

29 CODATA / NEWSLETTER

July 1984

Highlights

Beginnings	2
Books	14
China	1
Global Change	5
Hybridomas	11
Personalities	9
Profiles	3, 7
Proteins	4, 5
Reference Data	6
Thermo Tables	10
Thermophysics	8

People's Republic of China to Join CODATA

In an April 1984 telex to CODATA's President Dr. W.W. Hutchison from Feng Yinfu (Vice Chairman of the Committee on Scientific Publication, Library, and Information Services of the Chinese Academy of Sciences, Beijing, China) CODATA was informed of China's decision to become a participant in CODATA.

Mr. Feng comments: "Recognizing CODATA's very positive role in promoting world scientific activities, Chinese scientists have been long interested in joining this organization for exchanging useful experiences with their colleagues." Moreover, the prospect of China's membership has long been desired and discussed by administrative bodies within CODATA. Professor Paul Melchior (formerly President of CODATA), Professor Edgar F. Westrum, Jr. (formerly Secretary General of CODATA), and especially Professor Masao Kotani (CODATA's Past President) all endeavored on travels to Beijing to interest the Academia Sinica and the China Association for Science and Technology in membership in CODATA.

The Chinese Academy of Sciences not only is the highest academic organization in China, it also provides an integrated research center for the natural sciences. With about 120 research institutes and 40,000 researchers under its direction, the Academy is very actively conducting research in most areas of both pure and applied science.

The Committee on Scientific Publication, Library, and Information Services of the Chinese Academy of Sciences is one of the Academy's scholarly departments. It is responsible for organizing compilation and dissemination of the scientific data that the Academy produces as well as for making the Academy aware of outside scientific research results through its publication, library, and information services. The Committee is also responsible for establishing the Academy's scientific database system.

While the Republic of South Africa was welcomed to membership in CODATA by the Executive Committee earlier in 1984 (as noted in Newsletter 28), the question of China's membership will be addressed by the General Assembly in Jerusalem. Although China doesn't expect to participate fully until 1985, important CODATA guides for the publication of experimental data and of observational data from the geosciences have already been translated into Chinese and disseminated in appropriate journals by Chinese scientists.

Mr. Feng advised that when notified of CODATA's approval of the application, the Academy of Sciences will organize the China Committee for CODATA, and the executive body of this national committee will be the Academy's Committee on Scientific Publication, Library and Information Services.

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

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

CODATA's Beginnings

by Frederick D. Rossini
CODATA's First President (1966-70)

Since CODATA is now starting its 19th year of operation, I thought it would be interesting and informative to the participants in the 1984 CODATA Conference to have a brief historical review, including an account of the beginnings of CODATA and a note on the great increase in the activities and work of CODATA.

In the 16th century, most of the new results in science were communicated by personal correspondence among working scientists. After Gutenberg came printing, books, and journals. By the year 1800, about 100 different scientific journals had been established; by 1850, the number was 1000; by 1900, about 10,000; and by 1950, about 100,000. Similarly, the number of scientists generating and publishing scientific information has increased enormously. Rough estimates indicate that about 90 % of all the scientists that ever lived are living today, with well over one million scientific-technical papers appearing each year. The quantity of scientific information is said to be doubling about every 7 years.

shows the activities in this area in the principal countries involved:

- In Denmark, Julius Thomsen had published his four volumes of thermochemical data, 1882-86, under the title **Thermochemische Untersuchungen**.

- In Germany came the **Landolt-Börnstein Tabellen**: with 281 pages in 1883; 575 pages in 1894; 877 pages in 1905; 1330 pages in 1912; 8 volumes with 7500 pages in the 5th edition of 1923-36; and 24 volumes of 17,700 pages for the 6th edition of 1950-65.

- In France, the **Tables Annuelles des Constants** appeared in the years 1910-30 in ten volumes, and from 1936 to 1945 came 40 installments.

- In the United Kingdom, the National Physical Laboratory produced the Kaye and Laby **Tables of Physical and Chemical Constants**.

Because of my involvement in such matters in the U.S.A., and because the idea for CODATA was born in the U.S.A., I will cover developments in my country in more detail:

- In 1919, the International Union of Pure and Applied Chemistry, with the patronage of the International

Office of Critical Tables for the purpose of providing guidance, advice, support, and coordination for the numerous data-compilation projects which had come into existence in the U.S.A. Dr. Guy Waddington became Director of this new Office of Critical Tables and served in this capacity for 12 years, until his retirement in 1969.

Now, some words about the beginnings of CODATA...

By 1964, the Office of Critical Tables had been operating for 7 years under Dr. Waddington. In that period, the Office had been reasonably successful in carrying out its aims of coordinating, etc., the national data-compilation projects. By this time, Dr. Waddington and I knew that the time was ripe for international cooperation on a worldwide enterprise similar to the national Office of Critical Tables. He and I had several points strongly in mind: (1) Scientific inquiry is not confined by national boundaries; (2) No country has a monopoly on scientific intelligence; (3) The problem of data for science and technology is an international problem—not a national one; and (4) The most appropriate "umbrella" for such an international scientific enterprise is the International Council of Scientific

No country has a monopoly on scientific intelligence

Scientific inquiry is not confined by national boundaries

Years ago, the individual scientist had reached the point where he was beginning to spend too much time just digesting the original literature of his field, leaving him too little time for his own investigations. So it became necessary to interpose, between the original literature and the end-user investigator, a system of review and appraisal of all the scientific information by qualified experts. These critical appraisals were needed in all areas of science, but the prime area for first development was the field of numerical data for science and technology.

A brief sketch of the status of data-compilation from about 1930 to 1960

*Two years ago, Professor A.S. Kertes kindly invited me to participate in the Opening Session of the 1984 CODATA Conference In Jerusalem, but because of a schedule conflict, my participation was precluded. Recently, the Editor cordially invited me to present, for the Newsletter, the gist of what I would say at the Conference were I present. This invitation was happily accepted.

Council of Scientific Unions, approved a project called **The International Critical Tables of Numerical Data for Physics, Chemistry, and Technology (ICT)**. The U.S.A., through its National Academy of Sciences, assumed financial and editorial responsibility for the enterprise. With Professor E.W. Washburn as Editor-in-Chief and with the cooperation of 408 scientists in 18 countries, the complete work of 7 volumes of the **ICT** was issued in the years 1926 to 1930, with a separate index volume following in 1933. Most unfortunately for the **ICT**, Professor Washburn died in 1934.

- By the year 1950, a number of separate specialized data-compiling projects, operating on a continuing basis, had been established in the U.S., under the support and sponsorship of the American Petroleum Institute, the National Bureau of Standards, the U.S. Bureau of Mines, the U.S. Atomic Energy Commission, and others.

- In 1957, the National Academy of Sciences established the U.S.

Unions, or ICSU, for short.

Fortunately, the Foreign Secretary of our National Academy of Sciences was Professor Harrison Brown, who was also a member of the Executive Committee of ICSU. With this channel of contact, it was proposed to the Executive Committee of ICSU that ICSU provide international coordination and guidance in the area of data for science and technology. In June 1964, the Executive Committee of ICSU approved the proposal and established a Working Group under Professor Brown. The Working Group met in Washington in late 1964 and recommended the establishment, under ICSU, of a Committee on Data for Science and Technology. In April 1965, this recommendation was accepted by the Executive Committee of ICSU, which then requested the Working Group to prepare a Constitution and to seek nominations for membership from countries and Scientific Unions. The Working Group put the final touches on this assignment at a meeting in Frankfurt in the fall of 1965.

In January 1966, at the General Assembly of ICSU in Bombay, India, ICSU,

with Sir H.W. Thompson as Chair, approved the establishment, Constitution, and initial membership of a Committee on Data for Science and Technology. The first meeting of the Committee on Data for Science and Technology was held in June 1966, in Paris, under the chairmanship of Professor Brown. It was at this meeting that I was elected President, Professor Wilhelm Klemm of the Federal Republic of Germany and Professor Boris Vodar of France became Vice Presidents, and Sir Gordon Sutherland of the U.K., Secretary-Treasurer. In addition to being Director of the Office of Critical Tables, Dr. Guy Waddington was asked to become Director of the Headquarters Office of CODATA—an acronym coined by Dr. Waddington. So, for the time, the CODATA Office was assigned to the U.S. National Academy of Sciences, with quarters adjacent to those of the Office of Critical Tables.

Shortly after CODATA began its operations in Washington, Dr. Waddington and I agreed on the following points: (1) The start-up of CODATA was made financially viable by having the CODATA Office housed with the Office of Critical Tables at the National Academy of Sciences and operating under the part-time direction of the Director of the Office of Critical Tables; (2) After CODATA proved itself to be a viable scientific operation in Washington and became financially self-supporting through annual dues from the six National Members (which goals we hoped would be achieved in several years), the CODATA Office should be moved to one of the other member countries, preferably to Western Europe, to ensure international cooperation. This change occurred just as planned, with the CODATA Central Office moving to Frankfurt for a few years, and then to the present Secretariat in Paris.

CODATA's original National Members were six: France, Federal Republic of Germany, Japan, U.S.A., U.K., and U.S.S.R. Initially, there were 10 Union Members.

The Task Groups established in the first several years were three: Fundamental Constants, Key Values for Thermodynamics, and Chemical Kinetics.

This is an appropriate time for me to acknowledge the invaluable help of Professor Harrison Brown in the founding of CODATA and the very important cooperation and help provided by Professors Klemm, Vodar, and Sutherland in those formative years. Moreover, CODATA would never have gotten off the ground and survived through its early years had it not been for the dedicated work of Dr. Waddington.

(continued on page 7)

Frederick D. Rossini, CODATA's first President (1966-1970) was a "natural" for that position. His early association with Edward Washburn, the father of the International Critical Tables at the National Bureau of Standards (NBS), may have provided his initiatory inspiration. Subsequent to the production of the Bichowsky and Rossini book, he was the prime mover in the production of the massive and valuable NBS Circular 500 on inorganic chemical thermodynamics. On the organic side came the famous API 44 collection of thermodynamic data on hydrocarbons (1942)—also started at NBS. It moved to Carnegie Institute with Rossini in 1950 and today is being extended at Texas A&M University.



Frederick D. Rossini

These two giant compilation efforts quickly revealed the need for additional or new data—particularly the need for absolutely reliable key values. So in his own laboratories, with his own hands, and/or with the help of competent assistants (in part trained by him), Fred Rossini generated vast amounts of high quality heat-of-combustion data, mostly by bomb and flame calorimetry. These data were selected to increase the validity of the hoped-for internal consistency of Circular 500 and the tables of API 44.

