



38 CODATA / NEWSLETTER

1986 Recommended Values of the Fundamental Physical Constants

OCTOBER 1986

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An abbreviated set of some of the more useful values based on a least-squares adjustment with 17 degrees of freedom. The digits in parentheses are the one-standard-deviation uncertainty in the last digits of the given value. Since the uncertainties of many of these entries are correlated, the full covariance matrix must be used in evaluating the uncertainties of quantities computed from them.

Quantity	Symbol	Value	Units	Relative uncertainty (ppm)
speed of light in vacuum	c	299 792 458	m s^{-1}	(exact)
permeability of vacuum	μ_0	$4\pi \times 10^{-7}$ =12.566 370 614...	N A^{-2}	(exact)
permittivity of vacuum	ϵ_0	$1/\mu_0 c^2$ =8.854 187 817...	10^{-12} F/m	(exact)
Newtonian constant of gravitation	G	6.672 59(85)	$10^{-11} \text{ m}^3 \text{ kg}^{-1} \text{ s}^{-2}$	128
Planck constant	h	6.626 0755(40)	10^{-34} J s	0.60
$h/2\pi$	\hbar	1.054 572 66(63)	10^{-34} J s	0.60
elementary charge	e	1.602 177 33(49)	10^{-19} C	0.30
electron mass	m_e	9.109 3897(54)	10^{-31} kg	0.59
proton mass	m_p	1.672 6231(10)	10^{-27} kg	0.59
proton-electron mass ratio	m_p/m_e	1836.152 701(37)		0.020
fine-structure constant, $\frac{1}{2}\mu_0 c e^2/h$	α	7.297 353 08(33)	10^{-3}	0.045
inverse fine-structure constant	α^{-1}	137.035 9895(61)		0.045
Rydberg constant, $\frac{1}{2}m_e c \alpha^2/h$	R_∞	10 973 731.534(13)	m^{-1}	0.0012
Avogadro constant	N_A, L	6.022 1367(36)	10^{23} mol^{-1}	0.59
Faraday constant, $N_A e$	F	96 485.309(29)	C mol^{-1}	0.30
molar gas constant	R	8.314 510(70)	$\text{J mol}^{-1} \text{ K}^{-1}$	8.4
Boltzmann constant, R/N_A	k	1.380 658(12)	$10^{-23} \text{ J K}^{-1}$	8.5
Stefan-Boltzmann constant, $(\pi^2/60)k^4/\hbar^3 c^2$	σ	5.670 51(19)	$10^{-8} \text{ W m}^{-2} \text{ K}^{-4}$	34
Non-SI units used with SI				
electron volt, $(e/C) \text{ J} = \{e\} \text{ J}$	eV	1.602 177 33(49)	10^{-19} J	0.30
(unified) atomic mass unit, $1 \text{ u} = m_u = \frac{1}{12} m(^{12}\text{C})$	u	1.660 5402(10)	10^{-27} kg	0.59

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

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

The Inception, Beginning, and First Days of CODATA

My involvement in international scientific affairs and data for science and technology occurred after completing my graduate studies at the University of California at Berkeley in 1928. I was fortunate to receive an appointment at the U.S. National Bureau of Standards (NBS), in Washington, to work directly under the supervision of Prof. E.W. Washburn, Chief of the Chemistry Division, with an assignment to set up a thermochemical laboratory. Prof. Washburn was a member of the Commission on Thermochemistry of the International Union of Pure and Applied Chemistry (IUPAC) and also Editor-in-Chief of the International Critical Tables (ICT) of numerical data for physics, chemistry, and technology.

The ICT was founded in 1919, under the auspices of ICSU and IUPAC. Prof. Washburn had the cooperation and assistance of 408 scientists in 18 countries. The ICT produced 7 volumes, 1926-30, with an index volume following in 1933. Unfortunately, Prof. Washburn died in 1934 with the result that ICT lost its prime mover and the continuance of the ICT was lost.

Shortly after Prof. Washburn's passing, I was elected to succeed him as a Member of the IUPAC Commission on Thermochemistry. Two years earlier, Prof. Washburn and Dr. F.R. Bichowsky (Sub-Editor of the Thermochemical Tables in ICT Vol. 5) asked me to take the latter's old records and new references and revise the Thermochemical Tables of ICT. I did this on my own time and the book by Bichowsky and Rossini entitled "Thermochemistry of the Chemical Substances" appeared in 1936. My daily contact with Prof. Washburn, the Editor-in-Chief of the ICT, had had its effect.

I had already begun to take serious note of the data-compilation work completed or in progress in countries abroad. These included Julius Thomson's work in Denmark, Landolt-Börnstein Tabellen in Germany, Tables Annuelles des Constantes in France, and the Kaye and Laby Tables of Physical and Chemical Constants at the National Physical Laboratory in the U.K.

Following the demise of the ICT, a number of data-compiling projects in different areas appeared in the U.S.A. operating independently under industry and government sponsorship. These included projects sponsored by the National Bureau of Standards, the Atomic Energy Commission, the Bureau of Mines, the Office of Naval Research, the American Petroleum Institute and the Manufacturing Chemists Association. I was personally involved in three of these projects.

It had become quite clear that science is an international enterprise, not a national one, and that we can subscribe to the following two statements: (1) no one country has a monopoly on scientific intelligence; (2) scientific inquiry is not confined by national boundaries.

Looking at the number of data-compiling projects operating separately and independently in the U.S.A., it was clear that what was needed was a central office that would not compete with any of the projects but would provide services in the form of coordination, guidance on editorial and related matters, advice on sources of funding, etc. In 1955-58, I was Chairman of the Division of Chemistry and Chemical Technology of the National Research Council (NRC), and, at the same time, a member of the NRC committee dealing with data-compilation. The National Research Council approved the recommendation of this committee, chaired by Dr. Allen Astin, Director of the NBS, to establish, within the NRC, under the Division of Chemistry and Chemical Technology, a new Office of Critical Tables (OCT) which would provide the services mentioned above for all the data-projects operating in the U.S.A.

We were very fortunate in finding a highly qualified scientist to take on the job of directing the new Office of Critical Tables, in the person of Dr. Guy Waddington, then in charge of the Thermodynamics Section of the U.S.

Bureau of Mines at Bartlesville, Oklahoma. Dr. Waddington assumed his new position in 1957.

By 1964, the Office of Critical Tables had been operating for 7 years and our analysis indicated that the OCT was doing a reasonably successful job in providing coordination, guidance, advice, etc., to the data-projects operating in the U.S.A. I discussed with Dr. Waddington the possibility of creating an international organization that would do for data-projects world-wide what his Office of Critical Tables was doing on a national scale in the U.S.A.

