CODATA Newsletter Number 76- February 1997

HIGHLIGHTS

Highlights of the 15th International CODATA Conference

Representing more than 20 countries, over 200 scientists and engineers assembled in Japan's distinctive science city, Tsukuba, 30 September - 4 October, 1996, to exchange ideas and interests pertaining to *Scientific Data in the Age of Networking*. Some 204 presentations were given in plenary, parallel and poster sessions at the biennial conference.

In the keynote address Y. Nishijima, President of the Science Council of Japan, reminded the audience that in many instances, the integration of knowledge from various fields has led to significant scientific and technical advances--a fact that must be heeded in our current regard for the environment. He cited the establishment of a graduate School of Environmental Data at the University of Kyoto which merges studies in the social sciences, the basic, and natural sciences.

Y. Arskii and his collaborators reviewed how VINITI, the Russian Institute for Scientific and Technical Information, coordinates the sharing of ecological data and bibliographic information among countries of the former Soviet Union. Summarizing results from their recent survey on issues in the transborder flow of scientific data, US National Committee for CODATA spokesman P. Uhlir outlined a wide variety of concerns that had been identified. Too numerous to be listed here, they and other relevant papers will be made available on the World Wide Web[1] (WWW). In essence, the survey indicates that we now have the technological power to accumulate and disseminate vast amounts of data quickly and cheaply, but lack the social and economic infrastructure to exploit that power as fully as we might. In the final plenary of day one, J. Hiraishi of the Japanese Agency of Industrial Science and Technology reviewed the status of research and development in Japanese industry.

K. Neves, Boeing Information and Support Services, presented informatics aspects of their new 777 aircraft. The international, multi-dimensional system he described was truly a splendid example of the design, construct, and support role played by information technology in a major industry. A-M. Dubois of the Centre Scientifique et Technique du Bâtiment in France outlined the importance of international standardization programs that facilitate the sharing of data pertaining to all facets of the manufacturing process.

F. Webster, University of Delaware and Chair of CODATA's newly-approved Commission on Data Access, suggested possible roles for CODATA in dealing with the current flood of data and information relating to geophysics and the environment.

M. Krichevsky of Bionomics International outlined a program for addressing the outreach and education needs which have been identified in CODATA's long range plan. The strategy he proposed for addressing these issues became, in fact, the work plan of a new Task Group on Outreach, Education and Communication, approved at the General Assembly to be chaired by Dr. Krichevsky. T. Yamamoto of the University of Library and Information Science at Tsukuba dealt with searching/creating scientific information on the INTERNET and the role of the 'digital librarian'.

The three Kotani Memorial lectures were a highlight of the final afternoon session. Named in honor of Prof. Masao Kotani, esteemed ex-President of CODATA and one of its founders, these prizes were created to recognize young scientists' exemplary scientific data work. K. Berrington, Queen's University Belfast, gave an overview of two international collaborative projects involving the calculation of high quality atomic data from quantum-mechanical first principles. J. Green, NASA/Goddard Space Flight Centre, described how data and metadata generated in the International Solar Terrestrial Physics program are being disseminated to collaborators around the world for processing and analysis. R. Chen of the Chinese Academy of Sciences, Beijing, surveyed issues relating to exploiting the vast amount of information contained in the human genome both now and in the future. Complexity analysis, fractal dimension calculations, neural networks and cryptology are examples of the tools employed.

Y. Fukao of the Earthquake Research Institute at the University of Tokyo led his audience on a fascinating tour ranging from specifics of the 1995 Kobe earthquake to insights into current theoretical understanding of earthquakes.

Conference Opening Session, (l to r) Prof M Tasumi et al.

The variety and scope of papers given in parallel sessions reflected the multi-disciplinary nature of CODATA.

The **Life Sciences** began with a session on Genome Research, covering activities in a number of genetic, physical mapping, and related databases. Highlights included the bacteriophage T4 model database organism, the rice genome, the USDA Plant Genome program and the work of the Japanese center of the International DNA sequence database. The session on Biological Macromolecules featured reports from groups compiling the primary archives of protein sequences and of protein and nucleic acid structures. Reports were also received from other groups that collect related information on specific classes of biological macromolecules and link to the primary archives thereby integrating access to information from many sources.

In the Species Diversity session emphasis was given to the harmonious combination of informatics and biology. Those attending the symposium on Medical Biology heard overviews of databases related to thalassaemia, a common genetic disorder, and mutant haemoglobin, an historically important molecular disease.

Sessions constituting the **Physical Sciences** stream covered topics ranging from space to nanostructures. Participants heard about a new data management system planned for the Hubble Space Telescope which will be able to handle 400 to 500 Gbytes per month. A proposal to update existing systems for the dissemination of nuclear and atomic-molecular data was outlined and reports were given of projects associated with fusion data and solar energy mapping. The influence of the WWW in facilitating sharing of data, as well as computing resources, was evident as were the benefits to be reaped by wider adoption of standardized data formats and representations. Descriptions of systems and/or databases related to

organic chemistry, along with a new functional group database based on a charge density approach, were revealed.