Good experimental data require compounds of known high purity on which to perform measurements. So it was that Rossini brought the characterization method of freezing point depression to a high level of reliability for quantitative determination of the purity of individual molecular crystals, and particularly hydrocarbons.

To remedy the great gaps in knowledge of the composition of petroleum Rossini undertook (under API Project 42) separation of a representative crude oil into its component parts. A barrel of "Ponca City crude" was laboriously and systematically examined and many hydrocarbons were identified for the first time. Simultaneously, a program for preparation of substantial amounts of high purity hydrocarbons was initiated and samples were made available for experimentation.

Moreover, Dr. Rossini gained the volunteer support of many laboratories throughout the U.S.A. and elsewhere in making determination of numerical data that were needed to fill in important gaps in the tables of API 44.

These various activities reveal the depth of his vision and the scope of his organizational abilities. Rossini was an early advocate of international cooperation as a means of focusing the talents of scientists everywhere on achieving his aims. Thus it was that immediately after World War II, he became a force in the Commission on Thermochemistry of IUPAC which, under his influence, expanded its terms of reference to include essentially all aspects of chemical thermodynamics. His U.S.A. base for the IUPAC connection was the Division of Chemistry and Chemical Technology of the National Research Council of the National Academy of Sciences. When the time came in 1957 to establish the Office of Critical Tables of the NAS, Dr. Rossini naturally turned to that body for the human and other resources needed to take this step forward. Similarly, when the need for expansion of data compilation to the world level became apparent, the step to an ICSU-sponsored activity was a natural one.

There may be some who think that the compiling of tables of data is a sterile activity—merely filling in the squares of a giant matrix. Not so! To the scientist of insight and imagination, thermodynamic (or other) tables provide data on which industrial processes are based. Two examples from Rossini's early work substantiate this claim.

- The thermodynamics of the equilibrium among aliphatic hydrocarbon isomers, easily calculable from data in the publications of API 44, are the key to the tailoring of gasoline by catalytic means to yield maximum amounts of high-quality gasoline from crude oil. This power to control quality and increase yield has added enormously to the value of crude oil reserves. This application of good data is beneficial to the whole world.

(continued on page 9)

Protein Identification Resource Now Online

Since April 1984, updated tapes of the National Biomedical Research Foundation's Protein Identification Resource (NBRF-PIR) Protein and Nucleic Acid Sequence Databases are in the public domain and will no longer be licensed or copyrighted. Similarly, the programs of the powerful computer system for protein identification and for retrieval of associated information are in the public domain and tapes of the databases and programs will be available at nominal handling fees.

The world-wide accessibility of this tool will enable it to have a central role in the development of a human protein catalog and comes at a time, according to researchers at NBRF, when the rate of protein sequence information increase is so dramatic that many of the proteins corresponding to the nucleic acid sequences are poorly identified as to physiological function or even as to their actual existence.

The **NBRF-PIR Protein Sequence Database** now contains over 500,000 residues in over 2600 entries. Included in the databases are:

- All completely sequenced proteins
- Amino acid sequences translated from nucleic acid sequences, including "hypothetical" proteins from unidentified open reading frames
- Amino-terminal sequences and substantial fragmentary sequence data for many types of proteins for which complete sequences are not available
- Bibliographic citations for amino acid sequences, nucleic acid sequences, X-ray crystallography, active site determination, etc.
- Annotations identifying posttranslational modifications, active sites, signal sequences, activation cleavages, disulfide bonds, intron locations, etc.

The **NBRF-PIR Nucleic Acid Sequence Database** now contains more than 2 million basepairs. All entries are annotated to show the locations of protein coding regions, introns, and other features. The protein coding regions are carefully checked against the authors' translations and the sequences as reported from protein sequencing.

This Resource includes not only the two databases described but sophisticated retrieval, search, alignment, plotting, and other software tools to aid researchers in identifying unknown proteins.

The databases and programs of PIR will be accessible via TYMNET; user fees for nonprofit institutions will be subsidized by a grant from the Division of

Research Resources of the U.S. National Institutes of Health.

Information for ordering tapes of the programs or databases or for obtaining online access can be obtained by writing to Ms. K. Sidman, Protein Identification Resource, National Biomedical Research Foundation, 3900 Reservoir Road, NW, Washington, DC 20007, USA.

Coordination among Protein Sequence Databanks

Several databanks dealing with the primary structures of proteins already exist, and new databanks in this field are being planned as well. Their scope and activities—including software support and other services—are very diverse, cooperative efforts among them are limited, and distribution of the results is not always free. Moreover, increasing needs for access to collected data on various aspects of the primary structures of proteins are anticipated.

A group of scientists from France, Germany, Japan, and the United Kingdom met on February 3, 1984 in Paris to discuss in a preliminary way the problems enumerated below:

Current Priorities

- Searching for homologies among known proteins and between potential gene products and proteins.
- Analyzing evolutionary trees.
- Correlating primary sequence data with biological activity.
- Predicting sites of proteolytic cleavage.
- Ascertaining the relationship between the observed protein sequence and the original nucleotide sequence of the gene, e.g., excision of leader sequences.
- Post-transcriptional processing and modification, for example, phosphorylation.
- Correlating mutant sequences with clinical symptoms, for example, sickle cell anemia and effects of other mutant hemoglobins.
- Coordinating the development and distribution of computer programs for the utilization of the databases.
- Aiding in the identification and classification of the nature of proteins that are isolated and sequenced in advance of determining their function.
- Assisting work in protein sequence determination by avoiding unnecessary duplication of effort and simplifying the completion of sequences homologous to known proteins.
- Analyzing hydrophobicity profiles to identify domains and to identify regions of interaction, for example, with membranes.

Anticipated Concerns

- Supporting the design of synthetically-modified proteins by facilitating the application of known sequence and structural information.
- Providing a basis for research in problems for which no satisfactory solutions yet exist, such as prediction of secondary and tertiary structure.
- Helping to identify proteins or protein fragments, for example, from two-dimensional gel maps.

General Problems

- Encouraging the establishment of guidelines and use of standardized nomenclature.
- Helping to establish links—including cross references and compatibilities of formats—between protein sequence databases and other databases containing related information, i.e., between nucleic acid sequence databases and protein structural databases.
- Avoiding duplication and maximizing the effectiveness of the work of different groups in different countries by coordinating and fostering their cooperation.
- Identifying gaps in current programs and recommending new activities when appropriate.
- Guiding the design of the material distributed so that the exploitation of the results is maximally effective for the greatest number of users, including those without special training in computer science and those who only have access to relatively limited computer resources.

In conclusion they proposed, to make—as a working group—a preliminary survey of these problems to be completed before the General Assembly. The CODATA Executive Committee promptly established them as a Working Group; they will collect ideas from as large a community of scientists involved in related work as possible, including those groups which have already created protein sequence databases in widespread use.

Thus, CODATA proudly announces the birth of this new Working Group on Coordination among Protein Sequence Data Banks. The group met at the Secretariat May 11 and 12. Members are: B. Keil (Chairman, Institut Pasteur, France), A. Tsugita (Secretary, EMBL, F.R.G.), W.C. Barker (National Biomedical Research Foundation, U.S.), J.-M. Claverie, Institut Pasteur, France), B. Fortsch (Max-Planck Institut für Biochemie, F.R.G.), A. Henschen (Max-Planck Institut für Biochemie, F.R.G.), M. Kotani (past President of CODATA, Japan), A.M. Lesk (MRC Laboratory of Molecular Biology, U.K.), and H.W. Mewes (EMBL, F.R.G.).

Symposium on Global Change

The International Council of Scientific Unions (ICSU) is considering proposals for an international, inter-disciplinary program to study global change in the terrestrial environment (geosphere) and the life that inhabits it (biosphere) as a closely coupled system. The system is constantly undergoing change on time scales that range from hundreds of millions of years through the slow recurrence of ice ages to transient phenomena. Changes in the geosphere that embrace the land, oceans, atmosphere, and the solar terrestrial domain and in the terrestrial and marine biosphere arise from the interplay of physical, chemical, and biological processes. Over millions of years these natural changes have resulted in the evolution of delicately balanced ecosystems that constitute the global life support system and produce food, fiber, and shelter that sustain human life and give it meaning. To an increasing extent, these changes are influenced by the impact of human activity.

A central intellectual challenge of the next few decades is to deepen and strengthen our understanding of the complex, subtle, and often synergistic interactions between the several parts of the geosphere and biosphere. This knowledge base underpins societal management of our global life support system to enhance biological productivity and to respond to the increasing needs of a growing population.

Augmentation of established national and international programs will be required to illuminate the processes that govern the behavior of the oceans, atmosphere, lithosphere, biosphere, and the solar terrestrial domain by addressing the interfaces among them. This calls for a bold holistic approach which will require several years of careful planning and conceptualization to develop an appropriate scientific strategy. In view of the need to pursue and support existing programs in the several components of the geosphere and biosphere, at least three years will be allocated to formulate questions, to develop themes and sub-programs, to design observational networks responsive to particular research needs and to bring on-stream new technology. The decade of the 1990's appears to be an appropriate period for the proposed international program.

The first in-depth discussion of this program is planned for a scientific symposium to be held in Ottawa, Canada, on 25 September 1984 in conjunction with the ICSU General Assem-

(continued next column)

Protein Sequence Databanks Task Group Proposed

From responses to a survey of the biochemical community, the Working Group (see article page 4) perceived that extant protein sequence databanks reflect the interests of their authors and hence that they have uneven coverage, that they have divergent data organizations, formats, and systems, are seldom on common networks, and lack coordination in acquisition of data software, in its development, and in distribution procedures. The terms of reference of the Task Group proposed by Working Group members would include:

- collection of available information on the existing databanks and distributors of this information—contents, scope, software support, access procedures, future lines of development, etc.—and its dissemination through CODATA publications and professional journals.
- encouragement of the development of a common format for exchange of protein sequences and related data.
- identification and solution of problems of nomenclature and facilitation of discussion between developers and users of the databanks with the IUPAC-IUB Commission on Biochemical Nomenclature.
- coordination of the development of useful software for information retrieval by the collection and dissemination through CODATA of descriptions of available programs and software tools.
- encouragement and coordination of efforts for the development of specialized databanks complementary to the general ones
- organization of meetings at which developers, distributors, and users of databanks can exchange ideas and experience.

bly. Papers summarizing scientific developments over the past 25 years and assessing future prospects for illuminating disciplinary and interdisciplinary perspectives together with unifying concepts and new technologies will be treated. Important aspects of data management will be treated by Dr. W.W. Hutchison (Earth Sciences Sector, Energy, Mines, and Resources, Canada) and Dr. S. Bie (Norske Regnesentral, Norway).

