International CODATA Conference, *CODATA Bulletin*, No. 68, August 1988. (c)

Guide to Material Property Database Management, *CODATA Bulletin*, No. 69, November 1988. Editor: J. G. Kaufman. (d)

Directions for International Compatible Environmental Data, Vol. I. Report, *CODATA Bulletin*, No. 70-71, December 1988. Editor: Barry I. Diamondstone. (e)

1989 Bulletins

Directions for International Compatible Environmental Data, Vol. II. Position Papers, *CODATA Bulletin*, No. 72. Editor: G. Cynthia Carter. (f)

CODATA Directory of East-Asian Data Sources for Science and Technology, *CODATA Bulletin*, No. 73-74. (g)

....., *CODATA Bulletin*, No. 75.....

(a) Oxford University Press, January 1989. 266 pp., 35 figures, 27 tables. £25.00. ISBN 0-19-854218-6.

(b) Hemisphere Publishing Corp., New York, London, 1989. 271 pp. US\$59.50. ISBN 0-89116-758-7.

(c) CODATA Bulletin, 1988. x + 82 pp. Hemisphere Publishing Corp., New York.

US\$33 or by subscription. ISBN-336-757X.

(d) CODATA Bulletin, 1988. x + 50 pp. Hemisphere Publishing Corp., New York. US\$33 or by subscription. ISBN-336-757X.

(e) CODATA Bulletin, 1988. x + 169 pp. Hemisphere Publishing Corp., New York. ISBN-366-757X

(f) CODATA Bulletin, 1989. x + ca. 220 pp. Hemisphere Publishing Corp., New York, in press.

(g) CODATA Bulletin, 1989. x + ca. 240 pp. Hemisphere Publishing Corp., New York, in press.

Computational Molecular Biology Sources and Methods for Sequence Analysis

This 1989 monograph, edited by Arthur M. Lesk (MRC Laboratory of Molecular Biology, Cambridge, and European Molecular Biology Laboratory, Heidelberg), treats the field of computing with protein and nucleic acid sequences. It describes what data are available (e.g., databanks of protein sequences: the NBRF protein sequence databases, peptide and protein data banks in Japan, additional protein sequence data banks; data banks of nucleic acid sequences; GenBank; the EMBL data library; data banks of three-dimensional structures: the Protein Data Bank). It also explains the analysis and calculations that can be performed, the sources of the data and of software, and the intelligent interpretation of results in scientific applications.

The book arose in response to a CODATA Task Group initiative to bring together information of importance to a wide range of scientists working on sequence analysis in molecular biology. The field is growing in importance, and although the material presented is significant to people working in laboratories, it also has wide implications both on public health policy and on the way science is organized both nationally and internationally.

Readers interested in the developing importance of computing in molecular biology will find this book of interest. In its detailed contents, it should prove most valuable to investigators determining sequences, identifying unknown proteins and interpreting their function, and those interested in the three-dimensional structures of biological macromolecules and in sequence-structure relationships. (For further information, see page 5, CODATA Publications.)

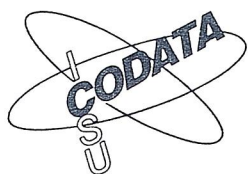
CODATA Key Values (cont'd. from p. 3)

bility, processing, management, and accessibility of data of importance to science and technology.



At a TGKVT meeting in the late 1970's. (left to right) Vadim Medvedev (Moscow) [Editor, deceased], Lev Gurvich (Moscow), J. Drowart (Brussels), William (Bill) Evans (Washington) [deceased], John Cox (Teddington) [Editor, TG Chairman 1974-80], Don Wagman (Washington/Vienna) [Editor]. (Taken by Stig Sunner.)

Although these data will find much application in current endeavors in subsequent updating of thermodynamics tables they provide also an archival record of the embodiment of newer techniques of evaluation. The current endeavors of the
(cont'd. on p. 8)



Task Group on Materials Database Management

Materials Database Newsletter

April 1989, Number 7

As reported in the previous issue of this Newsletter, the **Guide to Materials Database Management** has been published as *CODATA Bulletin No. 69*. The publication provides guidelines and recommendations covering: Management of Operations, including qualifications of personnel, standard procedures, and quality control; Data and Data Management, including documentation and consistency of data and data evaluation practices; System Capabilities and Content, including ease of access, help for users and testing of data systems; and Security, Legal and Pricing issues, including copyright. The Guide includes an extensive list of references and a glossary of technical terms and acronyms. The recommendations apply to databases in any form, whether PC disks, CD's or online systems. Editor: J. G. Kaufman. Publisher: Hemisphere Publishing Corp., 1010 Vermont Ave., NW, Washington, DC 20005, or 79 Madison Avenue, New York, NY 10016-7892, USA; *CODATA Bulletin Number 69*, 50 pp., single copy \$33/£19, or by subscription.