Two presentations on engineering were particularly noteworthy. In reviewing the data requirements for industrial ecology, the authors displayed an open-minded approach and admitted the difficulty of understanding and dealing with several important aspects affecting decision-making at a high level. T. Nelson--acknowledged as the father of the hypertext concept--intrigued the audience with his assertion that all information of value is disorganized; the challenge is to handle relationships between different and contrasting modes of representation of information.

A description of a series of virtual tools for manipulating and displaying three-dimensional geoscience data, important for applications involving ray tracing, tomography, as well as migration and simulation of complex geological structures, were described. It was observed that the Internet, while providing a powerful mechanism for the direct dissemination of data from collector to user, raises many new problems related to the quality of both data and metadata. INTERMAGNET, an international project which provides worldwide geomagnetic observatory data in nearly real-time, represents a major improvement in the delivery of such data.

Materials highlights included: an inventory to promote knowledge of available materials and chemical property databases on the Internet; databases on amorphous alloys and magnetic superlattices; modelling of the strength and toughness of materials to facilitate prediction of lifetimes under realistic conditions; an international project to incorporate all known structural, constitutional, property and bibliographic information on all ordered non-organic solids. The availability of high performance computers makes possible a shift in the paradigm of the exact sciences, wherein a problem is broken into smaller manageable pieces amenable to analytical descriptions, to a "brute force" approach wherein a complex problem is investigated as a whole. As an example, the author cited the rational design of nanoelectronic devices by modelling their operational characteristics at atomic resolutions in real-time.

Z. Pawlak, who introduced the "rough set" theory in 1982, showed how this *concept* could be applied in different fields, especially in data mining by finding hidden patterns of data and dependency of attributes in databases. Four *methodologies* of interest were sketched. One featured a general modelling approach applied to chemical structures which had been implemented in a system for structure manipulation and recognition. Another was a proposed extension of browsing strategies to assist the user in searching the Internet through the use of a decision support system or 'decision-agent'. The third was a proposal to develop so-called 'virtual activities organization' in information systems thereby intelligently assisting users to navigate heterogenous information environments more efficiently. Finally, a general framework to ensure data quality by systematic procedures in measurement and standards certification was proposed.

The first computational *tool* described was an extension of a B-tree scheme allowing for the search of a numerical value in some given range--a task often difficult in practice because of the imprecise nature of technical data. The second *tool* was an application of an expert system architecture to numerical data searching and retrieval by replacing the logical rules of expert systems by equations or formulae in which the appropriate laws of science and technology are expressed.

In the closing lecture J.-E. Dubois, as President, discussed two issues essential for CODATA. In the first part, he defined the position of CODATA today and its working connections with other bodies after the Chambéry Long Range Planning Workshop.

CODATA's areas of concern were gradually expanded and adapted to new technologies. All this experience and the originality of our action have been related in many papers given at previous Conferences. After recalling the more important milestones, J.-E. Dubois suggested that all interested participants look up the "Retrospect" presented at the Columbus Conference by J. Westbrook. (These papers can be found in the *Proceedings* and *Bulletins*.)

With the new orientations and the subsequent need for implementation of various computerized treatments of data and information for better communication (interpretability and the Internet), J.-E. Dubois stressed the growing importance of heterogeneous data in complex frameworks (similarity and scale aspects), sometimes involving subjective data evaluation (environment, quality excellence in industry, etc.).

In the second part, he outlined the changing aspects of our relationship to science and thus to information, leading primarily to the acceptance of different interpretations of objects, their properties and the correlation of these properties associated with different perceptions of the world, *e.g.*, the Galilean and its non-ambiguous spaces, quantum mechanics, and complexity.

The last two concepts and derived theories enabled him to introduce certain types of uncertainty at the microscopic and macroscopic levels, the growing importance of non-reversible phenomena, and the foundation of information theories. In this high-level overview, he first showed, then stressed, the real emergence of what he called "a science no longer limited to simplified situations." In conclusion, he quoted Ilya Prigogine, for whom this is "the true beginning of a dialogue with Nature."

> From this brief overview it is evident that, on the whole, these working units experienced productive biennia--laudable results given that CODATA functions primarily via suasion and volunteer efforts on a very limited budget.
>
> *--excerpted from a report (cf. Science International) by Dr. Gordon H. Wood*

CODATA General Assembly at Tsukuba, October 1997

Progress Review and Evaluation

One of the primary functions of the biennial General Assembly--involving about 45 participants and 20 observers-- is to receive progress reports from Task Groups, Commissions and Working Groups, as well as applications for new ones, and to determine which units should be approved for the next biennium. What was recounted will be summarized roughly along the lines of CODATA's basic objective: the promotion of the evaluation and, in general, the quality control of data as well as the improvement of the methods by which data are acquired, managed, and analyzed.

Major portion of the General Assembly

Treasurer J.Crease, President J.Dubois, Secretary General G.Wood at the Assembly

General Assembly Approves New and Continuing Task Groups

Three new Task Groups are supported for the biennium between General Assemblies (1996-1998):

Their anticipated productivity and *raison d'être* are presented. (A bit of the history of continuing Task Groups is also incorporated where appropriate).