In his daily tasks with the NRC, Dr. Waddington became acquainted with the officers and staff members of the National Academy of Sciences. At that time, Professor Harrison Brown was Foreign Secretary of the Academy and also a member of the Executive Committee of the ICSU. ICSU would be the ideal umbrella under which to operate a world-wide organization involving many disciplines.

Mr. Edward Rowan, on Brown's staff, was most helpful in the discussion Dr. Waddington had with him. Foreign Secretary Brown became much interested and took hold; under his leadership the following events occurred: (1) Prof. Brown convened a Working Group in Washington in late 1964, which recommended that ICSU set up a Committee on Data for Science and Technology; (2) the Working Group met in Frankfurt in 1965 and prepared a constitution with a list of national member countries and Union members; (3) in January, 1966, the General Assembly of ICSU, meeting in Bombay, India, with Sir H.W. Thompson in the chair, approved the establishment of a Committee on Data for Science and Technology, with its constitution and its list of initial national country members and Union members; (4) in June, 1965, Prof. Brown convened the Working Group in Paris for the first meeting of the new Committee.

At the first meeting of the Committee, the following elections were made: President, Prof. Frederick D. Rossini (U.S.A.), Vice-Presidents, Professors Wilhelm Klemm (Germany-Federal Republic) and Boris Vodar (France); Secretary-Treasurer, Prof. Sir G.B.B.M. Sutherland (U.K.); Director of the Headquarters Office, Dr. Guy Waddington (U.S.A.). By this time, it was quite clear that, because of the great interest of the U.S. National Academy of Sciences and the fact that it could provide quarters for the new enterprise with Dr. Waddington's Office of Critical Tables where he could serve as Director, in addition to his duties as Director of the OCT, it was agreed that the new enterprise would be located in Washington.

Initially, the member countries were six: France, Germany-Federal Republic, Japan, U.K., U.S.A., and U.S.S.R. The initial number of Scientific Unions was 10. In order to simplify communication, Dr. Waddington coined the acronym CODATA to represent Committee on Data for Science and Technology. The start of CODATA was made financially possible because of the quarters provided by the U.S. Academy and operationally successful because of the directorship of Dr. Waddington.

Dr. Waddington and I agreed that, because of the international character of CODATA, once CODATA was well started in the U.S.A. and it became financially independent through annual dues of member countries, the Headquarters Office should be moved to another country, preferably a member country in Western Europe, to facilitate travel and communication. Matters worked out satisfactorily, both financially and scientifically, so that after two years in Washington, the CODATA Office was moved to Frankfurt. Meanwhile, in these first several years, some additional Scientific Unions became members and Task Groups were established on "Fundamental Constants", "Chemical Kinetics" and "Chemical Thermodynamics".

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South African National Committee for CODATA

The composition of the 1986 South African National Committee for CODATA is summarized here:

Chairman:

Dr. E.N. van Deventer, Deputy President, CSIR

Members:

Dr. S.A. Fellingham, South African Medical Research Council

Dr. S. Hart, Chief Director, National Institute for Materials Research, CSIR

Mnr. J.S. van Rhyen, The Weather Bureau

Dr. C. Frick, Director, Mineralogy and Geochemistry, Geological Survey

Prof. C.J.H. Schutte, Department of Chemistry, University of South Africa

Prof. J.A. Thomson, CSIR Laboratory for Molecular and Cell Biology

Prof. P.H. Stoker, Department of Physics, Potchefstroom University for CHE

Mr. V.A. Shaw, Chief Director, National Institute for Informatics

Dr. G.E. Gibbs Russell, Botanical Research Institute

Secretary:

Miss G.U. Schirge, International Relations Division, CSIR, P.O. Box 395, Pretoria 0001, South Africa

International Conference on Thermodynamics of Aqueous Systems with Industrial Applications

This conference is sponsored by the Design Institute for Physical Property Data (DIPPR) of the American Institute of Chemical Engineers, the National Bureau of Standards and the National Science Foundation. It will be held May 10-14, 1987 at Airlie House, Warrenton, Virginia and will feature experimental data and techniques, basic theory, correlation and estimation techniques, data compilation, computer calculation of equilibria, industrial applications, and new directions. Attendance will be approximately 150 from industry, government, and academia.

Information on technical material may be obtained from: Dr. Noel C. Scrivner, E.I. du Pont de Nemours & Co., Louviers 1356, Wilmington, DE 19898, telephone: (302)366-4021. Registration material may be obtained from: Ms. Mary Pat Healy, DIPPR-AICHE, 345 East 47th Street, New York, NY 10017, telephone: (212)705-7332.

Indian National Committee for CODATA

The Indian National Committee for CODATA for the period July 1985 - June 1988 approved at a late 1985 meeting of the Council of the Indian National Science Academy is as follows:

Chairman: Dr. E.S. Raja Gopal, FNA, Professor, Department of Physics, Indian Institute of Science, Bangalore - 560 012.

Members: Dr. P.K. Iyengar, FNA, Director, Bhabha Atomic Research Centre, Trombay, Bombay - 400 085; Prof. R. Srinivasan, Senior Professor and Head, Department of Crystallography, University of Madras, Guindy Campus, Madras - 600 025; Dr. K. K. Lakshar, Centre for Cellular and Molecular Biology, Hyderabad - 500 009; Dr. N. Vijayaditya, National Information Centre, Electronics Commission, (Government of India), Pushpa Bhavan, Chirag Dilli, Madan-gir Road, New Delhi - 110 062; Dr. Kishan Lal, FNA, Deputy Director, National Physical Laboratory, Hillside Road, New Delhi - 110 012; Prof. A.P. Kudchadker, (Committee Secretary), Indian Institute of Technology, Powai, Bombay - 400 076.

SIGLE: System of Infor- mation on Grey Literature in Europe

To solve the problem of access to unpublished documents in scientific research, technology and social and economic sciences, European documentation centers, aided by the Commission of the European Communities, developed a cooperative information system to identify and supply this type of document, termed grey or nonconventional literature.

Grey literature comprises minutes, technical reports, papers, regulations, working documents and notices which are not published and which cannot therefore be obtained through the normal commercial publication channels.

Tremendous problems involved in the identification, acquisition and bibliographical control of this type of literature led to setting up SIGLE (System of Information on Grey Literature in Europe).

More than 80 000 documents are now stored in the SIGLE database and the number is growing steadily by some 30 000 documents a year.

The fields covered include: aeronautics; agriculture; phytology and veterinary sciences; the social sciences; biological and medical sciences; chemistry; the geosciences; electronics and electricity; energy; materials; mathematics; civil, industrial and marine engineering; methods and equipment; military science; missile technology; navigation and telecommunications; shipbuilding; physics;

propulsion and fuels; and space technology.

