

# 31 CODATA / NEWSLETTER

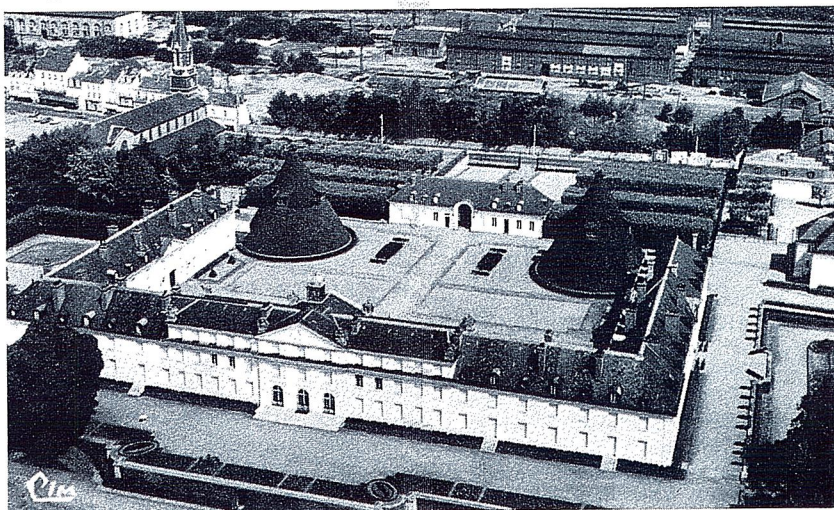
January 1985

## CENTRE BORIS VODAR

The former Bourgogne Secretariat headquarters of AIRAPT (International Association for Advancement in Technology of High Pressure) has been redesignated "Centre Boris Vodar." It retains similar program objectives, e.g., provision of conferences, summer schools, and data banks. The site is the famous Chateau de la Verrerie at Le Creusot, France, shown in the accompanying figure. Some secretarial aspects of the AIRAPT have been transferred to the Netherlands by Professor Trappeniers. The president-elect is Dr. Jean Loriers, Director of the Laboratory of Material Science by Advanced Techniques at CNRS, Bellevue, France.

The municipality of Le Creusot has been most accommodating in its arrangements and is expected to assist in the provision of financial aid for the organization of conferences.

Professor Vodar served CODATA from its inception, first as French Delegate (1966-1970), then as its second President (1970-1974). His



The renowned Chateau de la Verrerie at Le Creusot (Seine et Loire, France) the entrance portal of which (conical structure seen to the left in this view) has been designated in honor of Professor Boris Vodar.

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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.



## Quality Assurance of Chemical Measurement

Location: National Bureau of Standards, Gaithersburg, Maryland

Dates: May 1-2, 1985 and May 8-9, 1985

Seminar Leader: Dr. John K. Taylor, Coordinator for Chemical Measurement Assurance and Voluntary Standardization, Center for Analytical Chemistry

Description: These two-day seminars are concerned with techniques to improve the precision and accuracy of analytical measurements such as those needed in the compositional analysis of materials, process control, and regulatory enforcement.

Seminar Outline: Introduction; measurement as a process; statistical concepts; modeling; planning; sampling; calibration; methodology; quality control; quality assessment; control charts; corrective actions; measurement compatibility; traceability; reporting data; validation; laboratory evaluation; planning QA programs; good measurement practices.

Additional Information: The Seminars will be limited to 50 participants. It is open to all qualified applicants, subject to the availability of space, on a first-come, first-served basis. Interested persons are advised to contact Dr. Taylor at NBS as soon as possible.

Seminar Fee: \$325 per person. Fee includes: tuition, course materials (Instructor's Notes and NBS Handbook 91, "Experimental Statistics," by M.G. Natrella), and refreshments at breaks.

## Displaying Data

Since as much as one third of some scientific journals involve graphical presentations, guidelines for their effective use are relevant as noted by Gina Kolata (*Science*, 12 Oct. 1984, pp. 156-157). Slopes, areas, and vertical distances between curves are difficult to judge. Recent developments by statisticians in illustrating the behavior of data and in establishing criteria for choosing the kind of statistical analyses that are appropriate deserve much wider dissemination in scientific circles. The new volume by W.S. Cleveland (cf. *Newsletter*, p. 7)—when applied—should do much to enhance the quality of graphical presentation.

## Inorganic Data Banks

A colloque "Banques de Données en Chimie Inorganique" (B.D.C.I.) has been organized at Paris for 22-23 May 1985 by the C.N.R.S. Interested auditors should contact: Secrétariat du Colloque B.D.C.I., E.N.S.C.P., 11 Rue Pierre et Marie Curie, 75231 Paris Cedex 05, France.

## CODATA Personalities in the News

Dr. Ronald L. Wigington has been named Deputy Executive Director of Washington operations at American Chemical Society Headquarters, where he will oversee the Books and Journals, Education, and Membership Divisions, as well as financial operations, *Chemical and Engineering News*, public affairs, public relations, marketing, personnel, international activities, and data processing/word processing operations. Wigington was formerly director of the Chemical Abstracts Research and Development Division.