Data/Information and Visualization

Chair: *Dr. Nahum Gershon* (1996)

This group plans to write reports for the community, produce a glossary of terms of new technologies, establish a Bulletin Board on the network or an active WWW home page, organize two workshops on "Information Visualization: Where Are We and Where Do We Go from Here" and "The Applications of Web Technologies" (*e.g.*, distributed information systems and the Internet and its impact). After analysis of new technologies and their applications, the Task Group will systematically inform and assist CODATA Task Groups, Commissions, other ICSU bodies, and external bodies in the use of data and models appropriate to their projects.

CODATA and the World Wide Web

Chair: *Mr. James Crease* (1996)

This group will seek to enhance CODATA's presence on the Web and to help and advise member countries who wish to establish home pages. Output will include a report to CODATA that presents plans and recommendations to be posted on the Web for information and comment.

Outreach, Education, and Communication

Chair: *Dr. Micah I. Krichevsky* (1996)

Scientists and technologists throughout the world need better personal tools to utilize the information potentially--but not practically--available to them. In teaching courses on use of computers in microbiology and methods of international communication as well as courses on risk assessment of release of novel organisms into the environment, the students uniformly and globally react that they desire more time to learn with hands-on experience on the computers and networks.

Basic core course materials will be developed and edited. Appreciable progress and coordination with other groups will be set in place. One or more training courses will be held and one or more consulting offices established. The first output will be a detailed action plan (including a business plan projecting fiscal viability of the Task Group activities). Various paper and/or electronic documents will be produced, *e.g.* the completion of the initial needs assessment, the training materials, the roster of available faculty members, the lists of available resources in developing nations, etc.

This Task Group will fulfill two goals, organizational *within* CODATA (the activities of the Task Group will help the goal of outreach articulated in the Long Range Strategy Plan articulated in Chambery) and *externally* to provide a necessary service to the scientific and technical communities, with emphasis in developing nations. Moreover, it will be a major broadly *interdisciplinary* CODATA activity.

Two contrasting aspects of CODATA combine to make it the most appropriate body to undertake the activities: a unifying principle underlying all its components and disciplines and the diversity of the disciplines which facilitates adapting core educational materials to the needs of specific client groups. Many other components of ICSU as well as national societies have outreach and education programs involving training. In general, they are naturally focussed on a specific discipline and may or may not contain material on good data practices, access to data, and data dissemination. Close collaboration with these groups and other CODATA Task Groups is envisioned.

Two extant Commissions were also continued during the biennium:

Commission on Standardized Terminology for Access to Biological Data Banks (STABD)

Established 1988; Chairman: *Dr. F. A. Bisby* since 1994; Co-Chair: *Dr. Lois Blaine* (1996)

The STABD Commission is making a major impact on access to biological data, particularly in the modern world:

in the names and reference system for all organisms (Species 2000);

in directly stimulating databases for the reference and description of viruses and bacteria (ICTV Virus Database and Bergey's Manual);

in gradually working through some of the many areas where standardization of terminology is needed (*e.g.*, terminology of spores, then proteins).

The Commission has been highly successful in using CODATA funds to obtain much larger sums from other agencies. $168,000 was thus obtained in 1994-1996.

CODATA is the right organization for sponsoring these activities; data standards, nomenclature and terminology, and availability in worldwide networked databases are at the core of the activity.

Commission on Data Access

Established 1994; Chair: *Prof. Ferris W. Webster* since 1994

Data access issues span many disciplines, but common practice varies greatly among disciplines. A policy on data and information access that would be acceptable to scientists in one discipline might not be acceptable to those in another. To progress, it is likely that CODATA needs to address the problem one discipline at a time. Following that, a synthesis needs to be made, pulling together the various disciplinary views into a common policy. The first step has already been taken, with a meeting and reports of environmental and geoscientists last year.

The Commission will arrange for the first of a series of meetings looking at access issues from the point of view of the traditions and constraints in a scientific discipline, then evaluate how successful this approach is likely to be before proceeding with further meetings.

Seven previously established Task Groups were extended for the biennium.

Biological Macromolecules

Established 1984; Chair: *Dr. Arthur Lesk* since 1996

They will expand the Task Group WWW site to include linkages to WWW sites of other CODATA groups, of data banks related to biological macromolecules, of relevant discussion groups, as well as of groups that are providing nomenclature standards that may be useful to this community.

They plan also to provide publicity about the Task Group and its activities. These pages will include introductory educational materials to help new users become familiar with Web facilities and archives supporting research on biological macromolecules. Attention will be drawn to this site by announcements in suitable journals.

They expect to compile a thesaurus of anonymous terms (*e.g.* keywords, names of molecules) used in the major macromolecular databases, and reports summarizing symposia and workshops sponsored by the Task Group, including development of ideas relating to guidelines for electronic publication of scientific results related to biological macromolecules.

Global Plant Checklist Network

Established 1994 Chair: *Mrs. Karen L. Wilson* since 1994

Continued endorsement by CODATA of a flagship project, bringing together fundamental biological data that underpin biodiversity initiatives by IUBS, UNEP, and Unesco. Collaboration will be continued or sought with various related groups, including the Species 2000, TDWG, Species Planetarium Project of IPI, DIVERSITAS and other taxon-based global databasing projects. Data will be made available online via the IOPI Home Page.