Biological Reference Materials (BRM) Symposium

A symposium on BRMs held in Philadelphia in September 1983 evaluated the present availability, uses, and needs for BRMs for improvement of analytical methods, especially for nutrient analysis. (A proceedings volume edited by W.R. Wolf is listed in the Books Section.) The focus was on improving accuracy and interlaboratory comparability in measurement systems, especially for hitherto neglected organic constituents.

The formal presentations of the symposium concluded with discussions of the programs on Environmental Specimen Banking being carried out in Germany and in the U.S. The existence of these large-scale monitoring programs of a wide variety of biological materials—which are extremely well-characterized for a number of nutrients and which are appropriately documented and stored over long periods of time—can become a stable analytical base for measurement systems involving biological materials.

Further papers on BRMs were presented at the April 1984 American Chemical Society (St. Louis) meeting symposium on "Analytical Standards for the Eighties", organized by Dr. Curt Reimann, NBS. The fall ACS meeting in Philadelphia will include a symposium on "Validity of Nutritional Analyses" organized by Dr. Barbara Klein, University of Illinois, in which further papers on BRMs are to be presented.

In an endeavor to encourage further collaboration and enhance coordination, Dr. Wayne R. Wolf, research chemist at the Nutrient Composition Laboratory, U.S. Department of Agriculture, Beltsville, MD 20705, is soliciting information on availability and sources of BRMs.

Micros in 10% British Homes

Micros are often a youngster's fancy. So it's not surprising that at the end of last year the boom in micro sales coincided with the Christmas season. At the beginning of 1984 it is estimated that one in ten homes in Great Britain has a micro.

The intense interest in home computers has been encouraged and to some extent orchestrated by the Thatcher government—one of the few governments to be led by a former research scientist.

Government policy to place a micro in every school makes sure that the enthusiasm is passed on to the younger generations.

Standard Reference Data in Physical Chemistry *

The traditional approach to preparing tables of reference data on physical and chemical properties has involved the selection of "best values" from the data reported in the primary research literature. In the past 10 years new tools have become available for carrying out this process in a more systematic and comprehensive manner. This has come about first, through a gradual refinement of the theoretical framework which relates macroscopic physical properties to microscopic structure and second, through the availability of computers to carry out the calculations on such theoretical models. The modern approach to the preparation of reference databases thus involves the fitting or correlation of all available experimental data to an appropriate physical model. This helps not only to eliminate discrepant data points but also gives a basis for predicting properties in regions where no experimental measurements have been reported.

This symposium illustrated the way in which this approach is being used in a number of areas of physical chemistry. The first session dealt with thermodynamic and transport properties. Kenneth Pitzer reviewed the status of models of electrolyte solutions and discussed the evaluation and prediction of electrolyte properties as a function of ionic strength, temperature, and pressure. David Garvin described the handling of thermochemical data, stressing the analysis of very large sets of compounds that are "coupled" in complex ways by reaction data. This approach assures internal thermodynamic consistency of data collections such as the new NBS Tables of Chemical Thermodynamic Properties. Edward Mason discussed the use of the corresponding-states approach to correlate and predict the transport properties of gas mixtures. Finally, Jan Sengers discussed the application of critical-point universality to the prediction of thermophysical properties of fluids in the supercritical region.

The second session dealt with spectroscopy and kinetics. William Milne gave an overview of computer-readable databases available through interactive on-

line networks, stressing that the potential of present technology has not been realized because of a lack of validated data to put into the systems. William Stwalley described the determination of potential energy functions of diatomic molecules from high resolution spectroscopic data. Carl Lineberger reviewed the methods of measuring electron affinities of atoms and summarized the present state of our knowledge of accurate electron affinities. Fred McLafferty discussed the use of a mass spectral database for substance identification and the development of intelligent software for interpreting the mass spectrum of a previously unmeasured compound. Norman Cohen reviewed the evaluation of chemical kinetic data on gas phase reactions and showed how theory can be invoked in treating sparse data sets of low precision.

The symposium illustrated the application of a common conceptual approach to highly diverse physical and chemical properties. We can expect to see expanded use of this means of consolidating and extending the results of laboratory measurements.

—David R. Lide, Jr.
National Bureau of Standards

Workshop on Indicators of Data Document Quality

Meeting on 8-9 May at the National Library of Medicine, Bethesda, Md., about 65 selected experts (including participants from government, industry, and academia together with data users, compilers, evaluators, publishers, editors, etc.) deliberated on objectives and data categories concerning the quality of documentation from which the user can judge data validity. A 1982 workshop on indicators for the quality of data preceded the present discussion.

The (ambitious) objectives of the present endeavor—intended to provide the user with tools to assess the completeness of the information reported in a document and not to provide a judgement of the scientific quality or correctness of the data—were:

- to develop a set of indicators that characterize the completeness of reports of health or environmental data. The indicators will represent critical parameters that permit assessment of the reliability of the data.
- to recommend a format to the technical community for use of these indicators by authors, reviewers, abstractors, and database generators.

The five data categories selected reflect those measurement areas which

require documentation of a variety of parameters in order to draw comparative conclusions and which, without adequate documentation, raise questions as to data validity. They are:

- health effects—mammalian test species, laboratory tests of the effects of chemicals,
- health effects—in vitro tests of the effects of chemicals,
- ecological effects—aquatic/terrestrial, laboratory/field measurements,
- occupational measurements—physical/chemical agents in the workplace, and
- environmental measurements—air/water/soil effluents.

Among the CODATA members of the Steering Group roster were Dr. Cynthia Carter (NDAB) and Dr. George J. Cosmides (National Library of Medicine). Dr. L. Gevantman (ret., NBS) chaired a Work Group.

Information concerning the report of the Workshop may be obtained from R. Garrity Baker, Staff Executive, Chemical Manufacturers Association, 2501 M Street NW, Washington, D.C. 20037.

SIG/NDB Chairmen Plan ASIS Data Session

Chairman Cynthia Carter and Chairman-elect Helen Pfuderer are preparing the portion of the program that SIG/NDB (Special Interest Group/Numeric Data Bases) will sponsor at the 21-25 October American Society for Information Science (ASIS) Meeting in Philadelphia, Pa. Their current ideas include:

- data reporting in the literature—an exchange between reporting agencies (publishers) and users about the retrievability of numerical and factual data from published literature in view of current editorial policies with respect to figures, tables, etc.
- database on databases—for location of data sources.
- the future of computerized data dissemination—an interactive discussion with publishers, research scientists, data generators, computer and information scientists, and various data users.

Erratum

With demeanor abject and posture penitential, the Editor acknowledges confusion of Howard J. White, Jr. with Guy K. White (photo, page 8). It was the latter who received the Thermal Conductivity Award (Newsletter 27, page 1) and who should have been so credited. The former has claim enough to fame (see page 9 this issue).

* A Symposium at the American Chemical Society's St. Louis, Mo. Meeting, April 9-10, 1984.

NBS Workshop on Computers and Technical Data

A two-day workshop was held at NBS on March 19 and 20 to discuss the revolutionary changes that are occurring in the generation, dissemination, and use patterns of scientific and technical data as a result of the widespread introduction of computers. Participants included NBS staff and about 160 representatives from industry, professional societies, scientific publishing companies, universities, and other government agencies. The primary goal was to obtain input from a broad cross section of users to identify the proper role of government, and NBS in particular, in addressing these changes. The capabilities of computers in generating new types of data and establishing a better interface between the user and these data promise to greatly enhance the productivity of scientists, engineers, and all of industry.

During the first morning of the workshop, the broad issues to be considered by the participants were presented in talks by Dr. John McTague, Deputy Director, Office of Science and Technology Policy, Dr. Michael Wozny, Director, Center for Interactive Computer Graphics, Rensselaer Polytechnic Institute, Dr. Michael Jefferies, R & D Manager, Engineering Physics Laboratories, General Electric Company, and Dr. Ernest Ambler, Director, National Bureau of Standards.

In the afternoon session, speakers considered the implications of these issues in three broad technical areas. Fluid properties and thermochemical data were discussed by Dr. David Roth, Director, Office of Science and Technology, Allied Corporation, and Mr. Neil Olien, Chief, Chemical Engineering Science Division, NBS. Atomic, molecular, and nuclear data were considered by Dr. James Wynne, Watson Research Center, IBM, and Dr. Wolfgang Wiese, Chief, Atomic and Plasma Radiation Division, NBS. Finally, the broad area of materials performance data was discussed by Dr. Jack Westbrook, Materials Information Services, General Electric Company, and Dr. Louis Tescardi, Chief, Metallurgy Division, NBS.

These plenary presentations revealed a sharply enhanced interest in new capabilities brought about by the computer "revolution." The latest interactive computer manipulations and simulations for high-tech applications were described, including the opportunities for utilizing predictive modeling techniques as a method of provenance for technical data. The process of model building and

(continued on page 12)

Masao Kotani, the elected President of Tokyo Science University for three terms (1970-1982), also served as the President of CODATA from 1978-1982 and subsequently as Past President. As chairman of the effective Task Group on Accessibility and Dissemination of Data (1971-1978) during the earlier years of CODATA, he established many policies which still define programmatic thrusts.

No stranger to academe, Professor Kotani (born in Kyoto, 1906) graduated from the University of Tokyo in 1929 and became a lecturer in engineering. Only three years later, he became an associate professor in physics. In 1943, having acquired his D. Sc., he became a full professor of physics, and in 1966 he moved to a professorship in engineering science at Osaka University.



Masao Kotani

Although youthful educational experiences gave him an inferiority complex relative to experimentation, experiences in mountain climbing in the Japanese Alps and visiting the Bonin Islands enhanced his curiosity about and admiration for nature and these have guided his scientific pursuits through the years. His scientific investigations in quantum molecular science led to the evaluation of molecular integrals and the polarizability of the hydrogen molecule as well as to developments in our understanding of molecular orbital theory, ionic homopolar resonance, inorganic complexes of transition metals, magnetic properties, ligand field theory, and complex biological molecules such as myoglobins and hemoglobins. The trend first involved physical properties and later the biological activity of these life-supporting chemical species.