The SIGLE database is available for on-line documentary research via Euronet DIANE, accessed on BLAISE-LINE in the United Kingdom and INKA in the Federal Republic of Germany.

To facilitate the development of the SIGLE system, a European association has been set up under Luxembourg law: EAGLE (European Association of Grey Literature Exploitation), comprising major Belgian, British, French, German, Italian, Luxembourg and Netherlands information and documentation centers to promote the exploitation of European grey literature.

Information on EAGLE and the SIGLE database can be obtained from: Mr. Marcel Maurice, Commission of the European Communities, DG XIII/A/2, L-2920 Luxembourg.

Intl. Chemical Sciences

Scientists fortunate enough to work in developed countries, with comparatively rich resources in education, facilities, and funds, have a special obligation to share these resources and our energies with scientists in less developed countries and to work together to seek solutions to the world's most pressing problems. Among these problems are many areas (for example, improved control of disease and increased production of food) whose solutions may well be reached through the field of chemistry.

The International Organization for Chemical Sciences in Development (IOCD) was founded in 1981 involving chemists from Third World nations in the search for solutions to the urgent problems of their countries. To do this, IOCD uses two main channels: initiation of research programs and provision of services. Because scientists from industrial countries serve as scientific advisers and monitor IOCD research projects, technology transfer and the strengthening of institutions in Third World countries is also facilitated.

Professor Glenn T. Seaborg, University Professor of Chemistry and Chairman of the Lawrence Hall of Science, University of California, Berkeley, is the President of IOCD.

The IOCD has already made an impressive start in accomplishing some of its objectives in the brief period since its founding. A program of chemical synthesis designed to uncover new drugs for the treatment of tropical diseases has been initiated. Eleven laboratories (located mainly in developing countries) are participating in this program.

Reports on CODATA Activities by the National Committees

From Australia -

The CSIRO national computer network **CSIRONET**, which was previously closely linked with the CSIRO Division of Computing Research, has become an autonomous unit within CSIRO. This will ensure that the information needs of users in research and industry can be more adequately serviced.

The CSIRO Division of Information Technology, in collaboration with University Computer Centres, has commenced a review of the current status of networking within Australian research laboratories. It will focus on both internal interworking and the extent of international communications.

A new information service known as **CSIRO AUSTRALIS** has been established on CSIRONET to provide access to bibliographic, factual and numerical data. Some 21 databases are now included in this service.

ACI-AUSINET--a commercial computer network covering a wide range of business and non-scientific databases in addition to scientific ones--continues to expand, particularly in the bibliographic and factual fields.

In the field of biotechnology, particularly monoclonal antibody production, there is a quickening of interest in Australia in the CODATA-sponsored Hybridoma Data Bank.

From Canada -

The project for data bank transmission via satellite and other telecommunication systems based on micro-computer application has been carried forward to the state where micro-computer data banks for thermodynamic data have been made satisfactorily operational. Data transmission from micro to micro should be underway before the 16th CODATA General Assembly.

From China -

(See extensive report in Newsletter #37)

From the F.R.G. -

In Physics: FIZ Karlsruhe continues to act as a National Information Center for physics. Recent activities:

- The publication of data compilations in the series "**Physikdaten/Physics Data**" is continuing. Since 1984 some 7 more items have been published.

- A bibliographic database which gives reference to all worldwide existing **data compilations** in physics is regularly updated. It contains, at present, about 3 800 items. A printed version has been issued in 1986 in the series "**Physikdaten/Physics Data**" (No. 3-5).

- The establishment of a **computerized new database** containing **infrared spectra** has just been finished (produced by the BASF AG, Ludwigshafen). It contains 5 000 infrared spectra and will be offered for on-line access at FIZ Karlsruhe within the next three months.

- A database "**GAMCAT**", dealing with gamma-ray and alpha-ray decay of radioactive isotopes provides gamma-ray energies, intensities, etc.

- A project for the creation of an **Integrated Spectroscopic Information System** including various kinds of spectroscopic methods like HNMR, C13 NMR, Infrared, etc. has just been started. A first test version will be established by the BASF AG in Ludwigshafen by 1987.

- The establishment of a database of **Thermophysical Properties** by the "Institut für Kernenergetik und Energiesysteme" of the University of Stuttgart is underway. Data are expected for about 2 000 materials for thermal conductivity and 400 for heat storage. Implementation at FIZ Karlsruhe for on-line access of a later stage is envisaged.

In Chemistry and Chemical Engineering:

- **DETERM:** (Dechema Thermophysical Property Data Bank) which was already mentioned earlier consists now of three systems which retrieve (DETERM-SDS) physical data of chemical compounds and mixtures. DETERM contains 415 000 data records of more than 3 000 compounds and mixtures, and 140 calculation routines for the prediction of properties at any given state.

- **COALDATA:** (developed in a European Community project by Dechema/FRG, PPDS/Great Britain, LASSC/Belgium, and SBN/Netherlands) runs under the DETERM retrieval software and contains physical data on coals, coal liquids from liquefaction processes, and coal chemicals covering also the origin of the various coal types. COALDATA has run on the FIZ Karlsruhe host since August, 1986.

- **ELDAR:** a data bank for electrolyte systems (DECHEMA and University of Regensburg), runs also under the DETERM retrieval system and contains 180 000 data tuples from 8 000 documents on transport, phase equilibrium, surface, optical, electric, magnetic, acoustic, EMF, density and related properties of electrolytes. ELDAR will be available by the end of this year at the FIZ Karlsruhe host.

- **POLYMAT:** a polymer materials databank developed by DKI, Deutsches Kunststoff-Institut, Darmstadt. POLYMAT will contain up to 80 properties for each of the about 6 000 plastics materials (thermoplastics, duroplastics, casting resins). The retrieval system was developed by FIZ Chemie which will offer the data bank via the FIZ Karlsruhe host.

- **Gmelin** is preparing a numerical data file ("**Gmelin Online Data System**") from its vast amount of data contained in the Gmelin Handbook of Inorganic Chemistry. The data bank will also contain data of organometallic compounds.

- At Beilstein an on-line version of its Handbook of Organic Chemistry, **BEILSTEIN ONLINE**, will enable combined searching of data and structures or substructures. Over 60 out of more than 300 searchable items are numerical. These will be mechanical, thermal, transport, thermodynamic, optical, electrical, magnetic, phase equilibrium, chemical equilibrium, chemical reaction rate, and other data.