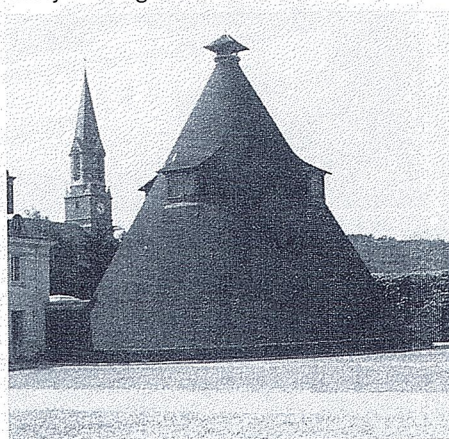
## CEC Data Bank Against Zoonosis

The Commission on European Communities has, on the advice of experts, appointed Unilever Computer Services, Ltd. to develop and market a data bank aimed at fighting infectious diseases transmissible between animals and humans. Some of the zoonotic diseases are fatal (rabies, anthrax), others are unpleasant (psittacosis, contracted from pet parrots). The data bank will provide updated information immediately on an international basis. The substantial need for this type of information from medical and veterinary groups, port authorities, pharmaceutical companies, and tourist organizations arises from the fact that more extensive travel (occasioned in part by the increase in leisure time) results in contact with unfamiliar environments.

## Centre Boris Vodar

(Continued from page 1.)

scientific work spanned many aspects of thermodynamics, solid state physics, and spectroscopy and their application to high-pressure science and technology. He was the founder and first Director (1948) of the Laboratory of High Pressures at Bellevue.



Entrance portal to the Centre Boris Vodar (in the right aisle of the Chateau.)

## International Association for the Properties of Steam

The 10th International Conference on the Properties of Steam in Moscow, U.S.S.R., September 1984, involved 200 participants from 14 countries for reports and discussions of work on the thermodynamic and transport properties of water substance and on solution chemistry problems of importance to steam power generation.

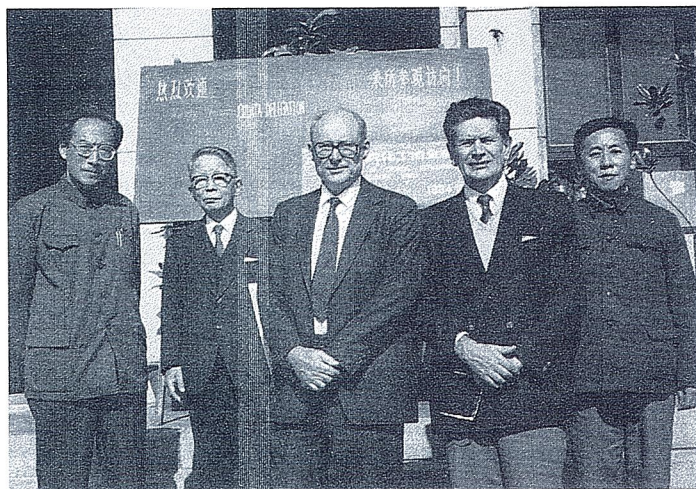
Results of these deliberations include new formal agreements by IAPS (International Association for the Properties of Steam) on formulations of the thermodynamic properties of light and heavy water substances. These agreements are documented in releases entitled "The IAPS Formulation 1984 for the Thermodynamic Properties of Ordinary Water Substance for Scientific and General Use" and "The IAPS Formulation 1984 for the Thermodynamic Properties of Heavy Water Substance." A separate release is to be prepared on new skeleton tables for density and enthalpy of ordinary water substance.

The subjects of invited lectures included non-equilibrium phase changes, the thermodynamics of aqueous solutions at high temperatures and pressures, critical anomalies in transport properties, the evaluation of solubility data in water and steam, and optimization of water chemistry for power plants. Scientific topics relevant to power plant efficiency and durability were covered in both invited and contributed papers. Invited lecturers included Prof. Kenneth Pitzer and Prof. Jan Sengers from the U.S.A.

During the next five years, the ongoing work of the International Association for the Properties of Steam will be carried out by two Working Groups and the Subcommittee on Industrial Calculations. Working Group A will be concerned with the thermophysical properties of normal and heavy water substance and aqueous systems. Working Group B will be concerned with the chemical thermodynamics of power cycles. An important part of the work of Working Group B will involve the preparation of recommended data on the thermodynamic properties of a variety of aqueous electrolyte systems. Working Group A will be concerned with aqueous systems with which Working Group B is not involved, although the two will coordinate their efforts very closely.

Further details on the program, on recent releases, and on the forthcoming proceedings can be obtained from the Executive Secretary of the sponsoring organization (IAPS): Dr. Howard J. White, Jr., Office of Standard Reference Data, National Bureau of Standards, Gaithersburg, MD 20899, U.S.A.