Thermodynamic Data for Key Chemical Substances

Established 1994; Chair: *Dr. Malcolm Chase* since 1994

Completion of evaluation and publication of the articles on barium and strontium. For each set of key chemical substances, an anticipated *CODATA Special Report* will provide the recommended values of the thermodynamic properties of interest and the associated documentation. The first article would be 'The recommended thermodynamic values for Sr(cr,l,g), Sr^{++}(aq), SrO (cr,l), and $SrCl_2$(cr,l). Even though the output each year is projected to be limited to a handful of chemical substances, over the course of years this collection will grow to become a reasonably-sized set of recommended temperature dependent data. Such data will help to form a consistent basis for the even larger sets of data employed by the user community.

Geothermodynamic Data

Established 1984; Former Chairs: *Dr. Igor Khodakovsky* and *Prof. Surendra Saxena*; Chair: *Professor Edgar F. Westrum, Jr.*

This Group will produce an initiatory volume on MgO-SiO_2 which will have data on about 30 phases (solids and melts) which will contain about 60 printed pages, a data and program diskette.

The work of this Task Group is indispensable in obtaining critical thermodynamic data to study problems of geological, geophysical, planetary, and industrial importance. Such studies include evolution of planets and man's impact on the natural processes operating in the earth's crust, hydrosphere, and atmosphere. The database will be crucial to all studies concerning global changes in the environment.

Materials Database Management

Established 1986; Chair: *Mr. J. G. Kaufman* since 1994

After completion of an excellent study on the "Costs of Building and Operating Numeric Databases: Results of a CODATA Survey", this Task Group is to meet in March 5 to make plans for the future. It continues to cooperate with ASM International and increase its focus on data quality for ecological attributes of materials. The General Assembly suggested that it might incorporate in its program some of the activities proposed by Prof. Oudar on surface and interfacial structure and composition, surface and interfacial thermodynamics and surface mobility. It will try to maintain international focus on materials data that has diminished significantly in the past several years with the demise of many national/international programs.

Survey of Data Sources in Asian-Oceanic Countries

Established 1986; Chair: *Professor Mitsuo Tasumi* until 1996, *Professor Akira Tsugita* 1996

Three subgroups of the Task Group will be studying Databases on Animal Viruses in Asian-Oceanic Countries, a Survey of Databases on Microbes in the area, and a Survey of Databases on Fishes in Asian-Oceanic countries. It plans to publish the proceedings of the Task Group meeting in Tokyo in 1996. The Chinese Academy of Sciences, Korea, Indonesia, and the Academy located in Taipei joined CODATA as

the result of the past activities of this Task Group. Countries in Asia and Oceania, for example Singapore, Thailand, and Pakistan are expected to become members of CODATA *(cf*. also Task Group TODAI Symposium report).

Fundamental Physical Constants

Established 1967; Chair: *Dr. B. N. Taylor* since 1994

It is now recognized that, because the fundamental physical constants of nature are the links in the chain that binds science and technology together, an internationally accepted set of recommended or "best" values of the constants must be made available periodically for the use of the scientific and technical communities. Further, these communities have now come to recognize that CODATA is a highly competent organization with broad scientific and technical representation and is thus the ideal international organization to assume the responsibility of providing such sets. No other international organization, e.g., IUPAC, IUPAP, CIPM/BIPM, has the depth and breadth of scientific and technical competence in the field of data analysis and compilation than does CODATA. Nevertheless, the Task Group maintains contact with such organizations to ensure that this work is acceptable.

CODATA Glossary of Terms Relating to Data, Data Capture, Data Manipulation, and Databases

Chair: *Dr. Jack H. Westbrook*

CODATA plans to complete an updated edition of the 1991 *Glossary* by introducing needed new terms and definitions, substituting standardized definitions where preferable to a*d hoc* definitions drafted for the first edition, improving present and *ad hoc* definitions where needed, deleting unnecessary, deprecated, or controversial terms, and supplement and improve the thesaurus relationships shown. (Although not defined as a Task Group, the updating group is endeavoring to expand the volume in time for 1997 publication.)

Officers:

President: Prof. J.-E. Dubois, *France* (1994-'98)

Vice-President: Prof. F. A. Kuznetsov, *Russia* (1996-2000)

Secretary General: Dr. G. H. Wood, *Canada* (1990-'98)

Treasurer: Dr. M. A. Chinnery, *U.S.A.* (1996-2000)

Members of the Executive Committee:

Prof. Jean-Loup Delcroix, *France* (1992-'98)

Prof. Ekkehard Fluck, *Germany* (1994-'98)

Prof. Ashok S. Kolaskar, *India* (1994-'98)

Mr. Keith W. Reynard, *U.K.* (1994-'98)

Dr. John Rumble, Jr., *U.S.A.* (1996-'98)

Prof. Honglie Sun, *Chinese Academy of Sciences* (1996-'98)

Prof. Mitsuo Tasumi, *Japan* (1994-'98)

Prof. Jen-Leih Wu, *Academy Located in Taipei* (1996-'98)

New Executive Committee meets in brief session after the Assembly

New National Members in CODATA

CODATA was pleased to welcome Senegal and Indonesia as national members. Attending their first CODATA General Assembly were Dr. Abdoulaye Gaye, the delegate from Senegal, and Dr. Rusik Dardjat, the delegate from Indonesia.