In Geoscience:

- In 1985 the Information Center for Mining, Geosciences and Water Management (GEO FIZ) was established at the Federal Institute for Geosciences and Natural Resources (BGR) in Hannover. The Information Center provides on-line access to databases of geoscience literature (for example, **GEOLINE** with 470 000, **HYDROLINE** with 40 000 and **MARINELINE** with 16 000 data); and in addition, off-line access to factual databases, like the **Mineral Deposit Database** of BGR with descriptions of 4 000 deposits worldwide, or data files on minerals with regard to reserves, production, supply, demand, imports and exports of the FRG.

From France -

The overall study of French production and needs has been undertaken to identify the gaps so that a proposal for new projects can be made to the French authorities at the end of 1986.

The sub-group on Metallurgy and Mechanics, led by Mr. Hocheid (Ecole Centrale and C.N.A.M.) has established links with the Société Française de Metallurgie and the C.E.A. It is preparing a questionnaire to ascertain French data needs and utilization which will be widely distributed to institutions and companies.

The sub-group on Polymers and Composites (led by Mr. Pabiot, Ecole Nationale Supérieure des Techniques Industrielles et des Mines de Douai) held a meeting on 6 February 1986 with about fifty participants: data bank

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Generating Instructional Data Modules

The creation of modular educational materials for use in data-related teacher-training courses and in instruction at the college and professional levels is proposed in a recent report.* Workshops are described that could be held to obtain formative evaluation of such materials and to foster their use.

The recommendation on generating instructional modules calls for mechanisms to be set up whereby instructional modules on data handling are produced for use in all levels of education, and to be of use in the classroom, laboratory, and place of work.

Each module should be short enough so that it can be used to teach a single data handling skill. It should also be short so that it can be easily updated in response to new professional and instructional insights. At the higher levels, the short modules should be designed so that they can also be easily combined in various ways to produce formal courses.

The modules should have audio-visual, laboratory, and computer project components where appropriate. Many of the modules could have separate versions with examples appropriate to specific disciplines.

The modules would be used mostly in the print medium at first, but they should be printed from standard electronically stored files for easy updating and inexpensive distribution.

The modules should be peer reviewed and extensively field tested and then revised as needed.

They should be listed in a printed catalog and made available by electronic retrieval. An electronic information system would also have aids for linking the modules in order to construct custom learning sequences.

Evaluative workshops should be held for prospective users of the instructional materials. Persons invited to these workshops would be typical of the target audience. They would examine the modules, learn successful techniques for using them, and give feedback to the developers of the materials. Such feedback could initially be sought on the acceptability of the modules, but could be held in conjunction with professional meetings. Workshop attendees would be encouraged to become collaborators in the generation, evaluation, and revision of the materials.

Peter Signell

**To obtain a complimentary copy of the report, "Improving the Treatment of Scientific and Engineering Data Through Education," published by the National Academy Press in 1986, contact Dr. Gesina C. Carter, Staff Director, Numerical Data Advisory Board, National Research Council, 2101 Constitution Avenue, N.W., Washington, D.C., 20418.*

Peter Signell is Professor of Physics and Astronomy at Michigan State University. He has been a member of the National Research Council's Numerical Data Advisory Board and was chairperson of the NRC panel that produced the report. Other members are: Carl O. Bowin, Gerald G. Johnson, Jr., Gunther Schlager, Edgar F. Westrum, Jr. and Gesina C. Carter, *ex officio*.

First CODATA Workshop on Nucleic Acid and Protein Sequencing Data

In supplement to the preliminary information in the July Newsletter, we note that the First International Workshop, to be held May 3-6, 1987 at the National Bureau of Standards, Gaithersburg, Maryland 20899 U.S.A., will address the fundamental aspects of data collection, management, quality control, and analysis of DNA, RNA, and protein sequences. Emphasis will be placed on methods of standardization, networking, and global interfacing of databases, as well as on exploration of the potential for the use of databases for storage and retrieval of higher

order information such as periodicity, pattern and signal, secondary and tertiary structures, and genome maps.

The goals of the First CODATA Conference on Nucleic Acid and Protein Sequence Data will be to provide a forum for the drafting of recommendations concerning:

Education
Analytical software needs
Subdisciplinary database responsibilities
Criteria for publication in scientific journals

Sessions will discuss the following topics:

Interfacing databases
Approaches to standardization
Communication

The Program Committee intends to follow a tradition of promoting the free exchange of ideas, providing a conducive environment for active discussions, and highlighting areas where new developments are needed. The Workshop will also herald new and innovative approaches in the fields of nucleic acid and of data processing.

A call for papers will be issued in December 1986. Additional information is available from: Mrs. Kathy C. Stang, U.S. Department of Commerce, National Bureau of Standards, A353 Physics, Gaithersburg, Maryland 20899.

CODATA Calendar

1986

November

- 20 CODATA France National Day
on Materials Databases, Paris, France

1987

January

- 13-14 Task Group on Coordination of Protein
Sequence Data Banks, Nice, France
13-14 Scientific Program Committee, International
Conference, Paris, France
15-17 CODATA Executive Committee,
Paris, France
19-20 Task Group on a Referral Data Base, Paris,
France

May

- 3-6 Workshop on Nucleic Acid and
Protein Sequencing, Gaithersburg,
MD

1988

September

- 26-29 International CODATA Conference,
Karlsruhe, Germany
30- CODATA General Assembly,
Oct 1 Karlsruhe, Germany

Reports on CODATA Activities by the Unions

The International Union of Crystallography -

In the field of numerical data the IUCr continues to promote the spreading of databases. At all its international and national congresses and in many summer schools the following databases have been demonstrated in action or by posters. They cover the most important fields of crystallographic data completely and they all are publicly available.

- Cambridge Crystallographic Data File - University Chemical Laboratory, Cambridge, U.K.

- Crystal Data - National Bureau of Standards, Gaithersburg, MD, U.S.A.

- Inorganic Crystal Structure Database - Fachinformationszentrum Energie Physik Mathematik, F.R.G.

- Metals Data File - National Research Council of Canada, Ottawa, Ontario, Canada

- Powder Data File - International Center for Diffraction Data, Swarthmore, PA, U.S.A.

- Protein Data Bank - Brookhaven National Laboratory, Upton, NY, U.S.A.

The accessibility of databases has been checked by a questionnaire distributed to 33 National Committees of the Union. The main conclusions which may be of importance for the whole field of information by databases are: Numerical databases are a highly acknowledged instrument to handle crystallographic (and other) data. Not all potential users are familiar with scientific possibilities of databases and technical possibilities to access them. High standards for contents of databases and for programs to handle them are expected.

Further activities are directed to the improvement of the data input. A "Standard Crystallographic File Structure" has been developed. A report about "The Deposition of Crystallographic Results" will be published and discussions about a stronger cooperation among authors, editors, referees, database producers and printers have been started. This cooperation should be possible by electronic mail or exchange of floppy disks. The International Union of Crystallography publishes journals which contain about 25% of the annual amount of relevant data. Thus this cooperation could be a pilot project for a general handling of numerical results.