*Left: CODATA leaders visit Beijing. (L to R) Professor Musun Guo, Professor M. Kotani, Dr. D.R. Lide, Jr., Professor J.E. DuBois, and Professor Zhihong Xu. (Professor Guo is the Chinese Delegate to CODATA and Director of the Institute of Chemical Metallurgy. Professor Xu is an Associate Research Professor at the same institution.) Right: CODATA's Secretary General (D.R. Lide, Jr.) and Vice President (J.E. DuBois) lunch in an open-air restaurant in the market by the ancient tombs near Xi'an, Shaanxi Province, P.R.C.*

## CODATA Leaders Meet with Chinese

Three CODATA leaders visited China October 19-29 at the invitation of the Chinese Academy of Sciences. They participated in formal meetings with the newly-formed Chinese National Committee for CODATA and others, banquetted, and visited institutes, colleges, and the computer center of the Academy.

The Academy Computer Center services the institutes in the Beijing region. It is well-equipped with recently-acquired IBM, Hitachi, and Wang computers and is also engaged in software development.

The Academy has received approval for a major program entitled "Science Databases". This involved development of a scientific and technical data network which is eventually to cover all of China. This program will, in fact, be a line item in the next Chinese five-year plan, to begin in 1986. It will fall under one of the "Four Modernizations," viz., the modernization of science and technology. The first phase will involve creation of a local area network linking about 30 research institutes in the "cultural area" of northwest Beijing. They will produce or buy numerical databases in various disciplines to disseminate on this network. The second phase will be to build regional networks patterned after the prototype in Beijing. The final phase will be to link these into a National Information System which will include economic and management information as well. Improvement of telecommunication facilities, which is also a part of the five-year plan, will be a prerequisite for the third phase.

Our conclusion from the visit was that China intends to take an active part in CODATA and views CODATA as a means of learning some of the methodology it needs to pursue its database programs. There was a

high level of enthusiasm and interest. The National Committee:

- agreed with my suggestion to name observers to CODATA Task Groups in 1985. The observers would receive the Task Group correspondence and have an opportunity to make suggestions. After determining which Task Groups are of most interest, the National Committee will propose individuals for consideration as full Task Group members.

- is interested in having CODATA organize a training course in China, perhaps on a regional (East Asia) basis.

- would like to have CODATA send one or more experts in data-base design to China for a two to three week visit. The Academy will cover expenses in China.

- intends that China participate in the 1986 CODATA Conference.

Finally, I should remark on the warm hospitality shown to the CODATA delegation by all of the organizations and individuals involved. The visit was a memorable experience, from both a scientific and cultural point of view.

-David R. Lide, Jr.

## Money/Science

Money is of course crucial for the progress of science, but money alone cannot make science. Science makes itself, grows itself, and is transformed by its own upheavals and surprises.

## ICSU Ratifies CODATA Statutes

The Executive Board of ICSU, meeting in Ottawa in September 1984, ratified the CODATA Constitution developed by the Executive Committee and accepted by the Jerusalem CODATA General Assembly in June 1984.

### ICSU General Assembly

The General Assembly passed a resolution expressing its "deep concern" that entry visas were still being denied to scientists attending international meetings. They mentioned the governments of India, the Soviet Union, and Canada.

The Indian National Science Academy's decision to withdraw its offer to host the next ICSU General Assembly is related. They have apparently been unable to meet the ICSU requirement that all scientists would be allowed entry visas. The 1986 General Assembly will be held in Switzerland.

The International Geosphere Biosphere Program (IGBP) received much attention. Specific proposals as to how to use available instrumentation in a coordinated fashion to monitor environmental changes and the influence of man on the environment were scarce. There was little doubt of the interrelatedness of these areas, but claims of woolly thinking and a lack of specificity in delineating what studies were needed were said to be evident.

The Assembly established an ad hoc planning committee to formulate objectives and proposals relative to IGBP. These included: understanding the interactions between physical, chemical, and biological processes; regulating the earth's unique environmental life; and monitoring the changes that are occurring in this system and the manner in which they are influenced by human action.



## Calendar of CODATA Meetings

1985

### February

- 4-5 Scientific Program Committee. Paris, France.
- 6-7 29th Executive Committee Meeting. Paris, France.
- 8-9 Task Group on a CODATA Referral Data Base. Paris, France.

### March

- 4-8 Coordination of Protein Sequence Data Banks. Paris, France.
- 15-16 Task Group on Geothermodynamic Data joint with Working Group on Thermodynamics of Natural Processes of the International Association of Geochemistry and Cosmochemistry (IAGC) and with the Commission on Thermodynamics of Minerals of the International Mineralogical Association (IMA). Suzdal/Moscow, U.S.S.R.
- Task Group on Multisatellite Thematic Mapping. Sophia Antipolis, France.

### April

- 15-16 Materials Data Systems for Engineering. Paris, France.

### June

- 10-15 Regional Meetings on Protein Sequence Data Banks. Tokyo and Osaka, Japan.
- 17-22 Software for Protein Sequence Data Banks. Georgetown, U.S.A.

### September

- 5-7 Task Group on Critically Evaluated Phase Equilibrium Data. Paris, France.
- 5-8 Task Group on Data for the Chemical Industry. Paris, France.
- 5-8 Task Group on Chemical Thermodynamic Tables. Grenoble, France.
- 7-8 Task Group on Geothermodynamic Data. Paris, France.
- 9-10 Chemical Thermodynamic and Thermophysical Properties Data Bases. Paris, France.
- 11-13 Critical Evaluation and Prediction of Phase Equilibria in Multicomponent Systems. Paris, France.
- 23-27 Workshop on Materials Data Systems for Engineering. Paris, France.