STANDARDS

The **British Standards Institution** has established a **Material Properties Panel (Panel 6)** which will provide a focus for the UK contribution to international standardization efforts in the area of computer-aided engineering, and will report to the BSI Advanced manufacturing Committee (AMT/4). The scope of the panel is to work towards the creation of a data model of materials property information that is required to support the life cycle of a product or component from design and analysis through use and maintenance to disposal and recycling. The panel will liaise with related standardization efforts in materials identification, terminology, materials data interchange, data reporting, software-based materials selection, materials databases, data evaluation models and other materials information issues. Anyone interested in contributing to the panel should contact the panel chairman, Dr. Philip Sargent, Department of Engineering, Trumpington Street, Cambridge, UK, CB2 1PZ.

A study to define a **Pilot Demonstrator project to Integrate Materials Information into the CAE Environment** is to be undertaken by Rolls-Royce plc under joint funding with the European Commission's Directorate General XIII/B. The initial proposal will be debriefed to interested parties in April this year. The proposal will incorporate an analysis of a materials engineering systems (as part of a larger engineering function). Based on the proposal will be a questionnaire which will be circulated throughout the European Community. Analysis of the survey will lead to a number of small follow-up meetings to identify the consensus. Rolls-Royce will then prepare a pilot demonstrator project proposal which will identify the methodology, scope/resources, key tasks and proposed participants. The definition study will be finished at the end of September 1989 when the results will be presented to the Commission and made available to participants. **FURTHER INFORMATION:** R. J. Bamkin, Project Leader, Rolls-Royce plc, PO Box 31, Derby, UK, DE2 8BJ.

ASTM Committee E49 will meet in Atlanta, GA, April 18-20, 1989, to deliberate on the advancement of a number of recommended standard formats for the description of materials and reporting of test results. The material classes include metals, polymers, and composites and the test types include tension, compression, bearing, notched bar impact and plane-strain fracture toughness. Significant studies have also begun on the search for standards related to data quality and reliability. International participation in these activities is strongly sought; interested parties should contact Don Viall at ASTM (see Calendar Listing for address).

The program for the **Second International Symposium on the Computerization of Materials Property Data**, November 29 - December 1 (see Calendar listing) will include some 30 technical papers from 8 countries, in addition to a large number of live demonstrations of PC, CD-ROM and online systems. The major emphasis of the papers will include international overviews, user interactions with data systems and specific applications.

DATA INTERCHANGE

The CEC's Petten Laboratory has commissioned a definition study into the problem of **Materials Data Interchange**. The study will define a Pilot Demonstrator Project to develop and demonstrate a

workable materials data interchange format, with the aim of promoting the market for materials information in Europe. The definition study will be carried out by Dr. P. Sargent, c/o Department of Engineering, Trumpington Street, Cambridge, UK CB2 1PZ.

NETWORKS Successful demonstrations of the enhanced version of the pilot **MPD Network** have been held at a number of ACS, ASM and ASME meetings. This is a forerunner of the production version to be available on **STN International** late next year, and is designed to aid engineers and materials scientists in locating and accessing data to update their own PC or CD-ROM based systems, independent of specific hardware or software.

DATABASES A feasibility study for a database comparing standard specifications of engineering materials is being carried out by Engineering Information Company (London) under contract to the European Commission. **FURTHER INFORMATION:** J. Vvedensky, Engineering Information Co., LTD., 15/17 Ingate Place, London, UK SW8 3NS. Tel: +44 1 622 8155. Telex: 94070600.

The American Society of Mechanical Engineers (ASME) has announced the availability of sections of the **ASME Boiler and Pressure Vessel Code**, including design values, on CD-ROM later this year. It will include sections of the Code, Code Cases, interpretations, referenced ASME standards and Addenda to the Code in later years. **FURTHER INFORMATION:** Information Handling Systems, Tel: 800 241 7824 (USA); or Technical Indexes Ltd., Tel: 44 344 426311 (UK).