Ideas continue to tumble out one after the other in his interdisciplinary pursuits and his scientific pilgrimage has continued unabated through administrative duties, conference planning, and other activities. Not only an inveterate traveller—one at home in many countries—he is so skilled in mathematical lore that friends have felt Kotani was himself scooting around on Riemann surfaces to achieve the desired results. His legendary inattention to time and his seemingly unbounded energy reserves have led to a Japanese laboratory designation for time in terms of a "Kotani"—roughly three hours. His seminars usually extended between one and two Kotanis.

His awards include the Japan Academy of Science Prize (1948) for work on magnetrons and microwave circuits, the Fujiwara Award (1974) for distinguished contributions in molecular- and biophysics (particularly to ligand field theory), and a commendation by the Japanese government for cultural service (1979). In the subsequent year, he received the Order of Cultural Merit in the presence of Emperor Hirohito.

His personal demeanor comprises modesty, reserve, and politeness to an extreme. Small only in physical stature and voice, he seems to have inspired tender affection from several generations of students who embrace a variety of physical disciplines as well as from colleagues and associates in many fields.

ROSSINI (continued from page 3)

CODATA was originally organized to provide a framework capable of expanding to cover new and broader activities. However, I doubt if any of us in those early years could have pictured the great growth in the scope of CODATA, both scientific and geographic, that has developed over its nearly two decades of existence: the number of Member Countries has gone from 6 to 17; the number of adhering Scientific Unions has increased from 10 to 15; the number of Task Groups has increased from 3 to 13; and in contrast with the early focus on physics and chemistry, the areas of science covered by CODATA have ex-

panded to include astronomy, biology, chemical engineering, computer-information, and geology, as well as the basic physico-chemical disciplines. It goes without saying that the number of scientists now associated with CODATA has increased enormously.

This great growth in the activities and work of CODATA has clearly come about because of the need for such work and services. It is a great tribute to those who have guided CODATA after its first several years.

I congratulate all the Officers of and participants in CODATA today and extend best wishes for a very fruitful 1984 Conference and continued success in the CODATA enterprise.

CODATA Task Group on Thermophysical Properties of Solids

Among the several endeavors of the CODATA Task Group on Thermophysical Properties of Solids since their September 1983 meeting in the U.S. are:

- an SRM project emphasizing experimental methods on such standard candidate reference materials as iron, austenitic steel, tungsten, and polycrystalline graphite,
- measurements on SRMs of low thermal conductivity materials (e.g., cordierite, Pyroceram 9606, etc.),
- critically evaluated tables of thermophysical properties of key solids, and
- thermophysical properties of SRMs.

The latter two projects are described in more detail below.

TABLES OF THERMOPHYSICAL PROPERTIES OF SOME KEY SOLIDS

This project, directed by Dr. G. K. White, CSIRO-NML, Australia, is producing internationally accepted recommended (critically evaluated) thermophysical properties of several key materials. These are to be published soon as a CODATA *Bulletin* documenting the results of the evaluation project.

This will include sections on:

- heat capacity of Al_2O_3 , Cu, and W;
- thermal expansion of Cu, Si, W, and Al_2O_3 ;
- electrical resistivity of Cu, Fe, W, and Pt;
- thermal conductivity of Cu, Fe, W, and Pt;
- thermal diffusivity of Cu, Fe, and W; and
- absolute thermopower of Pb and Cu

by analysts F. Castanet, CINDAS, S.J. Collocott, J.G. Hust, R.B. Roberts, H.E. Schmidt, C.A. Swenson, and G.K. White and reviewers J. Bass, D. Ditmars, M. Laubitz, P. Schroeder, and R.E. Taylor.

The Task Group believes that its projected publication will be a milestone both in terms of scientific content (critically evaluated data on key materials) and in terms of illustrating a sound methodology for critical evaluation in the thermophysics field.

THERMOPHYSICAL PROPERTIES IN THE GEOSCIENCES

Important objectives of this project include 1) thermal conductivity and

thermal diffusivity measurement technique intercomparisons where the focus is on obtaining reliable data on earth materials under mantle conditions, that is, at pressures up to 10 GPa and several hundred degrees Kelvin, and 2) evaluation of candidate standard reference materials in powder and solid (single crystal and polycrystalline) form. The proposed approach to attain these objectives includes interlaboratory measurements through the exchange of personnel between research groups and the exchange of reference materials and data.

Thus far, exchanges have occurred among the Potsdam, Kyoto, and London (Ontario) groups. Correspondence has been initiated by Prof. A.E. Beck of Canada with groups in Sweden, South Africa, U.S.A., England, Federal Republic of Germany, and Japan. This hopefully will lead to a broader base of exchanges.

One concern of the group is test materials. After a number of measurements on typical materials such as olivine, it became evident that several additional candidate calibration materials covering a range of properties needed to be identified. After consultation with the community, halite was selected because of its simple structure and known good behavior up to very high pressures, single crystal quartz because of its known anisotropy and behavior at

normal pressures and temperatures, fused quartz because of its importance at lower pressures to the geothermal community, magnesium oxide for reasons similar to those for halite, and potassium bromide because of its availability in pure form, its known phase transformation at

1.9 GPa, and because researchers in the field are already evaluating it.

Initially, material is provided from a single source, so that all measurements are performed on a common material; later, interlaboratory visits are proposed.

Results to date on KBr interlaboratory comparisons show significantly different experimental results, particularly near the phase change; those on NaCl indicate that measurement technique modifications may be necessary at high temperatures where radiation contributions are significant.

The Task Group consists of:

- Prof. A.E. Beck
The University of Western Ontario,
Canada
- Dr. R. Berman
Oxford University, U.K.
- Prof. F. Cabannes
Universite d'Orleans, France
- Mr. J.G. Hust
National Bureau of Standards, U.S.A.
- Dr. M.L. Minges, Chairman
Wright-Patterson Air Force Base,
U.S.A.
- Dr. G.K. White
CSIRO National Measurement Laboratory,
Australia

Stockholm Training Course on Non-Bibliographic Data Banks

With an international faculty of 27 (18 from Sweden, two each from U.K. and U.S.A., and one each from Austria, Denmark, Luxembourg, F.R.G., and France) almost as large as the participant group of 40 from such diverse origins as Australia (1), Columbia (3), Costa Rica (1), Denmark (1), Ethiopia (1), Finland (1), India (1), Kuwait (1), Malaysia (1), the Netherlands (1), Norway (1), Philippines (1), Poland (2), Singapore (1), Sweden (20), Syria (1), Thailand (1), United Kingdom (1), Yugoslavia (1), the course made a significant impact on its clientele. The course was held October 15-22 in Stockholm, Sweden under the auspices of Unesco, the Swedish DFI, and CODATA. Stephan Schwarz was the organizer and chari-person.

Such information as has filtered down through channels indicates that the October 1983 Stockholm course on data has to be acknowledged as a very successful endeavor by students, faculty, and bystanders. Accommodations and cuisine at Hasselby Slott were superb; generous financial support came from Unesco and the Swedish DFI; internationally known lecturers including CODATA stalwarts David G. Watson (Cambridge, U.K.), David R. Lide, Jr. (NBS, U.S.), and Alex Lorenz (IAEA, Austria) provided background; and a large number of scientists—mainly Swedish—provided specialty lectures covering a broad spectrum of topics for the students (and other teachers!).

Certainly the perennial dilemmas of lecturers' commitments and funding allowing but a single week must have taxed the absorptive capacity of the students with their differing backgrounds and language capabilities.

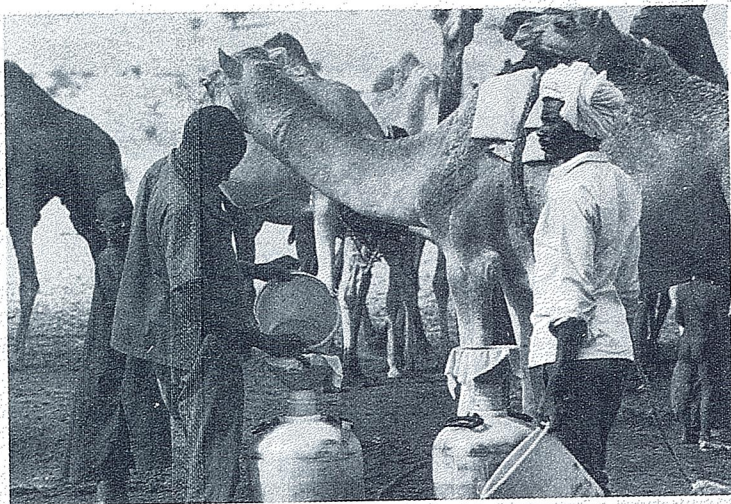


G. K. White

CODATA Personalities in the News

Professor A.S. KERTES of Hebrew University and Chairman of both the Scientific Program and the Organizing Committees for the Ninth CODATA Conference was also the recipient of the triennial International Solvent Extraction Conference Award "for outstanding accomplishment and meritorious achievement in solvent extraction." The award was made in Denver, Colorado (U.S.A.) in September 1983.

(Incidentally, the Editors would appreciate identification of other achievers from among CODATA adherents.)



Sampling a shallow nomad-used well in a section of the Sahel northeast of Lake Chad called the Kanem for the analysis of carbon 14 to determine the age (time since equilibration with atmospheric radiocarbon) of the water.

Courtesy of A.B. Muller, OECD

ROSSINI PROFILE (continued from page 3)

- The determination by Rossini and colleagues of the heat of transition of graphite to diamond, as a part of the determination of thermodynamic properties of key compounds, has been a key datum in selecting conditions for the catalytic production of industrial diamonds.

In summary, we see in Fred Rossini a man who has spent a lifetime pursuing a clear, integrated plan to determine experimental property values of pure substances and to encourage others to help in the collection, evaluation, and compilation of such values and to activate successfully a world-wide program to make good data available from all branches of science for the benefit of both science and technology.

Additionally, from his birth in Monongahela, Pennsylvania, in 1899 through an earned doctorate from the University of California at Berkeley in 1928, seven honorary doctorates, NBS section chiefdom, named professorships, departmental headships, directorships, deanships, University of Notre Dame Vice Presidency for Research, lectureships, fellowships, and society offices as well as 14 medals, awards, and prizes, Fred found time enough to author 263 publications including 11 books.

His national and international professional service would require another "Profile" just to list in outline. Is it any wonder that the the Rossini Lecture-ship is the highest award for thermodynamicists?