### December

- 9-11 Task Group on a Hybridoma Data Bank. Nice, France.

1986

### May

- Workshop on Standardization of Environmental Data (Tentative). Toronto, Canada.

### July

- 14-18 10th International CODATA Conference. Ottawa, Canada.
- 18-19 15th General Assembly. Ottawa, Canada.

## Chinese National Committee for CODATA

Moving rapidly toward full participation in CODATA in 1985, the People's Republic of China has identified officers and members of their National Committee for CODATA. These are listed below with their scientific affiliation. (CAS has been used as an acronym to identify the Chinese Academy of Science--Academia Sinica.)

**CHAIRMAN:** PROFESSOR ZHOU GUANGZHAO, Vice President, Chinese Academy of Sciences (CAS)

**NATIONAL DELEGATE:** PROFESSOR GUO MUSUN, Director, Institute of Chemical Metallurgy, CAS

**VICE CHAIRMEN:** MR. FENG YINFU, Vice Chairman, Committee on Scientific Publication, Library, and Information Services, CAS, and Project Manager of CAS Scientific Databases

MR. ZHU YONGHANG, Deputy Director, Foreign Affairs Bureau, CAS

MR. FANG JUN, Deputy Director, Department of International Affairs, China Association for Science and Technology

**MEMBERS:** PROFESSOR LIU YUANFANG, Dept. of Technological Physics, Beijing University, Ministry of Education

MR. CHEN JUNYONG, Chief Scientist, National Bureau of Survey and Mapping

MR. JIANG CHUSHENG, Deputy Chief Scientist, Bureau of Science and Technology, Ministry of Chemical Industry

MR. LI ZHOUQUN, Engineer, National Bureau of Standards

MR. DONG XIANQUAN, Engineer, China Research Institute of Metrological Science

PROFESSOR ZHANG TAO, Associate Research Professor and Secretary for Academic Affairs, Division of Earth Sciences, CAS

PROFESSOR XU ZHIHONG, Associate Research Professor, Institute of Chemical Metallurgy, CAS

PROFESSOR LIANG XIYUN, Research Professor, Institute of Chemistry, CAS

PROFESSOR WANG DINGSHENG, Associate Research Professor, Institute of Physics, CAS

PROFESSOR CHEN YIYUN, Associate Research Professor, Research Center for Space Science and Technology, CAS

PROFESSOR FENG BINGGEN, Assistant Research Professor, Institute of Computing Technology, CAS

PROFESSOR LI DIANMO, Assistant Research Professor, Institute of Zoology, CAS

PROFESSOR SHEN DIFEI, Assistant Research Professor and Head of the Preparatory Office for CAS Scientific Databases

MR. LIU SHENFANG, Chief, Division of International Organizations and Conferences, Foreign Affairs Bureau, CAS

MRS. WU GANMEI, Deputy Chief, Division of International Organizations and Conferences, Department of International Affairs, China Association for Science and Technology

**EXECUTIVE SECRETARY:** MR. ZHANG XIAOYANG, Program Manager, Committee on Scientific Publications, Library and Information Services, CAS

"Computers don't standardize; they promote diversity. We are coming closer to the time when the user can design the product and--in sensitive and high-quality work environments--the worker can change his environment and utilize an array of information that makes his or her contribution unique."

..... by Thomas J. Gordon



## Nuclear Data Conference

The International Conference on Nuclear Data for Basic and Applied Science will be held in Santa Fe, New Mexico, U.S.A., on May 13-17, 1985. This conference continues the series of nuclear cross-section and technology conferences begun in Washington (1966) and more recently held in Harwell (1978), Knoxville (1979), Kiev (1980), Antwerp (1982), and Kiev (1983). It will maintain the same general spirit and goals as earlier conferences, providing a forum whereby experimentalists, theorists, and evaluators involved in basic nuclear activities can communicate with scientists who utilize nuclear data in energy, shielding, medicine, space, and other areas of technology. Major emphasis will be placed on nuclear data measurement, analysis, calculation, and evaluation and on the requirements of the various applied areas for nuclear data.

The third mailing was to have been in December, 1984. Potential attendees should contact Phillip G. Young, Mail Stop B243, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, U.S.A.

## Chaos at IUTAM's ICTAM

The 16th International Congress of Theoretical and Applied Mechanics (ICTAM) was held August 1984 at the Technical University of Denmark. Special sessions on chaotic behavior and other sessions on turbulence captured a large share of the attendees at the conference.

This quadrennial event was held under the auspices of the International Union of Theoretical and Applied Mechanics (IUTAM) and was organized by the Technical University's Center for Applied Mathematics and Mechanics. Proceedings of the Congress (containing the full text of only the major lectures) will be published by the North-Holland Publishing Company.