CODATA Calendar

1997

March

23 CODATA Officer's Meeting. Paris, France

24-25 CODATA Executive Committee Meeting. Paris, France

1998

November

8-12 CODATA 16th International Conference. New Delhi, India

13-14 CODATA 21st General Assembly. New Delhi, India

Books and Databases

Journal of Physical and Chemical Reference Data. (1996, V25#1), 1-525. Heat Capacities and Entropies of Organic Compounds in the Condensed Phase. Volume III. E. S. Domalski and E. D. Hearing. [a]

DECHEMA Chemistry Data Series. Vol. XII, Part 1c. Electrolyte Data Collection. Part 1C: Conductivities, Transference Numbers, and Limiting Ionic Conductivities of Solutions of Aprotic, Protophobic Solvents. I: Nitriles. J. Barthel, R. Neueder, and P. Schröder. [b]

DECHEMA Chemistry Data Series. Vol. XII, Part 2. Electrolye Data Collection. Part 2: Dielectric Properties of Water and Aqueous Electrolye Solutions. J. Bartel, R. Buchner, and M. Münsterer. [c]

Survey of Thermodynamic and Kinetic Databases. Nuclear Science Committee. [d]

Gaphyor Handbook. Volumes 1 and 2 (1996). [e]

CODATA Books

Two more books in the Series **Data and Knowledge in a Changing World**:

Geosciences and Water Resources (Environmental Data Modeling). C. Bardinet, and J.-J. Royer (eds.). [f]

Industrial Information and Design Issues. J.-E. Dubois and N. D. Gershon (eds.). [g]

DIPPR® Books and Databases

DIPPR® Data Compilation of Pure Compound Properties. T. E. Daubert, R. P. Danner, H. M. Sibul, and C. C. Stebbins, eds. [h, i, j, k]

Transport Properties and Related Thermodynamic Data of Binary Mixtures. K. N. Marsh, Q. Dong, B. E. Gammon, and A. K. R. Dewan, eds. [l, m]

DIPPR® Publication Comprehensive Listing. [n]

An Update on DIPPR® Project Activities and Publications

The Design Institute for Physical Property Data (DIPPR)® of the American Institute of Chemical Engineers was organized in 1978 to meet the need for critically evaluated thermophysical property data on pure chemicals and mixtures for process design. Funded project work began in 1980. In the 18th year as the longest continually active of the six current sponsored research groups in AIChE, there are 36 corporate members. There have been 17 projects covering from one to 18 years in longevity based on individual member interests for continued annual funding.

The best known Project 801 - Data Compilation has been active for the full 18 years at The Pennsylvania State University Chemical Engineering Department. The contractor Professor Tom Daubert will be retiring from the project at the end of 1997. The new contractor team from the Department of Chemical Engineering, Brigham Young University, includes Professors Richard Rowley, Vince Wilding, and John Oscarson.

The project produces a numeric database containing inorganics, organics, and elements. It will contain 1700 pure chemicals by the end of 1997. The number of property constants (temperature invariant) has been expanded to 29 with addition of the standard state thermochemical properties S, $_{form}H$, $_{form}G$ at 298 K. Temperature dependent properties with regressed fitting coefficients have increased to 15 with inclusion of solid vapor pressure and solid thermal conductivity.

The 1996 public release of this extensive data collection is available in electronic format for both in-house use and on-line access as well as a hard copy version (*cf.* Books and Databases, page 4).

Project 882 - Evaluated Data of Mixtures has completed 8-1/2 years of operation under Ken Marsh at the Thermodynamics Research Center at Texas A&M University. The project goal is to satisfy industry needs for accurate and complete physical and transport property data for selected binary mixtures. Results are being published in both a hard copy series in four parts and in an electronic database called DIPMIX (*cf.* Books and Databases).

Project 931 - Property Estimation has been carried out under Professor Peter Jurs of The Pennsylvania State University Chemistry Department since 1993 using pattern recognition and neural networks. Methods were developed for estimating normal boiling point of hydrocarbons and hetero-atom containing organics. Additional work on estimating auto-ignition temperatures for pure organics is being completed. Results are being published in the *Journal of Chemical Information and Computer Sciences.*

Four experimental projects are currently active. Project 805 - Phase Equilibria measures VLE, LLE, VLLE on binary mixtures. Through 1995, contractors in the USA, Canada, Europe, and China--16 years--have measured data on 282 systems. Results on 196 have been published and 29 more were published in November 1996 in the Jou*rnal of Chemical and Engineering Data* (JCED).

The Liquid Vapor Pressure Project 821 under current contractor Bill Steele at the National Institute for Petroleum and Energy Research (NIPER) in Bartlesville, OK has studied 111 chemicals through 1995, published 79, and eight more are included in the above JCED issue.