International Union of Geological Sciences -

In the field of Stratigraphy, age boundaries (stratotypes) for the Precambrian-Cambrian, Ordovician-Silurian, all stages of Silurian, Silurian-Devonian, as well as of the Pliocene-Pleistocene boundary, have been established. A committee on Quantitative Stratigraphy focussing on the mathematical treatment of biostratigraphic field data in order to obtain a probabilistic biochronology has been established. In Geological Documentation, the main result is the completion of a Multilingual Thesaurus of Geology. In the field of Automatic Processing of Geological Data, new technologies such as optical disc storage and the use of expert systems to build knowledge bases of geological processes and to advise on procedural problems are being used to help the modelling and assessment of mineral and energy resources. In Marine Geology, the activities carried out in connection with the Scientific Committee on Oceanic Research (SCOR) are very important. The impact of comparative planetology on terrestrial problems is emphasized by the newest commission fostering the view that the geological history of Earth does not exist in isolation. The Commission on Igneous and Metamorphic Petrogenesis has been reorganized and will continue to promote interaction between the community of experimental petrologists and other geological disciplines. A Sub-Commission on Databases for Petrology will stimulate the development and exploitation of electronic databases by petrologists.

International Union of Geodesy and Geophysics -

The next quadrennial assembly of IUGG will be in Vancouver, 9-22 August 1987. CODATA particularly should be aware of a joint proposal of an IAU and IUGG working group to establish a new FAGS service assuming the activities of the Bureau International de l'Heure (BIH) and of the International Polar Motion Service (IPMS). The intention would be to provide a unified service to maintain both earth reference systems and astronomical reference systems for research and applications requiring precise spatial reference. This is particularly opportune as new techniques of location through (for example, VLBI) laser tracking of satellites and doppler tracking are making major advances in this field.

The IAPSO Working Group on Symbols, Units and Nomenclature has completed publication of the Report on Symbols, Units and Nomenclature. Pt. 1 contains a thorough discussion of the SI Units with special reference to oceanography and Pt. 2 tabulates the appropriate SI units for most of the derived units in active use in Marine Science.

International Union of Microbiological Sciences -

Interest of microbiologists in CODATA activities has increased. Microbiologists are represented on the CODATA Task Force for hybridoma data gathering and are also involved in the study group involved in planning a workshop on nucleic acid and protein sequencing data as a preliminary step for establishing a task group on nucleic acid sequence data. IUMS will co-sponsor the workshop on nucleic acid sequence data to be held at the National Bureau of Standards, Washington, D.C., May 3-6, 1987. Funds for the workshop have been provided by CODATA and a request has been submitted to IUMS for support of the workshop also.

The Microbiological Resource Centers (MIRCENS) Director's Council has established a network for microbiological workshop and electronic mail/computer conferencing.

International Union of Nutritional Sciences -

Committee III/5, Vitamin A Deficiency, of the IUNS published in May, 1985 the first edition of The IUNS International Directory of Scientists and Administrators Involved in the Alleviation of Vitamin A Deficiency and Nutritional Blindness. The proceedings of the workshop, "Towards Compatibility of Nutrient Data Banks in Europe," Wageningen, May 1983, were published in Annals of Nutrition and Metabolism 29(SI), 1-72, 1985.

Activities during 1985 as a result of the 1983 Wageningen workshop were:

- Work has been carried out on two projects: Collection of data related to nutrient losses and gains in the preparation of foods and on missing values in composition tables; quality of food analyses.

- An inventory of existing food composition tables in Europe was organized, published and distributed.

- Twenty food composition tables in Europe were compared with respect to layout (format), nutrients and non-nutrients included, modes of expression and units of measure of the components, and the extent of explanation and reference to sources of data.

- After a series of meetings in Luxembourg in December 1984 and Heidelberg in February and May 1985, a food coding system based on 14 major food groups was agreed on by representatives from 17 countries. The 14 sub-groups were sub-divided into 2500 sub-categories. The result is called EUROCODE 2 which is part of a food coding and descriptor system.

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● A market study to identify users and the needs of users of food composition tables/nutrient databases conducted in Denmark and the Federal Republic of Germany, indicated high interest, particularly in high quality data available on short notice, and more comprehensive than present data.

International Union of Pure and Applied Biophysics and International Union of Biochemistry (IUPAB and IUB) -

The structural, kinetic, thermodynamic and systematic data sources on which the biochemist and the biophysicist relies are very much identical to those of the basic physical, chemical and biological sciences and are shared with these. At present, the need for specialized databases in biochemistry or biophysics, beyond the existent ones on molecular structures and biopolymer sequences, is not considered an issue requiring intervention by IUB or IUPAB. The Interunion Commission on Biothermodynamics finished its formal existence after fulfilling its original task as a joint commission of IUB, IUPAC and (until 1984) IUPAB. The commission has published its recommendations in scientific journals, the Handbook on Chemical Thermodynamics Data in the Biological Sciences is in press. IUB and IUPAB were informed that some activities of this committee will be continued within an enlarged scope in the Working Party on Biophysical Chemistry in IUPAC's Division of Physical Chemistry. Neither the commission nor the joint groups of IUB and IUPAB are presently engaged in projects related primarily to the compilation of data. Both Unions are aware, however, of the growing activity of CODATA in the biosciences. In view of the rapid development of a new technology for the communication of information, at a time where the cost of maintaining exhaustive libraries in multidisciplinary fields has become a problem for many research institutions, the commitment of CODATA and its considerable help to ensure continuity to these initiatives is very much recognized.

International Union of Pure and Applied Chemistry -

The IUPAC Committee on Chemical Committee Databases met early in 1986 under the Chairmanship of Dr. David R. Lide, Jr. and Dr. S. Heller as Coordinator and Secretary.

The terms of reference of the Committee are:

● To advise the president and Executive Committee on all aspects of computerized databases of chemical properties, including division programs which produce databases, needs for standardization for databases and chemical structure records, and policy on database dissemination.

● To work with commissions on the design and implementation of databases and appropriate software and to encourage maximum compatibility of databases from different groups within IUPAC.

● To promote, in collaboration with other ICSU bodies, a higher level of awareness of the application of computers in the management, dissemination, and use of chemical data.

Candidate databases for initial endeavors were considered. In addition a number of educational activities on structural representation, proposed IUPAC chemical codes, computer term glossary for chemists, etc. were discussed.