Talks at the Congress covered the entire field of analytical, solid, and fluid mechanics. The 273 lectures and talks and 184 poster presentations were attended by approximately 750 participants. The U.S. had the largest representation (182) and Denmark (70) was second. The U.S.S.R. (12) had approximately the same number as in the two previous meetings, a vivid contrast with the 1200 Soviet participants in the 1972 Moscow meet. The French contributions to chaos and turbulence were said to be especially strong in both the experimental and analytical sides.

*Annual Meeting of the American Society for Information Science (ASIS) October 20-25, 1985, Las Vegas, Nevada.*

## Workshop on Environmental Data

A CODATA Task Group on environmental data met in Chambéry, France, in November 1984 to develop a program for a workshop on Directions for Internationally Compatible Environmental Data. Presentations by invited participants chosen for their special knowledge in data measurement fields will discuss the collection and organization of data in a form (also) appropriate for international exchange and use. This involves knowledge of existing standard measurement methods as adopted by standards organizations such as the International Standards Organization and numerous organizations that deal with the subject of standards within nations or small groups of nations.

The workshop is tentatively planned for one week in May 1986 in Montreal, Canada. Its objectives are assessments of the current status and projected needs for:

- measurement standards and methods for air, water, and soil environments.
- efficient dissemination of environmental data.
- background measurements and global monitoring.

The workshop concerns four broad topics: air, water, soil (including some tests on biota relevant to these), and the subject of data handling (and data systems that drive the needs for measurement standards). Position papers on each of these four subjects will initiate discussions and reviews of the subject by the participants even prior to the actual sessions. A follow-up committee will be selected involving the workshop program committee as well as chair persons and rapporteurs to produce a final report. The report will probably produce recommendations concerning needs for additional or improved standards and for additional or improved baseline data. It may identify organizations for which these recommendations are likely to be relevant and possibly topics for future workshops that may be developed.

The workshop program committee membership consists of

- Michael Martin-Bouyer, Chairman; Université de Chambéry, Chambéry, France
- G.C. Carter; Numerical Data Advisory Board, Washington, DC, USA
- John Clark; International Joint Commission, Detroit, MI/Windsor, Canada
- Barry Diamondstone; National Bureau of Standards, Gaithersburg, MD, USA.
- J. Hahn; Max-Planck-Institut für Chemie, West Germany

● Janne Forslund; Miljøstyrelsen, Denmark

● E.C. Halliday; National Physical Research Laboratory, South Africa

● Andre Marsan; Directeur de la Société Marsan, Montreal, Canada

● Mme. West; Association Française Pour La Normalisation, France

Corresponding members are:

● N.G. Rambidi; All-Union Scientific Research Institute of Metrological Service, Gostandard, USSR.

● Tomasz Plebanski; WZORMAT, Poland

● F. Khalaf; Kuwait Institute for Scientific Research, Kuwait.

(Additional corresponding members are to be added.)

## Tempus Fugit!

Peter Lykos, Professor of Chemistry at Illinois Institute of Technology, Chicago, Illinois, introduced the use of computers into undergraduate chemistry instruction in November 1959—25 years ago!

Using a Sperry Rand Univac 1105 based on vacuum tubes, punched paper tape input, and rudimentary assembly language, the students fit the vapor pressure of benzoic acid as a function of temperature. The instructor provided a subroutine for the evaluation of the Napierian logarithm in the expression  $\ln p = A - B/T$ .

Professor Lykos is the editor of Computer Education of Chemists (Wiley, N.Y., 1984, approx. \$36.60.) based on the American Chemical Society's 1982 Symposium.

## Irish Rock Band Produces Seismic Tremors

An October concert in Brussels rocked not only the audience but also seismic equipment at the Royal (Belgian) Meteorological Institute. Although five km away from the music hall, the earthquake detectors readily registered the vibrations of the percussion described by critics as "frightening" and "possessed."

## IUBS Explores Bio-Technology

One of many interesting endeavors initiated by the International Union of Biological Science (IUBS) Executive Committee at their October 1984 meeting in Paris was the establishment of an Ad Hoc Group for "Bio-Technology" to investigate potential development in this field and to report to the ICSU General Committee Meeting in 1985.



## Reporting Electrochemical Data

.....Petr Zuman

*... pertinent data-reporting details expanded from a Jerusalem CODATA Conference presentation. Not a "CODATA guide" but a considered recommendation that may stimulate more formal actions by appropriate bodies. Professor Zuman is from the Department of Chemistry, Clarkson University, Potsdam, New York.*

In the critical collection and compilation of electrochemical data information inadequate to critical evaluation and to the future use of published data is often encountered.

The names of all compounds studied, preferably in IUPAC or CA nomenclature, should be given together with CA registry numbers. Structural formulas for more complex compounds, source and purity of reagents, and methods of purification are relevant. Preparation of the stock solution (including solvent used, heat, if applied, etc.) and procedures used for establishing stability of the stock solution should be given as well as the purity and sources of all chemicals used in the preparation of supporting electrolytes. Solvent compositions (especially water content and methods for its determination), the nature and concentration of surfactants, ionic strength adjustment, the nature of the electrolyte, and detailed compositions of buffers should be given. "0.1 M ammonia buffer" is inadequate; only "0.1 M ammonia, 0.5 M ammonium chloride" sufficiently describes the buffer used.