CALENDAR

18-20 April 1989: Atlanta, GA, USA

ASTM Committee E49 on **COMPUTERIZATION OF MATERIAL PROPERTY DATA** Meeting. **CONTACT:** Don Viall, ASTM, 1916 Race Street, Philadelphia, PA, USA. Tel: 215 299 5546.

2 May 1989: New York, NY USA

Society of Plastics Engineers **Round Table Discussion of MATERIALS DATABASE Producers.**

7 June 1989: Birmingham, UK

MATERIALS SELECTION AND THE ROLE OF EXPERT SYSTEMS. **CONTACT:** Conference Dept., Institute of Metals, 1 Carlton House Terrace, London, UK, SW1Y 5DB.

27-29 June 1989: St. Louis, MO, USA

ASTM Committee E49 on **COMPUTERIZATION OF MATERIAL PROPERTY DATA** meeting.

27-29 November 1989: Orlando, FL, USA

Technical Committee Meetings of ASTM Committee E49 on **COMPUTERIZATION OF MATERIALS PROPERTY DATA.**

29 November - 1 December 1989: Orlando, FL, USA

Second International Symposium on **COMPUTERIZATION OF MATERIALS PROPERTY DATA.** **CONTACT:** Dorothy Savini or Don Viall at ASTM (see first listing).

15-19 July 1990: Columbus, OH, USA

Twelfth (Biennial) CODATA International Conference, **DATA FOR DISCOVERY.** **CONTACT:** 12th CODATA Conference, "Data for Discovery", Applied Information Technologies Institute, 1880 Mackenzie Drive, Suite 111, Columbus, Ohio 43220, USA

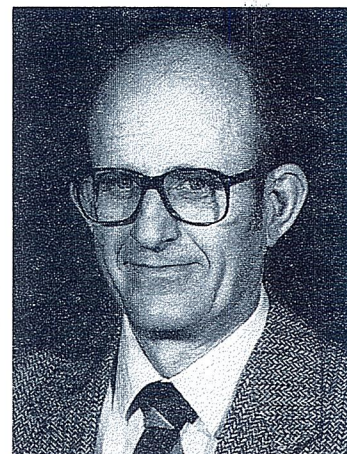
EDITOR: W. G. Jackson. **EDITORIAL OFFICE:** The Institute of Metals, 1 Carlton House Terrace, London, UK, SW1Y 5DB. Tel: +44 1 839 4071. Telex: 8814813. Telefax: +44 1 839 2289. There are no restrictions on the reproduction and distribution of the contents of this Newsletter.

CODATA Key Values (cont'd. from p.5)

CODATA Task Groups on Chemical Thermodynamic Tables and on Geothermodynamic Tables are firmly anchored by these initiatory selections and evaluation achievements. The production of CODATA's internationally generated comprehensive thermodynamic tables depends upon the essential foundation provided by these key values.

"This work chronicles the production of an internationally agreed data set for some basic thermodynamic properties of 151 key chemical species. The project was among the first to be launched by the Committee on Data for Science and Technology (CODATA) of the International Council of Scientific Unions, following its creation in 1966. When we joined the project we little realized that we would still be involved with it 20 years later! During the intervening years many scientists have helped the enterprise along, and we would like to emphasize that the work of critical selection of data, followed by further critical assessment of the initial selections, has been a cooperative, participatory process. We hope, therefore, that the results of the project presented here will find wide-spread acceptance among thermodynamicists, and that others will build our recommended data into more comprehensive data tables and thence into calculations in many branches of science and technology. The use of internationally agreed key values for thermodynamics should go far in assuring harmony among thermodynamicists worldwide." --The Editors.

The book represents the evaluations of the CODATA Task Group on Key Values for Thermodynamics (TGKVT). Their active program dates from their creation in 1968 to 1979, subsequent to their termination in 1979, the editors--and others--devoted much time to the preparation of this report.



Professor Stig Sunner [left] (Sweden, TG Chairman, 1968-74), Professor Loren Hepler [right] (Canada).

C.B. Alcock (Canada, U.S.A.), D.M. Newitt (U.K.), J.B. Pedley (U.K.), I. Wadsö (Sweden), and L. Waldman (F.R.G.) have also served as members of, or consultants to, TGKVT.

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COMMITTEE ON DATA FOR SCIENCE AND TECHNOLOGY



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