International Union of Pure and Applied Physics -

IUPAP is an organization primarily directed towards the general furtherance of physics through sponsorship of conferences and workshops; there is little direct support of data compilation and evaluation within the Union, although the individuals and organizations associated with its commissions contribute to the general data field by

virtue of their associations with academic or national laboratories.

The Union has however recently increased its activities in the applied and industrial aspects of physics, recognising the increased importance of these areas. Concomitant with this there should also be an increase in the emphasis on data. The Commission on Symbols, Units, Nomenclature, Atomic Masses and Fundamental Constants has, as an example, revised its mandate to include a more active concern with metrology and standards. Since the 1984 General Assembly, the new review by Wapstra and Audi on Atomic Masses and Nuclear Reaction Energies has been published and the Commission is preparing a new edition of the handbook on "Symbols, Units and Nomenclature in Physics," which should appear within the next year.

Federation of Astronomical and Geophysical Services -

The activities of FAGS have continued in a regular way. The Services are storing, evaluating and disseminating a very large amount of data pertaining to their individual fields. The methods are of course permanently improved to take advantage of the new facilities for the treatment of information.

The list of the Services is as follows:

	Since
International Polar Motion Service	1895
Bureau International de l'Heure	1911
International Gravity Bureau	1953
International Centre for Earth Tides	1960
Permanent Service on Mean Sea Level	1933
Permanent Service on Geomagnetic Indices	1932
Quarterly Bulletin on Solar Activity	1928
Permanent Service on the Fluctuation of Glaciers	1967
International Ursigram and World Days Service	1962
Centre de Données Stellaires	1985

This last Centre installed at the Observatoire de Strasbourg is a new one accepted in the Federation in 1985. There is however a problem now with the International Service of Geomagnetic Indices which has been discontinued in De Bilt-Utrecht and must be transferred to another Institute or Observatory.

International Council for Scientific and Technical Information -

The Executive Board of the ICSTI commissioned a Task Force on Numerical Data at its meeting of June 2, 1985, in Baden-Baden, Federal Republic of Germany to determine whether the establishment of a Special Interest Group on Numeric Data in ICSTI would be a useful adjunct in furthering relationships between CODATA and ICSTI.

The Task Force reached the conclusion that such a Special Interest Group would indeed offer the opportunity to build on the relationship being established with CODATA, to help ensure that the efforts of the two organizations are optimized in useful linkages of bibliographic, factual, and numeric data information systems. Those findings were endorsed by the ICSTI General Assembly, which met in May 1986 in York, England. The first meeting of the Numerical Data Group will be held in December 1986.

World Federation for Culture Collections -

The World Federation for Culture Collections is an organization to promote and foster activities that support the interests of culture collections and their users. A struc-

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producers (both from banks which are operational and banks which are being created), data users (manufacturers of plastics, machines, etc.).

The sub-group on Civil Engineering and Construction (led by Mr. Puccini, Société Eternit) held a smaller meeting on the same day to study the following themes: hosts and network systems, data evaluation, data bank coordination, cost, promotion.

The sub-group on Electronics and Electrotechnics has been created to coordinate cooperation between public research institutions (E.S.S., Université de Paris VI, C.N.E.T., L.E.T.I.) and industrial companies (C.G.E., Thomson, Metallimphy, etc.).

From the G.D.R. -

The Central Information Institute for Chemistry and the Central Institute for Molecular Biology (Academy of Sciences) built new bioscientific and chemical data centers. The conclusions and recommendations resulting from a careful state-of-the-art analysis made of the handling of scientific and technical data were presented to the Government and to the heads of various research institutes in different fields, in particular to the Academy of Sciences of the G.D.R.

Technical support and the use of computers and networks were a further consideration in the work of the N.C.-G.D.R. The computer network DELTA was constructed to create computer links between the research and education communities, i.e. between computer centers in the Institutions of the Academy of Sciences and certain universities. This network is mainly used to access and disseminate data.

From Hungary -

In the series "Publications of the Hungarian National Committee for CODATA" the following reports were published:

No. 2. Recommended Consistent Fundamental Physical Constants (Hungarian translation of CODATA Bulletin No. 11).

No. 3. Computerized Cartographic Information System for Soil Mapping (in Hungarian - the English version of this Report is in preparation).

From India -

The importance of critical data/reviews in various branches of science and technology is being increasingly recognized. Serious programs in biotechnology and library information have been finally started with the principal support of the National Biotechnology Board (Government of India) and the University Grants Commission. As in many areas the early lukewarm phase is giving way now to an enthusiastic participative acceptance. The earlier programs on crystallographic and nuclear material databases are progressing well. The Department of Science and Technology, Government of India, organized a meeting in April 1985 of several potentially interested groups like those working in bio-resources, industrial toxicology, thermophysical data, petrochemicals, medicinal plants, earth resources, energy research, meteorology, environmental problems and natural products. There was an awareness of the utility of modern computer-based data systems and a consequent desire to start serious activity in this direction.

The national committee noted that while it can play a useful role in catalytically increasing the tempo of these activities, it has no financial resources to support large projects. It was therefore decided to concentrate on the promotional aspects. As a part of this effort, it was decided to hold a national symposium in December 1986 at the Indian Institute of Science, Bangalore.

From Israel -

As a follow-up of the Ninth Conference, and on the initiative of the National Committee, the National Center of Scientific and Technological Information (COSTI), which is an agency of the Ministry of Energy and Infrastructure, has published in February 1986, under the editorship of Dr. Hoffman, the "Directory of Special Data Bases in Israel." Listed are complete bibliographic details, scopes, contents and services provided of 50 databases, some 34 of them factual databases in natural sciences. The compilation, first of its kind in Israel, is probably incomplete. Publication of a revised, expanded and more complete version is anticipated within the next two years. Having accumulated this experience, they plan to conduct a countrywide survey of individual scientists, rather than institutions, to determine the degree of interest in databases and information activities in general, and in that of CODATA in particular.

From Japan -

Collection, compilation, and evaluation in Japan of physical and chemical property data of substances have been left mainly to voluntary activities of a smaller number of eager scientists on the plea of the necessity of special knowledge for these works. This trend has made it difficult to accumulate data systematically and to maintain them routinely, and has, furthermore, caused these data to be available only to a limited number of scientists.

As an attempt to improve these circumstances, they are developing the Thermophysical and Thermochemical Property Database System (TH System) with the following intentions:

1) To promote the collection and compilation activities carried out in some special data centers in Japan, by organizing these data into a database.

2) To disseminate this database to all classes of users at a reasonable price through a public information service center (JICST).

The TH System is being developed as one of the components of the Integrated Chemical Database System, supported by the funds of the Science and Technology Agency of the Japanese Government. Therefore, the TH System is also intended to be capable of combined use with other database systems in the integrated system.