The type and geometry of the electrolytic cell should be stated in detail together with whether a two- or a three-electrode system was used and the way the reference and auxiliary electrodes were separated from the examined solution.

The indicator electrode should be described in sufficient detail, i.e., drop time; outflow velocity; material of the electrode, its shape, surface area, dimensions, mode—stationary, rotating, vibrating, hanging, etc.—unstirred or stirred solution, etc., to allow reproduction of results. Less common types of electrodes, pretreatment of solid electrodes, and reference and counter (working) electrodes should be described in sufficient detail to allow repetition. Composition of the electrolyte (nature and concentration of salt and solvent) should be given for less commonly used electrodes. Methods of calibration of the potential of the reference electrode (measurement, pilot ion used, etc.) should be given.

The electrochemical technique used should be described, if possible, using the IUPAC-approved nomenclature [Meites, Nurnberg, and Zuman, *Pure Appl. Chem.* 45, 81 (1976)]. when a new or rarely used technique is used,

it should be described in sufficient detail so that consultation of previous publications is unnecessary. Experimental parameters such as range of applied current or potential; rate of scanning or rotation of the electrode; frequency, amplitude, and phase angle of a periodically applied signal; current-reversal time; etc., should be given. Correction for the iR-drop, counter-current compensation, instrumental subtraction of the residual current, use of the oxygen-removing agent, and mode of data handling should be stated.

The composition of the supporting electrolyte concentration of the ligand and also pH, ionic strength, and temperature for each measured value should be given. For each solution the number of waves, their character (diffusion, kinetic, adsorption, catalytic, etc.), and the characteristic potential, half-wave potential in dc polarography, quarter-transition time in chronopotentiometry, summit potentials in ac and pulse polarography, peak and half-peak potentials in linear sweep voltammetry, etc., should be stated. If this potential is expressed against electrodes other than aqueous SCE, this should be clearly indicated.

The response constant and the independent variable (usually current) should be given both in terms of the experimentally obtained value and in the derived form. Diffusion coefficients should be calculated from current values instead of from experimentally obtained current intensities.

The statement of the total number of electrons should be supplemented by information on how this value was obtained (e.g., by comparison of limiting currents with specified standards and media, from the shape of current-voltage curves for reversible processes, or by coulometry, together with specification of indicator electrode used) and the method of evaluation.

Electrokinetic data should be presented as heterogeneous rate constants at standard potential or, for multistep processes, by information on wave shape.

In preparative electrolysis, products formed, applications of a micro- or macroelectrode, and methods used to isolate or identify products or intermediates should be described in detail. Physical constants or spectral properties of such species should be reported.

Finally, it should be clearly indicated whether the observed process is cathodic or anodic, or if so-called "latent currents" are involved. The shapes of maxima or of unusual waves should be mentioned. If the characteristic potential of the response constant has been proved to be a function of some experimental

parameter (such as concentration, pH, drop time, rate of scanning, starting potential temperature, time, etc.) the relationship should be reported. Similarly, correlations of the characteristic potential or the response constant with other experimental values (such as  $\Delta$ ,  $\gamma$ ,  $\lambda$ , or pKa), with substituent constants  $\sigma$ , or with quantities obtained by quantum chemical calculations  $\beta$  should be stated.

In proposing a mechanism, how it was deduced from experimental data and the degree to which observed variations in experimental data correlate with predicted relationships should be indicated.

## BIOMASS Data Center

The SCAR (SCAR/SCOR/IABO/ACMRR Group of Specialists on Southern Ocean Ecosystems and their Living Resources) BIOMASS Executive accepted a proposal from the British Antarctic Survey for the provision of adequate analytical computing facilities, data management, and infrastructural support.

BAS is to fund a data base manager and a programmer to run a BIOMASS system, so that the costs to BIOMASS would be confined to the recurrent costs of computing and workshops, computer time, and travel expenses for the data manager in the event that workshops are held in locations other than the data center. The BAS offer, which fully supported hardware, software, and personnel costs, (and another from the Alfred-Wegener Institut, Bremerhaven) was generous.

The BAS Institute is well endowed with mini and micro computers and other ancillary equipment which would enhance the data base facility. In addition, data transmission to other centers at which workshops may be held is possible provided adequate links and compatible equipment are available at proposed workshop sites. Since transmission of data via telephone links is expensive, the use of tapes is more feasible. The Executive decided that, in view of the more advanced state of the BAS system and the urgency with which such facilities are required, the BAS offer should be accepted.

The broad direction of the system will be the responsibility of the Group of Specialists, but more detailed administration and supervision will have to be undertaken by the host institute. To enhance such an arrangement the Executive decided that a small Data Systems Advisory Group would be constituted. This group will receive annual written reports from the Data Base Manager and report directly to the Executive on matters relating to the Data System. The Executive will in turn report to the Group of Specialists on these matters.