President of CODATA? Yes—while serving simultaneously as President of the World Petroleum Congress, Vice President of Associated Midwestern Universities and of Argonne Universities Association, etc.

(The Editor acknowledges with appreciation the knowledgeable and enabling contribution of Dr. Guy Waddington to the preparation of this profile.)

Incentives for Evaluators

The Numerical Data Advisory Board (NDAB) has asked a small group to explore incentives. T. Massalski (Chair, Carnegie-Mellon, Pittsburgh), J. Rumble (National Bureau of Standards, Washington), and B. Carroll (Oak Ridge National Department of Energy, Oak Ridge) formulated some suggestions within a national framework. However, they have a broader application in promotion of critical evaluation endeavors elsewhere.

Their conclusions, tersely phrased, are that:

- Adequate, direct grant support is the best incentive. Consequently, in evaluation programs with good funding, incentives are not a major problem. For new evaluation programs in which funding is neither secure nor sufficient, incentives can be useful.

- Incentives that can attract the best people to evaluation work include:

Monetary incentives

- Extra research money as a reward for evaluations
- Summer support money to faculty
- Grants to institutions for evaluation activity

Other incentives

- Publication credit
- Preferred access
- Awards

Preferred access implies obtaining access to other evaluated data projects such as the American Institute of Chemical Engineers' DIPPR Project in which supporters get priority in exclusive use of the data for a year.

Money is seldom the key to get management to permit senior people in industry to devote time to evaluation. Here, other incentives are more meaningful.

They suggest:

- NDAB should work actively with leading scientific and engineering societies to have them establish prestigious awards for evaluation work.

- NDAB could compile a list of groups which support and encourage evaluations. Not only could this be distributed on an individual basis, but a news article in the popular scientific press would call attention to it.

- NDAB could send a letter to department chairmen at universities encouraging them to give appropriate weight to evaluation publications in tenure and promotion situations.

Thermodynamic Tables – An Interview with TGCTT Chair Howard White

CODATA probably has made more extensive data endeavors in chemical thermodynamics than in any other single disciplinary field. In view of the wide interdisciplinary utilization of thermodynamics, this has been an appropriate allocation of manpower and funding. The CODATA Task Group on Chemical Thermodynamic Tables (TGCTT) under the direction of NBS's Dr. Howard White, Jr., chair, is presently undertaking a major new international project in chemical thermodynamics. It involves far-reaching implications in complex data manipulation, compilation, evaluation, and presentation and represents a new departure even among CODATA projects. This is revealed—at least in part—by the following interview with Dr. White.

Editor: Howard, during much of the past decade your industrious Task Group has been developing formats, procedures, and a whole modus operandi to enable the production of a master set of international thermodynamic tables to which additional volumes may be added from many sources and yet, as Ward Hubbard once said, " . . . will be totally self-compatible, self-consistent, etc. They'll 'fit' on the same shelf." What is the current status of this endeavor?

Dr. White: Briefly, Edgar, we have worked out a plan to produce such an international set of tables and have convinced ourselves of its soundness by producing a small set of tables according to that plan. In our minds feasibility has been established; what remains is to obtain the acceptance and cooperation of the thermodynamics community.

To show what we have been doing in somewhat more specific terms, it is instructive to think about merging two tables. There are two classes of problem. The first, and easier, involves conventions: the units used, the reference states, the functions tabulated, etc. These generally can be converted from one to the other. It may be complicated, tedious, and a lot of work, but it can be done. The other class is harder. How is a given number in a table related to the experimental data on the one hand and to the other numbers in the table on the other? If I wish to change a number, either because of new data or to be consistent with another table, what other numbers must I change to maintain internal thermodynamic consistency? By how much? Will I like the overall result? These have always been very hard questions to handle. So hard that the tables usually were done over completely.

Several developments make it possible to answer such questions now. What might be called an automated chemical accounting system has been devised which can provide answers to each of the questions asked above. It also can document the relationship between numbers in the table and given experimental measurements. Also, a body of automated methods have been developed to treat the effects of changes in temperature and in composition.

We have adopted a set of conventions and a set of automated methods so that it is possible to add to or change numbers in the tables more or less at will. This makes it possible to produce the tables in a decentralized way, although, as you would expect, there must be an eventual step drawing things together.

Editor: And at this stage, what has been produced to acquaint the interested scientific community with your progress?

Dr. White: There are two major reports, Edgar. The first is "A Systematic Approach to the Preparation of Thermodynamic Tables", which is available as CODATA Bulletin No. 47 of May 1982. In this we discuss the preparation of large sets of tables of thermodynamic properties. We then make a step-by-step analysis of the flow of work during the process of

data evaluation and use this analysis to define the structure of an international program to prepare a wide-ranging set of thermodynamic tables. It represents, if you will, a systems analysis of the process of evaluating thermochemical data and a plan for further action. Anyone interested in understanding the basis for what we are doing should read this.

The second report is entitled "CODATA Thermodynamic Tables: Tentative Selections for Some Compounds of Calcium and Related Mixtures. A Prototype Set of Tables." This is in the final stages of preparation and will also be published by CODATA. As the name states, these are prototype tables. They represent on the one hand implementation of the plan discussed above and on the other hand our conception as to what a definitive set of international thermodynamic tables might look like. That they are international is beyond dispute. There are major contributions from France, the U.K., the U.S.S.R., and the U.S.A. There are data for an alloy, a molten salt mixture, an aqueous solution, thermal functions, and formation properties for the individual substances and mixtures. The data cover a range of temperatures and, where relevant, of concentrations. All results are based on the CODATA Key Values. We think that we have covered the important classes of substances and properties with the important caveat that we have not yet dealt with the effects of pressure, so we are considering condensed phases at moderate pressure.

Editor: How will you get feedback from the scientific community?

Dr. White: We hope that the prototype tables will be examined by many people. The "Systematic Approach . . ." has been out for a while, but it's a bit abstract. The prototype tables are concrete examples.

Several of us have given brief reports at meetings and David Garvin and I have a paper on the program for the Joint Calorimetry Conference/IUPAC Thermodynamics Conference in Hamilton, Ontario in August. We hope to have copies of the tables available there and at least a few at Jerusalem for the CODATA Conference.

Finally, we have talked with a number of people and have had several attend Task Group meetings. I think that everyone wants the end result that we are working toward and so is well disposed toward such an effort. It remains to be seen to what extent we have met their expectations.

We will, of course, revise the prototype tables and plans in accordance with comments we receive. There is also the problem of getting people familiarized with our ideas. After all, we have been working on the problem for some time and other people haven't. It took a lot of time and discussion for all of us to reach agreement and it is reasonable to expect that others will have to chew on things for a while, too.

Editor: Once the constructive criticism has been assimilated, what is the next step?

Dr. White: At its meeting in Kyoto in 1982, CODATA endorsed the basic plan and told the Task Group to set out to prepare a comprehensive set of international tables. The prototype tables represent the first step. They set the conventions, the format, and the style. If other tables are prepared in the same way, and this includes using the same computer programs to produce some of the material as well as the conventions and formats, it will be possible to make these tables consistent with the prototype tables and with each other. In this way, comprehensive tables can be built up. It will be necessary for cooperating workers to work closely with the Task Group particularly in the early stages because the system is anything but routine at this stage.

(continued on page 15)

Hybridoma Data Bank Nearly Ready

Despite the longstanding use of antibodies as immunological tracers in medical diagnosis, bacteriology, veterinary science, agriculture, biochemistry, etc., the invention by KOHLER and MILSTEIN, in 1975, of permanent lymphoid cell clones (immunoclones, IC's)—or hybridomas—was a major step toward the goal of obtaining monospecific reagents: monoclonal antibodies (MA's) and pure immunological factors (such as T cell clone factors, etc.). These MA's can be used to detect and titrate almost any immunogenic substance (or by the use of coupled carriers, any hapten). Consequently MA's have been used in the medical diagnostic field (bacteria, viruses, parasites, hormones, enzymes, transplantation antigens, allotypes, etc.) as well as in veterinary science, genetics, neurophysiology, agriculture, biochemistry, organic chemistry, etc. As a result of their exquisite specificity in an immunoabsorbant system, MA's can uniquely "pick" a given substance which is present in small amount in a mixture of other substances and serve as a preparative agent. A good example is the recently achieved preparation of blood interferon.

While the use of MA's in therapeutics, both human and animal, is not as widespread as it is in the diagnostic and preparative applications, the motivation for finding a cure for certain fatal diseases, such as cancer, is so great that the search for new MA's as therapeutic agents is developing very rapidly. IC products other than MA's, such as T cell factors, macrophage factors, etc., have been produced and are useful for understanding the mechanism of immune response. Finally, IC's can be the source of non-secreted products such as membrane components, RNA, DNA, etc., are indefinitely renewable, and are of major interest for cellular immunologists, molecular biologists, genetic engineers, etc. The production of IC's and MA's has rapidly risen in the last five years so that the number of reagents available today is possibly as large as 10^4 with the annual production of new MA's probably also approaching this figure. The cost of establishing a given IC has been estimated to be about 25 k\$.

It seems obvious that some kind of a list of extant MA's and IC's should be established and made available to the scientific community.

This catalog should meet the following minimum requirements:

- It should be international in scope for entries and for distribution of information.
- It should be computerized.
- It should be easily accessible to everybody.
- Its use should be cheap.

The first point is related to the fact that the seekers of MA's or IC's are unconcerned by the nationality of the producer. Building, as it has been suggested, databanks at the national, then regional, and finally international levels would be a waste of time, engender duplication of information, and would be a costly procedure. It is much wiser to establish a central databank immediately at an international level for the collection and storage of data.

In contrast to the collection and storage of data, the distribution (output) of information in answer to queries may use a decentralized structure of "satellites" or "nodes" at a regional or national level.

A comprehensive, computerized, international, readily accessible, and inexpensive databank, the Hybridoma Data Bank (HDB) has been created (NL #26) by CODATA and the International Union of Immunological Societies (IUIS), both components of ICSU.

The HDB will serve as a basis for information exchange on hybridomas and other cloned cell lines producing immunoreactive substances, as a source for locating hybridomas of

given specificity, and as a means for maintaining background information on the hybridomas for comparative studies of methods and species used in their production. Duplication of effort in hybridoma development may be avoided by searching the bank for existing cell lines prior to setting up research projects.

Categories of information will include such diverse aspects of hybridoma technology as the availability of cell lines and products, specific reactivities of the monoclonal antibodies, methods for developing hybridomas, and characteristics of the hybridomas. New categories will be added as needed.