The Critical Properties Project 851 currently under Loren Wilson at Wiltec Research Co. in Provo, UT has studied 105 chemicals, published 84, and covered 14 more in the above JCED.

Project 871 on Enthalpies of Combustion and Formation under Bill Steele at NIPER has studied 72 chemicals, published 32, and covered 17 more in the above JCED.

In the past, experimental results were published by AIChE in their Symposium *Series* and *DIPPR Data Series*. Future results will appear in JCED. Moreover, all of these results are included in the Data Compilation Source File as a repository.

Other areas covered by projects have been electrolyte thermodynamics, property estimation, polymers. Two active projects at Michigan Technological University, Chemical Engineering Department under Profs. Mike Mullins and Tony Rogers cover 56 properties of more than 600 chemicals in the environmental regulatory domain. Project 911 is developing a computerized numeric database; Project 912 is working on property estimation methods based on structure.

Ted Selover retired as Technical Director and has been replaced by George Thomson--formerly of Phillips Petroleum Company at Bartlesville, Oklahoma.

--Theodore B. Selover, Jr., DIPPR Technical Director (Retired)

CODATA, WWW, and Databases

Leading the way for CODATA onto the WWW, the Working Group on **Electronic Information Transfer** established an international site, at the National Research Council in Canada, which was designed not only as a working tool for those involved in CODATA but as a means of introducing CODATA to the world. *CODATA Newsletters* are readily available there (with colored illustrations).

The **Biological Macromolecules** Task Group published its symposium *Proceedings* on the WWW rather than in the more conventional hard copy form. Furthermore, listings of the fundamental constants, the major product of our Task Group by that name, appear on many WWW sites throughout the world, thereby expanding their availability and importance.

The **Materials Database Management** Task Group has produced an important report entitled *The Costs of Building and Operating Numeric Databases: Results of a CODATA Survey* which will be adapted to become part of a book to be published in 1997. This summary is especially noteworthy in that it represents one of the first attempts to quantify the costs of developing and maintaining materials databases.

Task Group on Biological Macromolecules

A Task Group meeting was held in Tokyo September 28-29, 1996, just prior to the 15th International CODATA Conference. The first day was an open symposium including the genome project. Each representative from DDBJ, PIR, MIPS, JIPID, and PDB reported their current and future activities. Subsequently, regional database developments were reported from India, Australia, Taiwan, and China. Prof. Y. Sakaki from the University of Tokyo comprehensively reported the status quo of the human genome project in Japan. Dr. D. Bigwood from the US Department of Agriculture explained their plant genome database system.

The members met on the second day and discussed plans, which included proposals for the following specific activities: development of the Task Group's home page; collection of information on quality control systems from different archival database projects; data archives for the "Proteome"; and continuation of support to nucleic acid structure databases, carbohydrate databases, as well as standardization of terminology.

TODAI Symposium: Sharing and Utilization of Engineering Data in Asian-Oceanic Countries

*T*he Symposium organized under the direction of Professor Shuichi Iwata and supported by the Inoue Foundation which was held at the University of Tokyo September 27-28, involved more than 24 presentations from Asian-Oceanic countries with more than 40 participants. Dr. Hiroyuki Yoshikawa, President of the University, welcomed the participants and opened the meeting.

Presentations ranged over perspectives of information flow within Asia, between East and West, the role of copyrights, the outlook on relevant aspects of sustainable development, sharing medical information, and database development, together with developments in specialized areas (geomagnetism, fish, astronomy, etc.), as well as new approaches for sharing; e.g., virtual reality, multimedia, strategic computing, virtual engineering as well as the Task Group's action plans for the near future. A summary document is expected.

In spite of the recent drastic changes in communication infrastructures represented by the designation "Internet", it is not so easy to realize fluent transborder, trans-discipline and trans-generation data flows in Asian-Oceanic countries due to not only their different historical, economical, technological, cultural,

environmental and other backgrounds but also to the status of the science and technology themselves. To share and utilize scientific and engineering data as public goods suitably, certain developments are essential.

The first concerns awareness provided earlier by CODATA directories and more recently by browsers like NETSCAPE with many new capabilities for data retrieval and capture. Communication comes second, and it is the key issue for sharing and utilization. Different kinds of schemes for terminology, classification systems, metadata, etc. have been prepared for more effective data communications by CODATA and/or other international/domestic activities and some of them are implemented as browsing tools. The third step is utilization of data which requires understanding on essential semantics of each data set and also infrastructure to verify/realize the semantics. (This subject recently became a popular one as demonstrated partly by image objects described by VRML and Java.) In these contexts the Task Group would like to develop feasible action plans for the future.

OECD Megascience Forum Working Group on Biological Informatics

The OECD Megascience Forum Working Group on Biological Informatics held its first meeting on June 6-7, 1996, in Washington, D.C., to delineate a model for harnessing informal technology to meet the challenges of international data management in the biological sciences. The meeting was attended by 44 delegates from 15 OECD member countries, three delegates from the Russian Federation, one delegate from Poland, eight delegates from the European Commission, and one member of the OECD Secretariat.