## New CODATA Publications

**Data in Modern Biology.**<sup>a</sup> Bulletin No. 56 (Nov. 1984). Phyllis S. Glaeser, Editor.

**The Role of Data in Science.** Phyllis S. Glaeser, Editor.<sup>b</sup>

## Books for the Bookshelf . . .

**The Effect of Computers on the Generation and Use of Technical Data.**<sup>c</sup>

**Data Sources Quarterly Periodical.**<sup>d</sup>

**Science Software Quarterly.**<sup>e</sup>

**Application of Minicomputers and Microcomputers to Information Handling.** Jose-Marie Griffiths.<sup>f</sup>

**Encyclopedia of Information Systems and Services 1985-86, Sixth Edition.** John Schmittroth, Jr., Editor.<sup>g</sup>

**The Elements of Graphing Data.** William S. Cleveland.<sup>h</sup>

**Phase Diagrams for Ceramists. Cumulative Index.**<sup>i</sup>

**CRC Handbook of Data of Organic Compounds.** Robert C. Weast, Editor.<sup>j</sup>

**Japanese R & D Centers - 1984.**<sup>k</sup>

**The Infrared Spectra Handbook of Inorganic Compounds.**

**Standards Activities of Organizations in the United States.** Robert B. Toth, Editor.<sup>m</sup>

\* Further details on content, identification, price, source, etc. for above items (if available) are referenced below.

a. CODATA Bulletin. Subscriptions: Regular, US \$45; Personal, US \$15. Individual copies (#56): US \$10. Pergamon Press, Ltd., (UK) Headington Hill Hall, Oxford, United Kingdom OX3 0BW, (Americas) Fairview Park, Elmsford, NY 10523, U.S.A.

b. Proceedings of the Ninth International CODATA Conference, 24-28 June 1984, Jerusalem, Israel. Published by North-Holland Publishing Co., P.O. Box 1991, 1000 BZ Amsterdam, The Netherlands.

c. (1984.) Available from U.S. Department of Commerce, National Bureau of Standards, Office of Standard Reference Data, Gaithersburg, MD 20899. NBSIR 84-2907.

d. Formatted listings of 37 k products and 9 k companies including hardware, software, data communications, local area networks, company profiles, and product comparison charts. US \$150/year. Ziff-Davis Publishing Company, 1 Park Ave., New York, New York 10016.

e. This publication is a resource for natural scientists who use computers. As such, it depends on input from computer users, software vendors, developers and writers, and anyone else interested in the use of computers for natural science applications. (1984.) Center for Environmental Studies, Arizona State University, Tempe, AZ 85287.

f. Up-to-date assessment of the most advantageous applications of small-scale computing equipment in automating information handling procedures. Analysis of the impact of computer technology, present-day applications in libraries and information centers, and recommendations for the future. (1983.) 102 pp. Paper. US \$13.50. UNIPUB, 205 East 42nd Street, New York, NY 10017.

g. Included are information providers, information access services, information sources on the information industry, and support services. (1984.) The International Volume (669 pp., US \$165.00, ISBN 0-8103-1537-6) covers more than 1100 international and national information organizations, systems, and services located in some 65 countries excluding the United States. The United States Volume (about 1400 pp., US \$190.00, ISBN 0-8103-1541-6) covers about 2200 information organizations, systems, and services of international, national, or regional scope. Set = US \$325.00. Gale Research Co., Book Tower, Detroit, MI 48226. ISSN 0734-9068. ISBN 0-8103-1537-8 (set).

h. Deals with improving and expanding graphical data display in science and technology, principles of graph construction, graphical style, graphical methods, high-interaction graphical methods, and graphical perception. (Feb. 1985.) 350 pp. Paper. US \$18.95. Wadsworth Advanced Books and Software, 10 Davis Drive, Belmont, CA 94002. ISBN 0-534-03730-5.

i. This cumulative author and subject index for Vols. I through V in the Phase Diagrams for Ceramists series was compiled at the National Bureau of Standards and edited and published by the American Ceramic Society. (1984.) 96 pp. Soft bound. Nonmember: US \$15; member: US \$10. ISBN 0-916094-60-x.

j. Approximately 27,000 compounds are described in detail. Each table included extensive, yet concise data such as trade names, synonyms, flash points, boiling points, formulas, formula weights, melting points, purity, color, odor, specific gravity, solubility, shipping quantities, and sources of information for each compound. Periodic up-

dates are planned. (due 1985.) 7 x 10. ca. 2000 pp. (2 vol.) US \$200. CRC Press, Inc. 2000 Corporate Blvd., N.W., Boca Raton, FL 33431. ISBN 0-8493-0400-8.

k. Available from Euralia, 3 Rue de l'Arrivee, Cit Boite 144, 75749 Paris Cedex 15, France.

l. Mid-IR reference spectra for 345 inorganic compounds selected from the Sadler Spectra Collections. The spectra are arranged by groups in the periodic chart for easy location and comparison of similar classes of materials. Compounds containing 32 principal elements are presented: B, Al, C, Si, Ge, Ti, Zr, Sn, N, P, As, Sb, Bi, V, Nb, Ta, O, S, Se, Te, Cr, Mo, W, F, Cl, Br, I, Mn, Re, Os, Co, U. Sadler Research Laboratories, 3316 Spring Garden Street, Philadelphia, PA 19104.

m. NBS Special Publication 681. This directory is a guide to mandatory and voluntary standards activities in the United States at Federal and state levels and by non-government (trade associations, technical and other professional) societies. It excludes standards that are proprietary and that originated at local levels of government. It supersedes the 1975 edition (NBS SP 417), "Directory of United States Standardization Activities" and, for the first time, includes standards distributors, libraries, and information centers, and union lists of standards repositories by regional areas. It also lists organizations that no longer develop standards or that have become defunct since the previous directory was issued. 572 pp. Order from Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402. LCC 84-601084.