Data for the bank are being provided by hybridoma investigators through the use of standardized data reporting forms. Other means of data collection are: search of catalogs from monoclonal antibody distributors, and integration of existing data collections from major research centers. Literature search is used primarily to identify individuals and laboratories involved in hybridoma technology. Since the HDB will contain much unpublished information, it will serve as a means to bridge the time gap between laboratory discoveries and publication. The bank will be available to the scientific community by fall 1984.

The address of the headquarters of the HDB is: CODATA/IUIS HYBRIDOMA DATA BANK, Ms. Lois Blaine, 12301 Parklawn Drive, Rockville, Maryland 20852, U.S.A. It is located at the American Type Culture Collection (ATCC) in Rockville. Computer facilities are housed at the National Institutes of Health in Bethesda, Maryland.

Identical copies of the databank will be housed on mainframe computers at cooperating centers or "nodes" established at the Institute for Physical and Chemical Research (RIKEN) in Japan and at a European location which is currently under negotiation. Each node will be responsible for data entry and quality control as well as dissemination of data.

Frequent exchanges between nodes will update the continuously growing file. When sufficient data have been entered, each node will answer queries from the public free of charge. Funding for this project includes grants from government agencies in the United States, France, Japan, Switzerland, and the United Kingdom, as well as from scientific groups such as the World Health Organization.

United States agencies involved are the National Institute of Allergy and Infectious Diseases, National Institute of Dental Research (NIDR), National Institute of General Medical Sciences, National Cancer Institute, NIH Division of Research Resources, Food and Drug Administration, and the U.S. Department of Agriculture.

The policies, planning, and monitoring of performance of the HDB are the responsibilities of a formally constituted Task Group of CODATA composed of scientists involved in hybridoma technology:

Dr. R. Accolla (Switzerland)
Prof. A. Bussard, Chairman (France)
Dr. G. Hammerling (F.R.G.)
Dr. V. Houbi (WHO)
Dr. B. Janicki (U.S.A.)
Dr. M. Krichevsky, Secretary (U.S.A.)
Dr. E.S. Lennox (U.K.)
Dr. J. Natvig (Norway)
Dr. T. Tada (Japan)

An excellent, more detailed article appears in *Biotechnology*, April 1984, pp. 338-341. Further questions can be answered by Lois Blaine, Data Bank Manager, at 301-801-2600 or at the address above.

Data Handling in Astronomy and Astrophysics

This international course in data handling in astronomy and astrophysics to be held at the International Center for Theoretical Physics at Trieste July 9-13, 1984 is designed to enable astronomers interested in this field to meet scientists intensively engaged in data handling. Although the importance of data has been recognized by astronomers since the first star catalog was established by Hipparchos in the second century B.C., the current era is characterized by a veritable data explosion. This arises from the construction of giant telescopes and the launching of astronomical satellites and mandates such a course.

The program of this course will include lectures by astronomers from the Stellar Data Center at Strasbourg (Prof. C. Jaschek,* Dr. F. Ochsenbein*), the NASA World Data Center (Drs. J. I. Vette,* J. Mead, W.H. Warren), the NASA Space Telescope Science Institute (Drs. R. Albrecht,* H. Jenkner, D. Rosenthal, C. Stoll), the European Southern Observatory (Dr. P. Grosbol*), and various observatories as well as by scientists from other disciplines (P. Linda, Trieste, chemometrics; H. Behrens, FIZ, physics) and specialists from IBM.

The main topics will be:

- Data management for data banks
- Astronomical catalogs
- Information transfer systems and standards
- Extraction methods for observational data
- Data handling in other sciences

More than fifty applicants from Europe, North America, Africa, India, and Japan had submitted dossiers by mid-April. The Scientific Organizing Committee is co-directed by Professor B. Hauck (Lausanne University) and Dr. G. Sedmak (ASTRONET) and includes Drs. L. Benacchio (ASTRONET), O.B. Dluzhnevskaya (ACAS, U.S.S.R.), M. Hack (GNA CNR, Italy), and T.F. Howell (ESRIN) as well as the speakers indicated (*) above.

WORKSHOP (continued from page 7)

testing is an iterative one, and it has already been carried out effectively in selected areas of the NBS Standard Reference Data Program. The papers provided a re-examination of the classical approach to the generation, compilation, and dissemination of scientific data.

Ten working panels charged with identifying general issues in the context of

their specific disciplinary classes of data met the next morning. One of the panels addressed the broader questions of standardization and compatibility of databases. The other groups investigated in more detail the impact of rapidly advancing computer capabilities on specific disciplines, including nuclear physics, thermodynamics, corrosion science, mechanical properties, and alloy, ceramic, and polymer phase diagrams.

Conclusions of the workshops generally pointed to (1) the significant positive impact that reliable automated databases have on R & D and (2) the increasing dependence of R & D on computerized databases.

The panel chairmen recommended that NBS should take a leadership role in focusing the efforts of all institutions involved. Proceedings summarizing the talks presented and the recommendations of the ten panels are being prepared by the Office of Standard Reference Data, NBS, and are expected in June.

The workshop was convened by Dr. Ernest Ambler in cooperation with Dr. David R. Lide, Jr., both of the National Bureau of Standards, Washington, DC 20234.

Database Management in Science and Technology

A CODATA Sourcebook on the Use of Computers in Data Activities

Edited by JOHN R. RUMBLE, Jr., National Bureau of Standards, U.S.A. and VIKTOR E. HAMPEL, Lawrence Livermore National Laboratory, U.S.A.

1984 xiv + 264 pages US \$45.00/Dfl. 135.00 ISBN 0-444-86865-8

This book is designed as an introduction for scientists and engineers into the use of computers to store, manipulate, and distribute collections of numeric data. The basic theme is simple: think before doing. Stated another way, successful computer database projects first require careful plans and designs followed by rational selection and implementation. This work introduces to people interested in scientific data, the important and useful concepts developed over the past decade to control computer data projects and improve the chances of success.

ORDER FORM

Send to:
ELSEVIER SCIENCE PUBLISHERS
Book Order Department
P.O. Box 211
1000 AE Amsterdam, The Netherlands

In the U.S.A./Canada:
ELSEVIER SCIENCE PUBLISHING CO. INC.
P.O. Box 1663, Grand Central Station
New York, NY 10163, USA

Please send me ... copy(ies) of DATABASE MANAGEMENT IN SCIENCE AND TECHNOLOGY, Rumble/Hampel (eds), at US \$45.00/Dfl. 135.00.

Orders from individuals must be accompanied by a remittance.

☐ Payment enclosed:

(Bank Draft/Eurocheque/International Money Order/Personal Cheque/Postal Cheque)

☐ Charge my credit card:

☐ Access ☐ Eurocard ☐ MasterCard ☐ American Express ☐ VISA

Card No. _____ Valid Until _____

Name _____

Professional Address _____

Date _____ Signature _____

NORTH-HOLLAND

0882NH/BK/LIS

Database Management in Science and Technology

This book, edited by **JOHN R. RUMBLE, JR.**, National Bureau of Standards, Washington, DC, U.S.A., and **VIKTOR E. HAMPEL**, Lawrence Livermore National Laboratory, Livermore, CA, U.S.A., is designed for scientists and engineers as an introduction to the use of computers to store, manipulate, and distribute collections of numerical data. Since successful computer database projects require first careful plans and designs followed by rational selection and implementation, this work introduces people interested in scientific data to the important and useful concepts developed over the past decade to control computer data projects and improve the chances of success. A major feature is the clear introduction of important database management concepts and ideas. The chapters, each written by an expert in scientific database management, cover three main topics. First, an overview of the concepts is given; then, a detailed discussion of each phase of a database project follows; and finally, the book concludes with a discussion on computer communications and linkage to other scientific database work. Extensive annotated bibliographies are incorporated.

This sourcebook is also designed to be a succinct yet clear reference manual to the topical literature in database management in general and to the requirements of using data in science and technology. The volume is intended as an introduction for scientists and engineers who are—even though newcomers to the database field—interested in the use of computers in data activities.

The following chapters are included: Foreword; Chapter 1: Data, Computers and Database Management Systems (J.R. Rumble, Jr.); Chapter 2: Data Types and Structures in Science and Technology (A.A. Brooks); Chapter 3: Database Management Systems in Science and Technology (F.D. Gault); Chapter 4: Analysis and Display of Data in Science and Technology (J.R. Rumble, Jr. and N.L. Seidenman); Chapter 5: Planning for Database Management in Science and Technology (F.J. Smith); Chapter 6: Designing the Database Management System (H. Bestougeff); Chapter 7: Selecting a Suitable Database Management System (M.A. Hufferberger and C.A. Schermer); Chapter 8: Implementing and Using the Database Management System (J. Russell and D.E. Cullen); Chapter 9: Integrating Your System with Data Communication Networks and to Other Database Activities (J.R.U. Page); Chapter 10: Database Management Concerns at the International Level (C. Gottschalk).

North Holland Publishing Co., Amsterdam, produced the 264 page book in March 1984. It costs US \$ 45 or 135 Dfl. ISBN 0-444-86865-8.

Database Management Systems

A short, select list of other useful books on database management systems has been compiled by John Rumble, Jr. for the Newsletter:

- C.J. Date, *An Introduction to Database Systems*, 3rd Edition (Addison-Wesley, Reading, MA, 1981)
- M. Flavin, *Fundamental Concepts of Information Modeling* (Yourdon Press, NY, 1981)
- J. Martin, *Computer Data-Base Organization*, 2nd Edition (Prentice Hall, Englewood Cliffs, NJ, 1977)
- J. Martin, *An End User's Guide to Database* (Prentice Hall, 1981)
- J. Martin, *Principles of Database Management* (Prentice Hall, 1976)
- M. Page-Jones, *The Practical Guide to Structured Systems Design* (Yourdon Press, NY, 1980).

Conference on Computers in Science

The second in a series of conferences on computers in science sponsored by the periodical Science in conjunction with Scherago Associates will be held in Washington, DC, 28 October-1 November 1984. Dr. Steve Heller, EPA, PM-218, Washington, D.C. 20460 is Conference chairman. The gamut of subjects to be covered includes Artificial Intelligence, Biology Workstations, Computer-Aided Molecular Design, Databases . . . through Robotics and Workstation Hardware.