The developing of the TH System started in 1981. This system will be in operation after 1987.

The TH database system has been designed for thermophysical and thermochemical property data of pure substances which comprise elements, inorganic compounds, and low molecular weight compounds, and of mixtures composed of three or less components. Data covered by the database are divided into two types: 1) about 40 kinds of fundamental thermophysical and thermochemical property data such as PVT data, vapor pressure, etc.; 2) 15 kinds of physical and chemical property data of inflammable substances, such as ignition temperature, flame temperature, inflammability limit, etc.

These data are collected from primary journals and data books, and will total 50 000 sets by 1987. Evaluation of these data will be done by data center experts.

From Poland -

The Polish National Committee for CODATA for 1984-1986 has been appointed by the decision of the Praesidium of the Polish Academy of Sciences as a Scientific Committee directly attached to the Praesidium and the present composition of the Committee was slightly extended. This reflects the fact that the CODATA sphere of activities became more interdisciplinary and the number of disciplines in which activities are undertaken has been augmented. Direct reporting to the Praesidium of the Academy (previously the Committee reported to the

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15th CODATA General Assembly Sets Scientific Direction

The 15th CODATA General Assembly, which followed the Conference, authorized 11 Task Groups for the 1986-88 period. These include new projects on the implementation of a prototype Microbial Strain Data Network and the establishment of standard formats and terminology for engineering materials databases. The new roster of officers and members of the Executive Committee is as follows (asterisk denotes members and officers newly elected at the General Assembly):

President: David R. Lide, Jr. (National Bureau of Standards, U.S.A.)*

Past President: William W. Hutchison (Energy, Mines and Resources Ministry, Canada)

Vice-President: Andrzej Bylicki (Polish Academy of Sciences, Poland)

Vice-President: Jacques-Emile Dubois (ITODYS, France)

Treasurer: David G. Watson (University Chemical Laboratory, Cambridge, U.K.)

Secretary General: Alain Bussard (Pasteur Institute, France, retired)*

Members:

David Abir (Tel Aviv University, Israel)*

James Crease (U.K. Institute of Oceanographic Sciences, U.K.)*

Akira Tsugita (Science University of Tokyo, Japan)*

Lev V. Gurvich (Institute for High Temperatures, U.S.S.R. Academy of Sciences, U.S.S.R.)*

Edgar F. Westrum, Jr. (University of Michigan, U.S.A.)

Heinrich Behrens (Fachinformationszentrum Energie, Physik, Mathematik, F.R.G.)

Marcello Carapezza (University of Palermo, Italy)

The General Assembly accessed both the reports from the National and Union members and the extant task group and the analysis of rapporteurs for the bio and geosciences, chemistry, and chemical engineering, physics, technology, as well as data management and handling. On the basis of this and other information sources, decisions were made on the renewal of the extant task--and/or working--groups as task groups for the biennial period.

Among the renewed groups were the following (the name of the chairperson is included):

Chemical Thermodynamic Tables, H.J. White

Fundamental Constants, T.J. Quinn

Critically Evaluated Phase Equilibrium Data, A. Bylicki

Multisatellite Thematic Mapping, C. Bardinet

Geothermodynamic Data, I.L. Khodakovsky

CODATA Referral Database, E.F. Westrum, Jr.

Hybridoma Data Bank, B.W. Janicki

Coordination of Protein Sequence Data Banks, B. Keil

Internationally Compatible Environmental Data, M. Martin-Bouyer

Microbial Strain Data Network, M.I. Krichevsky

In addition, two new task/working group proposals were accepted by the general assembly:

Material Database Standards, (to be named)

Computer Graphics for Data Capture and Presentation, (to be named)

In as much as financial restrictions do impose a restraint on the total scope of endeavor that CODATA can mount in any particular period--other proposed endeavors were not approved by the delegates at this time and both the Executive Committee and the delegates themselves will probably present modified or new proposals for consideration in the near future.

FIRST DAYS OF CODATA

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Though CODATA was organized to provide a framework capable of expanding to cover new and increasing activities, it is unlikely that any of the original officers foresaw what has actually happened: member countries, 6 to 18; Scientific Unions, 10 to 15; Task Groups 3 to 13.

As the first President, I can say that the first several years of CODATA went so well because of the great co-operation among the representatives of the six member countries and the Director of the CODATA Office. With great thanks, I record the immeasurable assistance received from Professors Klemm, Kotani, Styrikovich, Sutherland, and Vodar. I believe that every one of these men agreed with me that the dedicated work of Dr. Guy Waddington in those first two years made CODATA become a viable enterprise.

Credit for the remarkable growth of CODATA must be shared all along the line, from top to bottom, from the inception to the present. All of the past and present delegates have made contributions, each in his own way, to the development of CODATA.

While all participants in the work of CODATA can heave a sigh of relief regarding its first 20 years, we must keep firmly in mind that what lies ahead is an even greater work, which will challenge the talents of those who carry on.

Frederick D. Rossini
First President of CODATA, 1966-70

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ture of committees for Education, Patents, Postal and Quarantine, Publicity and Endangered Collections exists to carry out the current programme. In addition, the Federation sponsors two major international data activities, the World Data Centre (WDC) for Collections of Microorganisms and the Microbial Strain Data Network (MSDN).

The WDC has pioneered the collection of microbiological data and because of the retirement of its first Director, Professor V.B.D. Skerman, must now be relocated. In the summer of 1985 the WFCC invited proposals from organizations to take over the database and following assessment of the proposals by a committee set up for the purpose, agreed to relocate the WDC to the Institute of Physical and Chemical Research, RIKEN, Japan. Accordingly, a Letter of Agreement between WFCC and RIKEN has been prepared and arrangements for transfer of the database are under way. The database will be operating from RIKEN as of July, 1986, and the WFCC is confident of the competence and enthusiasm of RIKEN to develop the WDC to the benefit of culture collections worldwide.

A Steering Committee has been set up to support the development of the WDC and provide close liaison between RIKEN and WFCC.

(--abstracted from Union Reports submitted to the 15th CODATA General Assembly, Ottawa, Canada, July 1986)

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Department of Technical Sciences) reflects the multidisciplinary character of CODATA.

From South Africa -

New data centres or data programmes:

- A Computing Centre for Water Research is being established at the University of Natal in Pietermaritzburg. It is sponsored by the Water Research Commission and its purpose is to provide an incentive and an aid to water researchers throughout the country. The Centre will ultimately provide a powerful means of processing research information for any water research project requiring relational data and computer graphics capabilities.

- A centralized database for weather, climate and atmosphere-related data will be established in the Eastern Transvaal. Such a database would provide an important service function primarily to the research community, but would ultimately become a facility of national importance. In view of the existing infrastructure and expertise on information management and database management and research within the CSIR, there was a strong possibility that this database would be established at the CSIR.