## Meeting of Task Group on Coordination of Protein Sequence Data Banks

At its General Assembly in June 1984, CODATA established the Task Group on Coordination of Protein Sequence Data Banks. The main task of this Group is to enhance the cooperation among existing data banks on proteins and among their distribution networks, to encourage the creation of new specialized data banks, to facilitate efficient contacts between data bank creators, distributors, and users, and to encourage the solution of technical problems (e.g. nomenclature, format, and software).

The Task Group has formed two subcommittees, both of which met in Paris during the week of 10-14 December 1984. The Task Group also met informally. One subcommittee is preparing a Protein Data Bank Inventory to be published in a CODATA Bulletin. A questionnaire was sent to more than 600 scientists and answers were received from over 25 % of them. The responses were analyzed and additional questionnaires were designed to obtain more detailed information from those scientists having collections of sequences or computer programs for their analysis. The subcommittee on formats addressed the question of devising an exchange format for protein sequence data. The participants identified areas of general agreement and remaining problems. The subcommittees were greatly assisted by several expert consultants, including Drs. S. Sakakibara and Y. Seto (Japan), Dr. J.-M. Claverie (France), and Dr. B. Foertsch and H.W. Mewes (F.R.G.).

The Task Group is chaired by Prof. B. Keil (France) and its members are Prof. A. Tsugita (EMBL, F.R.G.), Dr. W. C. Barker (U.S.A.), Dr. A. Henschen (F.R.G.), Prof. M. Kotani (Japan), Dr. A.M. Lesk (U.K.), and Dr. J.R. Rogers (Canada).

Winona C. Barker



Paris Meeting of Task Group on Protein Sequence Data Banks. (L to R): Drs. A. Henschen, A.M. Lesk, W.C. Barker, B. Fortsch, H.W. Mewes, J.-M. Claverie, B. Keil, A. Tsugita.

Petr Zuman noted in the Sunday Times (London) an article on women in the computer industry reporting that, "Around a quarter to one third of the women recruited to IBM and ICL as graduate trainees are female."



## Hybridoma Data Bank

A meeting of the Hybridoma Data Bank Task Group was held in Geneva on 17-19 December. Task Group members attending were: A. Bussard, Chairman; M. Krichevsky, Secretary; V. Houba; B. Janicki; E. Lennox; and T. Tada. Invited observers were R. Bell, L. Blaine, P. Glaeser, P. Reiniger, R. Stevenson, H. Sugawara, and G. Torrigiani.

The HDB has been officially opened to the scientific community for queries. The bank is being operated as more of an information center than a single database. Questions on cell lines and products not in the bank are researched through outside sources, such as commercial databases, science and medical libraries, and investigators working on projects related to the query. All information gathered through these channels is entered into the bank in proper format and a report is sent to the requestor. Thus, the growth of information in the HDB is partly controlled as a self-organizing data flow. The priority of entry is decided by the nature of the queries received.

The HDB not only provides directory information regarding development and availability of specific immunoreactive products of cloned cell lines but can supply the complete background for each cell line and product in textual or tabular format. Data analyses can also be performed using the powerful capabilities of the MICRO-IS software. Cluster analyses showing taxonomic similarities among virus strains by monoclonal antibody reactivity patterns were demonstrated to the Task Group.

The pilot phase of the HDB project will end in December, 1985. Attendees were briefed on the financial and technical status of the HDB. 1986/87 will be a transition period during which the funding base will be broadened to include donations from private industry. Core support will still be solicited from current funding agencies which indicate willingness to continue their support. It is proposed that during this period, all inquiries to the bank be

answered free of charge as they have been during the pilot period.

After the transition period the HDB will attempt to recover its operating costs through subscription-type charges and fees for special services performed by data bank personnel. These special services will include workshops on storage and retrieval of cell line and product data for major centers of hybridoma development, analysis of data, and creation of custom-designed charts and tables of hybridoma data.

Priorities for the final year of the pilot project include increasing publicity about the bank, establishing a network of contacts at universities and research centers who will supply data to the HDB, and establishing a node in Europe to facilitate data collection and dissemination within the European community.

---Lois Blaine



CODATA Hybridoma Task Group meets in Geneva. (L to R): Dr. E.S. Lennox, Prof. T. Tada, Dr. H. Sugawara, Dr. R. Stevenson, Dr. B.W. Janicki, Dr. V. Houba, Prof. A.E. Bussard, Dr. M. Krichevsky, Ms. L. Blaine, Dr. P. Reiniger.

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