ICSU Press Takes Off

ICSU Press Newsletter No. 1, April 1984, announces a welter of serial publications (4), symposia and monographs (7), semi-popular volumes (3), and service projects (4) completed or in hand and offers samples for evidence. Three months beyond their first anniversary, they are already implementing their aims:

"...to initiate interdisciplinary projects that are beyond the scope of any one ICSU member, to cooperate with individual members in their own publication projects by giving advice or by engaging in joint publication, to produce service publications, to introduce new communication technologies, to raise the profile of ICSU and its members among individual scientists, among the educated lay public and bodies outside the ICSU organization, to publish material that will be of real service to science and to help bring a financial return to the ICSU family for support of our various activities."

Although their initial bias is definitely biological, they are eager to cover the entire ICSU family. BioEssays (News and Reviews in Molecular, Cellular, and Developmental Biology) is to be a monthly current-awareness journal devoted to reviews, comment, debate, and progress in the above three frontier areas as well as to their impact on science and society.

Materials Properties Data Network Created

This national network, a cooperative, not-for-profit venture, was incorporated 24 January 1984 in a Philadelphia meeting of the Metal Properties Council (MPC). The action culminates four years of study of the growing need for computer access to numerical data for the design and evaluation of engineering structures. The Network will coordinate the activities of the autonomous computerized data centers maintained by societies, private companies, universities, research institutes, and government agencies and/or contractors. Users may include designers, material producers, manufacturing and engineering corporations, regulatory agencies, R & D organizations, and those involved in the development of codes, specifications, and standards.

Further information may be obtained from Dr. Martin Prager at The Metal Properties Council, Inc., 345 E. 47th Street, New York, NY 10017. The telephone number is 212-705-7673.

I might add that we have had quite encouraging inquiries from possible collaborators recently.

Editor: What do you see as the role of the Task Group in this era?

Dr. White: The Task Group would have several roles, Edgar. First of all, most of the members are involved in evaluating data themselves. They are continuing to contribute to the international tables. Second, there still is much to be done before a truly automated system is attained. We have all read and used automated products from one another and have exchanged software. There is more software to be developed; however, most of the members of the Task Group are experts in this area. Finally, although much of the work can be done in a decentralized fashion, there must be a central group to organize and manage the effort, maintain quality control, solve problems, and settle differences. The Task Group would undertake to fill this role also.

Editor: Who, though, do you envision as actually producing and marketing these rather extensive tables?

Dr. White: I don't have a detailed answer to this question, Edgar. To some extent the answers are probably not mine to give but may need to be given by CODATA. The detailed plan hasn't been made as yet.

All of us on the Task Group feel that truly international tables need an international sponsor. That is one of the reasons that we recommended to CODATA that a set of CODATA thermodynamic tables be prepared. On the other hand, many of the groups producing sections of the tables can be expected to have responsibilities to other sponsors which the tables fulfill. Any detailed plan must be flexible enough to allow specific responsibilities to sponsors to be met at the same time that sections for the international tables are prepared. I feel sure that appropriate arrangements can be made, but the problem hasn't been faced as yet.

Editor: And how will CODATA itself be related to these tables? What kind of a time scale is involved?

Dr. White: The tables will be prepared under the aegis of CODATA. A recognized international organization is needed to provide legitimacy and recognition to an international project, and CODATA is the appropriate organization for an international project on thermodynamic tables which crosses the boundaries of several scientific and engineering disciplines.

It is particularly difficult to set a time scale right now. Because of the existence of the CODATA Key Values and new computer bookkeeping techniques, it is not necessary to evaluate data throughout the periodic table in the rigid systematic fashion used in the past. If there are a number of participants, the work will go rapidly; however, it is conceivable that some portion of the periodic table would be left behind. Then the Task Group would need to assume responsibility for such a neglected area. The real advantage of the new system is not so much speed (although it should be considerably faster than its predecessors), but that it is cumulative. Little or nothing will be lost or need to be done over simply because no one can figure out how to incorporate it.

Editor: One of CODATA's major—now, almost historical—endeavors (apart from fundamental constants) has been in key values for thermodynamics. The final hardbound volume from that task group's endeavor will (hopefully) be published in late 1984. But will you not need to revive that activity for your tables project?

Dr. White: Yes, Edgar, we intend to remain active in the "Key Values" area. In fact the Task Group has a subcommittee on the topic. As I have already indicated, the existence of the Key Values has been a great help to the Task Group. By basing our tables on the set of Key Values we are able to treat sections of the periodic tables in parallel rather than in a strictly serial fashion.

Probably the set of key substances should be reconsidered and the Key Values updated every 5 to 10 years.

a. Containing over 10,000 terms in English, German, French, and Russian, the dictionary covers: technology and logic structure of high-integrated circuits; circuitry and functional components of microprocessor systems; microcomputer peripherals; application-oriented design of microcomputers and structure and maintenance of microcomputers; microcomputer programming; microcomputer information processing; application-oriented practice. 1983. 320 pp. US \$74.50. Elsevier Science Publishing Co., Inc., 52 Vanderbilt Avenue, New York, NY, 10017. ISBN-0-444-99645-1.

b. A Reference and Referral Guide to Libraries, Information Firms, and Other Sources Providing Computerized Information Retrieval and Associated Services Using Publicly Available Online Databases. This Directory provides detailed descriptions of the online information retrieval services offered to outside users by public, academic, and special libraries, private information firms, and other organizations in the United States and Canada. The work serves as a link between the users in need of online information and the libraries or organizations that are able to search the particular databases that meet those needs. Entries furnish up to 17 points of information about each organization, including: full name, address, and telephone number; year service established; key contact person; number of staff conducting searches; online systems accessed; subject areas searched; most frequently searched databases; associated services; service availability; fee policy; names of search personnel; etc. Six indexes provide in-depth analysis of the information contained in the entries and assist users in locating the most appropriate search service for their needs. The six indexes are: organization index, index to organizations by online systems accessed, index to organizations by databases searched, index to organizations by subject areas searched, search personnel index, geographic index. Part 1 of 2 Parts, December 1983 (Entries 1-634). (Part Two to be published August 1984). Subscription to the two parts: US \$75. Gale Research Co., Detroit. ISBN-0-8103-1698-6.

c. A Guide to University-Related and Other Nonprofit Research Organizations Established on a Permanent Basis and Carrying on Continuing Research Programs. Contains 6314 listings of university-related and other nonprofit research

centers throughout the U.S. and Canada. Arranged by major subjects and indexed by subjects, institutions, and research centers. Typically covers mailing address, phone number, status (affiliation), sources of support, staff size, annual budget, principal fields of activity, special facilities and their availability to outsiders, publication of research, seminars, and library facilities. 1983. 1082 pp. US \$235. Longmans, London. Also available from: Gale Research Company, Book Tower, Detroit, MI 48226. ISBN: 0-8103-0458-9.

d. A periodic supplement to Research Centers Directory, 8th edition (see c above). Covered are centers established since the current edition went to press and those for which complete information is just becoming available. 1983. Inter-edition subscription, US \$190. Longmans, London. Also available from: Gale Research Company, Book Tower, Detroit, MI 48226. ISBN: 0-8103-0451-1.

e. 3000 leading research centers are identified in this revised reference tool. Arranged by country, with individual facilities in alphabetic order, it includes research centers operated by or affiliated with government agencies and universities as well as independent commercial facilities. Typical entries provide name, address, and telephone number of the center, name and title of the director, government or university affiliation when relevant, a description and breakdown of the staff, fields of research and ongoing projects, scope of library, and details on publication and seminar programs. 1984. 750 pp. US \$250. Longmans, London. Also available from: Gale Research Company, Book Tower, Detroit, MI 48226. ISBN: 0-8103-0467-8.

f. Supplement to e above which includes more nations and organizations. Inter-edition subscription, US \$140. Longmans, London. Also available from Gale Research Company, Book Tower, Detroit, MI 48226. ISBN: 0-8103-0468-6.

g. A Guide to Laboratories, Consultants, Firms, Data Collection and Analysis Centers, Individuals, and Other Facilities in the Private Sector Which Conduct Research. Lists companies providing research services on a contract or fee-for-service basis. Emphasis is on the small research and development firms and independent researchers and consultants who specialize in specific areas or industries. Among the services they offer are testing and analysis, new product development, market research, data collection and analysis,

experimental review and synthesis, policy research, feasibility studies, surveys, space evaluation and planning, systems design, identification of natural phenomena, opinion research, and technological and other types of forecasting. Areas covered include business, education, energy and the environment, agriculture, government, public affairs, social sciences, art and the humanities, physical and earth sciences, life sciences, and engineering and technology. 1982. 379 pp. US \$235. Longmans, London. Also available from: Gale Research Company, Book Tower, Detroit, MI 48226. ISBN: 0-8103-0248-9.

h. Periodical supplement to the Research Services Directory, 2nd Edition. 1984. Inter-edition subscription, US \$140. Longmans, London. Also available from: Gale Research Company, Book Tower, Detroit, MI 48226. ISBN: 0-8103-0249-7.

i. Some 1642 research and development facilities funded by the U.S. government either as parts of its agencies or as private contractors are identified. Represented are organizations including testing and experiment stations, computation centers, statistical laboratories, survey units, grant and contract offices, and research and development bureaus, etc. Entries typically provide name, address and telephone number of the center, the name and title of the director, parent agency and federal affiliation, a description and breakdown of the staff, fields of research and ongoing projects, scope of library, and description of publication and seminar programs. 1982. US \$260. 434 pp. Longmans, London. Also available from: Gale Research Company, Book Tower, Detroit, MI 48226. ISBN: 0-8103-0461-9.

j. 1984. US \$150. Longmans, London. Also available from: Gale Research Company, Book Tower, Detroit, MI 48226. ISBN: 0-8103-0462-7.

k. Supplement 1. The purpose of the original volume was to provide an organized literature reference source allowing easy access to data published between 1900 and early 1977 on mixing and excess properties. The rapid expansion of available information—over 2,500 new references in the past

(continued on page 15)

New CODATA Publications *

Scientific Program and Abstracts: Ninth International CODATA Conference, Jerusalem, Israel. Bulletin 54 (Mar. 1984)

Directory Chapter 11: Chemical Thermodynamics. Robert D. Freeman, Chapter Editor, Bulletin 55 (April 1984).

CODATA Bulletin. Subscriptions: Regular, US \$45; Personal, US \$15. Individual copies: (#54) US \$10; (#55) US \$15. Pergamon Press, Ltd., Headington Hill Hall, Oxford, United Kingdom OX3 0BW.