The Megascience Forum had designated the United States as the lead country, to supply administrative support and to provide a chairperson. Dr. James Edwards was chosen to chair the group.

The first priority of the Biodiversity Informatics Subgroup is to produce a report on the state of biodiversity informatics in OECD countries and to evaluate the opportunities for collective progress. The Neuroinformatics Subgroup focused on defining the new field of neuroinformatics, integrating neuroinformatics into the community of neuroscience researchers, and identifying gaps in neuroinformatics tools. They discussed beta testing and documentation of neuroinformatics software, as well as ways to reward people for contributing to neuroinformatics resources.

Another meeting of the OECD Megascience Forum took place in Paris on 28-29 January 1997. Bioinformatics, considered as an emerging science, was investigated in the course of three Sub-Working Groups: two Group sessions on biological informatics biodiversity and neuroinformatics, presided over by U.S. representatives, took place simultaneously with a Group on Intellectual Property Rights and Ethics, presided over by Ms. Michèle Durand from the French Ministry of Education and Research. This Group was divided into two sessions, i.e., IR and Ethics in Biodiversity and Neuroinformatics, on the one hand, and Database Ownership and Access Issues on the other. Professor J.-E. Dubois, president of CODATA chaired the latter session, where Dr. Micah Krichevsky, of the U.S. CODATA Committee on Issues in the Transborder Flow of Scientific Data, presented the conclusions of their report on "Bits of Power." The concepts of free and open circulation of information were extensively examined. Dr. J. Franklin, a former CODATA associate, gave a paper on "Publishing and Free Information." The discussion was very constructive and lively, as the OECD Group and the European Commission representatives (DG XII) are deeply involved in biodiversity problems and the ethical aspects associated with patenting the genome findings.

Report on Informatics

Most of the work of CODATA and its affiliated bodies done in the Informatics area is in the context of individual disciplines and, of course, a great deal has been accomplished in that regard, as noted by the other rapporteurs. However, this report focuses on Informatics, or Information Science, issues and work

largely independent of specific disciplines, and in this context a review of the reports submitted to the 20th General Assembly shows very little attention to Informatics topics. (I define Informatics to include not only research on the methodology, techniques, and organization of scientific and technical data and information, but also the use of information systems in the work of CODATA.)

CODATA and Its National Committees. A review of the National Committee reports shows little research in Informatics per se by those committees themselves, and some spotty information provided about national informatics research activities. Brief descriptions of ongoing work may be found in the National Committee reports of China, France, Poland, Russia, and the United States.

CODATA and four of the National Committees--Canada, China, France, and the United States--have established World Wide Web sites in the past two years. Although all those involved in these activities should be commended for their initiative, these Web sites remain underutilized for CODATA work. Moreover, most CODATA national members still do not have a Web site.

CODATA Working Groups, Task Groups, and Commissions. Until this General Assembly, there were no Task Groups or Commissions focused on Informatics. Only the Working Group on Web Technologies, which established the CODATA Web site, has been active to date. However, three proposals for new Task Groups in this area at this 20th General Assembly were voted into existence.

With regard to the use of information systems in CODATA work, all Task Groups and Commissions have made extensive use of computers and electronic networks for years. Moreover, a number of them have also developed Web sites as part of their activities; this should be encouraged for them and for CODATA National Committees.

Corresponding ICSU Bodies. A review of the reports to CODATA by the corresponding ICSU bodies shows different levels of accomplishments in Informatics activities as well, although most of these are understandably done in the context of specific discipline projects and programs. The notable exception to this is the work done by the International Council on Scientific and Technical Information (ICSTI). Also, it should be noted that the use of electronic networks and the establishment of Web sites has grown considerably in the past two years. At the same time, it is worth noting that in its recent review of U. S. involvement in and support of ICSU activities, the National Science Foundation emphasized that future support of these activities was contingent in part on the expanded and improved use of electronic networks by the ICSU community.

In summary, CODATA and its affiliated groups have made significant progress in the Informatics area, particularly in the use of information systems, in the past two years. However, much more can and should be done.

--Paul Uhlir, Rapporteur to Tsukuba General Assembly

Retiring CODATA Treasurer presented with Blue Diode-Activated Modern Sculpture

An award cleverly devised by the French electronic sculptor, Gilles Roussi, whose modern interactive electronic sculptures can be seen at the Cité des Sciences and at the Ecole Polytechnique in Paris and who is the official sculptor for Hewlett-Packard, was presented to CODATA's retiring Treasurer, Mr. Jim Crease at Tsukuba, to honor his eight years of devoted service to CODATA. The blue diodes were intended to represent the ocean, Mr. Crease's specialty.

Interdisciplinary Harmonization of Terminology used in Describing Spore-forming Microorganisms

The October 22-25, 1996 Workshop held at Santa Maria Imbaro, Italy and organized by Micah I. Krichevsky, Lois D. Blaine, and Miriam Balaban for the Co-Sponsors: UNEP, U.S. National Science Foundation, and CODATA is not an isolated event but rather the beginning of an organized endeavor to resolve an important issue in biology. Some 15 scientists from about 6 countries participated. The lack of a comprehensive, authoritative treatment of the description of spores and spore types means that many biodiversity and systematics studies are either in error or not understandable due to the resulting misidentifications or confusing descriptions. This problem must adversely affect many such studies. Furthermore, the lack of consistent vocabulary with respect to spores has legal and regulatory consequences.