Books for the Bookshelf.....

Dictionary of Microprocessor Systems. D. Müller.^a

Online Database Search Services Directory, First Edition, Issue Number One. John Schmittroth, Jr. and Doris Morris Maxfield, Editors.^b

Research Centers Directory, 8th edition. Mary M. Watkins and James A. Ruffner, Editors.^c

New Research Centers, 8th edition.^d

International Research Centers Directory, 2nd edition. Anthony T. Kruzas and Kay Gill, Editors.^e

International Research Centers Directory, 2nd Edition Supplement.^f

Research Services Directory, 2nd Edition.^g

Research Services Directory, 2nd Edition Supplement.^h

Government Research Centers Directory, 2nd edition. Anthony T. Kruzas and Kay Gill, Editors.ⁱ

Government Research Centers—2nd Edition Supplement.^j

Mixing and Excess Thermodynamic Properties. A Literature Source Book. J. Wisniak and A. Tamir.^k

Heats of Phase Change of Pure Components and Mixtures. A. Tamir, E. Tamir, and K. Stephan.^l

Handbook of Glass Data, Part A: Silica Glass and Binary Silicate Glasses. O.V. Mazurin, M.V. Streltsina, and T.P. Shvaiko-Shvaikovskaya.^m

Nuclear Data Standards for Nuclear Measurements.ⁿ

Chemical Graph Theory, Volume 1. Nenad Trinajstić.^{o,p}

Chemical Graph Theory, Volume 2. Nenad Trinajstić.^{o,q}

CRC Handbook of Solubility Parameters and Other Cohesion Parameters. Allan F.M. Barton, Editor.^r

Solar-Terrestrial Data Access, Distribution, and Archiving. Joint Data Panel of the Committee on Solar and Space Physics, Space Science Board, and Committee on Solar-Terrestrial Research, Board on Atmospheric Science and Climate, Commission on Physical Sciences, Mathematics, and Resources, National Research Council.^s

Practical Applications of a Space Station. Space Applications Board.^t

Computer Modeling of Complex Biological Systems. S. Sitharama Iyengar, Editor.^u

Information Sources in Biotechnology. Anita Crafts-Lightly.^v

Biological Reference Materials: Availability, Uses, and Needs for Nutrient Analysis. W.R. Wolf, Editor.^w

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

(continued from page 14)

four years—has necessitated the compilation of a supplement to the main volume which covers the literature that appeared between 1977 and 1981, as well as some references that were overlooked in the original work. 1982. 734 pp. US \$138.25. Elsevier Science Publishing Co., Inc., 52 Vanderbilt Avenue, New York, NY, 10017. ISBN-0-444-42072-X.

l. Physical Sciences Data, 14. Provides an up-to-date review on the theories and equations for the heat of vaporization of mixtures and pure substances as well as for new methods for predicting this property for mixtures, and secondly, an organized literature reference source allowing easy access to data published between 1900 and 1981 for the heats of melting or fusion, sublimation and vaporization. In addition to the heat of phase change data, the book includes all references containing pertinent data on vapor pressure versus temperature from which the heat of phase change can be calculated by means of the Clausius-Clapeyron equation. 1983. 754 pp. US \$149.00. Elsevier Science Publishing Co., Inc., 52 Vanderbilt Avenue, New York, NY 10017. ISBN-0-444-42170-X.

m. Physical Sciences Data, 15. This is the first part of a five-volume reference work designed to provide comprehensive information on the properties of one-component, binary and ternary oxide glass-forming melts and glasses. Part A deals with silica glass and binary silicate glasses. The main body of the book contains the most important and dependable numerical and graphical data on the following properties: glass formation, crystallization, density, thermal expansion, optical properties, absorption spectra (references only), specific heat, thermal conductivity, surface tension, viscosity, elasticity, internal friction, strength, microhardness, electrical properties, chemical durability, diffusivity, solubility and permittivity of gases, ion diffusion, magnetic properties (references only), volatilization, and glass transition temperature. 1983. 686 pp. US \$149. Elsevier Science Publishing Co., Inc., 52 Vanderbilt Avenue, New York, NY 10017. ISBN-0-444-42215-3.

n. This handbook was published in the IAEA Technical Reports Series No. 227. It contains the 1982 version of the

international Nuclear Standards File maintained and updated under the auspices of the International Nuclear Data Committee (IANDC) and the OECD/NEA Nuclear Data Committee. 1983. 98 pp. Austrian Schillings 240 (A limited number of copies is available free of charge to scientists in developing countries). IAEA Nuclear Data Section (NDS), P.O. Box 100, A-1400 Vienna, Austria.

o. These volumes provide a detailed introduction to the field of chemical graph theory and clear-cut instructions on how and when to apply the graph-theoretical methods in research. Mathematical and chemical graphs are defined and topological matrices and characteristic polynomials are discussed in detail. In addition, the books present the topological aspects of simple molecular orbital theory, the topological theory of aromaticity, and isospectral and subspectral molecules. Also reviewed are the enumeration of valence bond structures, resonance-structure theory, the conjugated circuits model, and the application of graph theory to valence bond theory. Applications of graph-theoretical techniques to structure-activity relationships via topological indices and isomer enumeration are included. Each chapter concludes with a comprehensive list of references.

p. 1983. 7 X 10. 160 pp. US \$66 within the U.S., \$76 outside. CRC Press, Inc., 2000 Corporate Blvd., N.W., Boca Raton, Florida 33431. ISBN-0-8493-5273-8.

q. 1983. 7 X 10. 184 pp. US \$71 within the U.S., \$82 outside. CRC Press, Inc., 2000 Corporate Blvd., N.W., Boca Raton, Florida 33431. ISBN-0-8493-5274-6.

r. For the first time, all scientific information published worldwide on solubility parameter values and their diverse applications is collected in one convenient reference source. Scientists and technologists will find comprehensive solubility data on polymers, polymer blends, plasticizers, solvents, pigments, paints, dyes, inks, lubricants, adhesives, membranes, chromatographic materials, colloids, and biocompatible materials. Scientists involved in fundamental research of liquids and gases, as well as surfaces and reaction kinetics will also find this reference valuable. The data are presented both as numerical tables and as solubility maps. Materials

are presented in order of increasing complexity. This format allows you to familiarize yourself only with those aspects of the theoretical background necessary for an understanding of the particular type of system under investigation. 1983. 608 pp. Hardbound. US \$99.50 in the U.S., \$115 elsewhere. CRC Press, Inc., 2000 Corporate Blvd., N.W., Boca Raton, Florida 33431.

s. Due to the successful operation of existing large mass-storage systems and the impending availability of video disks and digital optical disks, data storage is no longer the problem it has been in the past. Consequently, the Data Panel focused on the problem of data accessibility as the present highest priority problem in solar-terrestrial data management. In developing a solution to this problem, both today's technological capabilities and the economic realities of funding agencies have been considered. 1984. National Academy Press, Washington, D.C. Available from Committee on Solar and Space Physics or Committee on Solar-Terrestrial Research, National Research Council, Washington, D.C. 20418.

t. 1984. 101 pp. Available from the Space Applications Board.

u. Computer modeling of biological systems, a process of building new sets of conceptualizations, theories, and implementations, is covered in depth. The emphasis is on how computer modeling encompasses three distinct areas of science (computer science, biology, and medicine) for building a framework for investigating the behavior of a complex biological system. Simulation and modeling are discussed because these two factors provide the methodology for the design, development, experimentation, analysis, and evaluation of an experiment under study. 1984. 7 X 10. 152 pp. US \$59 within U.S., \$68 outside. ISBN-0-8493-5208-8.

v. This book reviews books, conferences, trade periodicals, computer databases, etc. It is an essential working reference in biotechnology. Publishers and addresses are also included. 200 pp. £ 40. Globe Book Services, Brunel Road, Houndmills, Basingstoke, Hants, UK RG21 2XS. ISBN-0-333-36178-4.

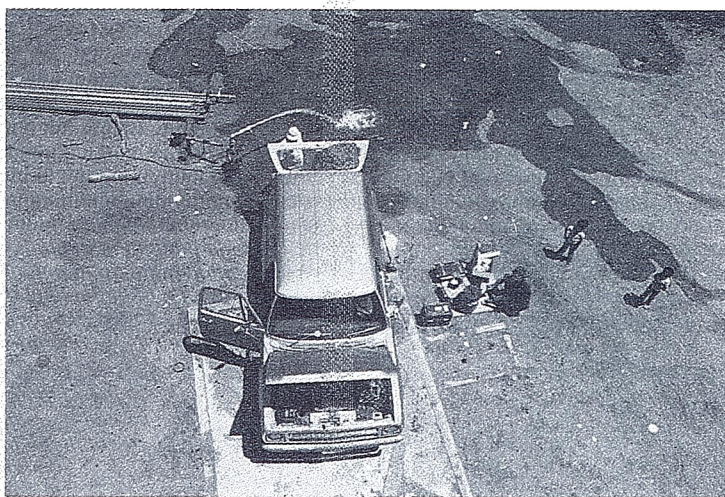
w. 1984. Wiley-Interscience, New York.

Data Evaluation

"Data evaluation is an unglamorous activity, unlikely to win Nobel prizes for its practitioners. Moreover, the very modesty of its cost tends to obscure its importance. It is thus not surprising to learn . . . that current U.S. activity is about one-third to one-half that required to keep pace. If this situation is to change, a greater awareness of the need for and importance of data evaluation on the part of the scientific community seems essential."

Walter H. Stockmayer, Professor of Chemistry, Dartmouth College, Hanover, New Hampshire 03755

From Guest Editorial in *Science* (18 Aug. 1978).



Windmill-top view of sampling at the Stripa Mine in Sweden. This mine is a test facility to study the feasibility of disposing of high level nuclear wastes deep in granite.

Courtesy of A.B. Muller, OECD

Editor pro tempore: Edgar F. Westrum, Jr.

Department of Chemistry, University of Michigan,
Ann Arbor, MI 48109

Telephone: (313) 764-7357/ Telex: 8102236056

Published four times per year (January, April, July, and October)

Associate Editor: Phyllis Glaeser

CODATA Secretariat, 51 Blvd. de Montmorency,
75016 Paris, France

Telephone: 525-04-96/ Cables: ICSU Paris 016/ Telex: 630553

Assistance in dissemination provided by National Committees.

CODATA Secretariat
51 Boulevard de Montmorency
75016 Paris, France

Here is CODATA's latest Newsletter for