The subject of the workshop was the rationalization and codification of the terminology of spore descriptions for all these types of microorganisms. The immediate output of this effort was a terse report containing the proceedings of the workshop. The substantive outcome of the workshop is the template for data entry which resulted from the most important conclusion by the participants that it was possible and useful to create a "universal" template. The template will be used to build a database of terms, their definitions, and pointers to applicable taxa. The database, in turn, will be the basis for building a comprehensive manual (to be published by CRC Press, Inc.) on spore terminology with illustrations and recommendations to aid the non-expert in describing spores they may encounter in their work. The agreed working title is: Handbook of Spires and Cysts: Algae, Bacteria, Fungi, and Protozoa.

In Memoriam

GUY WADDINGTON 1904-1996

Guy Waddington died March 18, 1996 in Victoria, British Columbia, Canada. Born: Victoria, B. C., Canada, May 22, 1904; B. A. and M.A., University of British Columbia; Ph.D., California Institute of Technoloy, 1932; Professor and Department Head, Rollins College. His major professional activity was at the U. S. Bureau of Mines, Bartlesville, Oklahoma (1943-1955), where he became Chief of the Petroleum Thermodynamics Branch. In the era of 1940-1960, in conjunction with Professor Hugh Huffman, the outstanding chemical thermodynamics laboratory in the USA was developed. Guy served also in the Reference Data Headquarters Operation of the National Reseach Council in Washington, D.C. with Professor F. D. Rossini, CODATA's first President, and played a seminal role in getting CODATA launched as a worldwide operation prior to the establishment of the Central Office in Frankfurt am Main, Germany and, indeed, trained the personnel for that endeavor. He was active in fabricating bolo ties by lapidarial work from native Oregon stones in his retirement days and maintained an enthusiastic interest in the work of the Canadian National Committee for CODATA.

GESINA CATHARINA CARTER ("CYNTHIA") 1939-1996

Gesina Carter, 57, a program manager in the Division of Advanced Energy Projects of the Department of Energy, died of breast cancer December 22, 1996. Dr. Carter was born in Nootdorp, Netherlands IN 1939. She came to the United States at 17, graduated from the University of Michigan, and received a Doctorate in Physics from Carnegie Mellon University in Pittsburgh. She moved to the Washington area in 1966, and her career there included teaching physics at Catholic University, working as a staff physicist at the National Academy of Sciences, where she specialized in data standardization, and, since 1991, working at the Department of Energy. She was active in the Reference Data Headquarter Operation, the U. S. National Committee for CODATA, as well as the international CODATA scene over many years. Dr. Carter was captain of the U.S. Women's Fencing Team at the World Championships in 1974 at Grenoble, France, and was a volunteer at fencing events at the 1996 Olympics in Atlanta. Her husband, Forest Lee Carter, died in 1987.

LOREN HEPLER 1928-1996

Following heart surgery, Loren Hepler died in Edmonton, Alberta on June 8, 1996. He was born in 1928 in Ottawa, Kansas--was an errand boy, railroad hand, and a minor league baseball pitcher in his youth. He took his Ph.D. at the University of California, Berkeley (W. M. Latimer) and had an academic career in five universities (1954-'96). He was active in CODATA's Chemical Thermodynamics Task Group for many years He taught at the University of Lethbridge in Alberta, Canada, from 1968-83. From there he became AOSTRA Professor of Chemistry and Chemical Engineering at Alberta's principal research school, the University of Alberta in Edmonton. His research was in the field of thermodynamics, especially solution thermodynamics, and he did applied research in tar sands and heavy oil, devised comprehensive critical reviews of the thermochemistry of transition elements and their compounds, as well as employed the Picker heat-capacity calorimeter. He traveled extensively, and was a visiting professor on three continents and published 250 papers. After retirement, he continued research and writing and served as Adjunct professor at the University of Lethbridge

MICHAIL A. STYRIKOVICH 1902-1995

Academician Michail Adolfovich Styrikovich died in Moscow October 27, 1995 after a serious illness at the age of 93; he was born November 16, 1902. He was an outstanding scientist in energetics, heat, and mass transfer, thermal engineering and thermophysics. Professor Styrikovich developed methods for dynamic thermal calculations of vapor boilers. His studies were connected with the investigation of the hydrodynamics of two phase flows, the generation of mercurial vapors, the prognostication of energetics development and the structure of future energy consumption. He also created a theory of gas phase solutions of inorganic substances--particularly in steam. These and related Styrikovich works are well-known. He was President of the Soviet National CODATA Committee from 1965 to 1973 and Vice-President of International CODATA for eight years. He was also President of the International Heat and Mass Transfer Center; the Academician-Secretary of Physical and Technical Problems of the Energetics Division of the USSR Academy of Sciences from 1964 to 1980. Many international organizations sought his consultation. He was a very erudite, wise, witty and warm man and made significant contributions to the stature of CODATA in the world.

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