- The South African Water Information Centre is about to produce a new computerized hydrological Southern African data register.

From the U.K. -

1) Imperial College Thermophysical Properties Data Service (Department of Chemical Engineering):

The Imperial College Centre includes the IUPAC Thermodynamic Tables Project Centre and the IUPAC Transport Properties Project Centre. The IUPAC Thermodynamic Tables Project Centre is responsible for the preparation of internationally agreed equations of state for the thermodynamic properties of pure fluids. The work is carried out either independently by the Centre or by means of collaboration with recognized authorities throughout the world. Thermodynamic tables for chlorine have been published recently and tables for oxygen, ethylene, fluorine, and methanol are in preparation.

2) Physical Properties Data Service, National Engineering Laboratory, East Kilbride, and Institution of Chemical Engineers, Rugby:

The NEL and IChemE data package, PPDS, provides critically evaluated data for over 1100 chemical compounds for chemical engineering design. Data are stored for pure components on 17 constant and 15 temperature-dependent properties, together with mixing rules for the generation of values for multicomponent systems. There are also special routines to provide data on petroleum fractions, vapour-liquid equilibrium and others such as LOADER (correlation and/or estimation data generator), PSYCHO (moist air), REFRIG (refrigerants), FASTWS (fast water/steam), and other water packages based on IAPS international standards.

3) Chemical Kinetics Data Centre, University of Birmingham (Department of Chemistry)

The Chemical Kinetics Data Centre at the University of Birmingham compiles kinetic data on homogeneous gas phase bimolecular atomic and radical reactions. Kinetic data compilations have been published at about three-year intervals and data evaluations less regularly. The Centre works in liaison with the NBS Chemical Kinetics Data Centre and with the IUPAC Commission on Chemical Kinetics Subcommittee on Data Evaluation for Atmospheric Chemistry. No direct services are offered but queries are dealt with concerning the published output.

From the U.S.S.R.

In 1985-86 the Soviet National Committee-CODATA carried out the scientific and methodical coordination of the data centres such as: Scientific Information Centre on Molecular Spectroscopy of the Siberian Division of the Academy of Sciences of the U.S.S.R., Information Thermophysical Centre (IVTAN), Data Centre of the GSSSD on thermophysical properties of hydrocarbons and petroleum products of the Ministry of Oil and Chemical Production of the U.S.S.R., and the Thermocentre of the Academy of Sciences of the U.S.S.R. They enabled the development and establishment of the Bank on Kinetic Constants, banks on physical and chemical gas dynamics, on chemical data, on data for comparative planetology, on hydrological and on seismological data, as well as on fields of raw materials, blood data, nucleic protein, and metabolic pathways.

The elaboration of the plan for creation and introduction of "Georesource" multibranch systems and on the publishing of determination of x-ray data on new minerals was carried out. Organization of the distribution bank on crystallostructural data, unification and standardization of lexical means of handling and searching mineralogical information, and elaboration of the format for x-ray data for publications and databases were achieved.

From the U.S.A. -

The Toxicology Information Program (TIP), Specialized Information Services Division (SIS), National Library of Medicine (NLM) has the responsibility for all of the "fact" information databases offered under the auspices of the Library. These online, publicly accessible files include RTECS (Registry of Toxic Effects of Chemical Substances), Toxicology Data Bank (TDB), and the Hazardous Substances Data Bank (HSDB).

RTECS is produced by the National Institute for Occupational Safety and Health (NIOSH) as part of its legislative mandate. The revised and updated file is supplied by NIOSH to NLM quarterly and the new "edition" is immediately made available to NLM's online user community. The NLM version does include several features which make searching and retrieving more convenient than other services provide. As in the printed edition, which is released irregularly and infrequently, the file contains data and information in a telegraphic format which reports the experimental type, species, route of administration, dosage, and effect(s) for in vivo and in vitro studies demonstrating effects in various test systems.

The TDB was the first effort by SIS to produce a database containing factual information (as opposed to bibliographic and pointer references) concerning a limited set (now more than 4000) of chemicals of regulatory and biomedical interest because of their toxicity, wide use, etc. The HSDB has many more data elements than TDB, (138 vs. 95) and the improved coverage is predominantly in the areas of environmental impact, and handling and disposal of hazardous substances. Each HSDB record represents a comprehensive, intellectually complete review of what is known about the compound, its manufacture and use, the hazards associated with it, signs and symptoms of its effects, antidote and treatment, etc.

(--abstracted from National Member Reports submitted to the 15th CODATA General Assembly, Ottawa, Canada, July 1986)

Reminder: The VIIth International Conference on Computers in Chemical Research and Education is scheduled for Beijing China on August 25-30, 1987. for information contact: Prof. Cheng Qian, c/o Shanghai Institute of Organic Chemistry, 345 Lingling Road, Shanghai, People's Republic of China.

New CODATA Publications.....

Recommended Consistent Fundamental Physical Constants
(Hungarian translation of CODATA Bulletin No. 11).^a

Books/Microcomputer Programs.....

Thermochemical Data of Organic Compounds (Second Edition). By J.B. Pedley, R.D. Naylor and S.B. Kirby.^b

Guidelines for the Organization of Short Courses and Workshops on the Dissemination of Data in Science and Technology. By David G. Watson.^c

Copper, Silver, Gold & Zinc, Cadmium, Mercury Oxides & Hydroxides. Edited by T.P. Dirkse.^d

Propane, Butane & 2-Methylpropane. Edited by W. Hayduk.^e

Metals in Mercury. By C. Hirayama, Z. Galus, and C. Guminski.^f

Sulfites, Selenites & Tellurites. Edited by M.R. Masson, H.D. Lutz, and B. Engelen.^g

Handbook of Thermodynamic and Transport Properties of Alkali Metals. Edited by R.W. Ohse.^h

Chlorine: International Thermodynamic Tables of the Fluid State. Edited by S. Angus, B. Armstrong, K.M. de Reuck.ⁱ

Enthalpies of Organic Compounds. Edited by V. Majer and V. Svoboda.^j

Handbook of Information Technology and Office Systems. Edited by A.E. Cawkell.^k

A Guide to, and Commentary on, the Published Collections and Literature of Mass Spectral Data. by R.W.A. Oliver and K.R. Davis.^l

International Data Series. Contains physical and thermodynamic properties of binary mixtures of organic compounds. These data are selected and evaluated at the University of Paris with cooperation and support from TRC.^m

New Data-Related Software.ⁿ

The Scientific Desk.^o

Computer-Aided Second Virial Coefficient Data for Organic Individual Compounds and Binary Systems. By Jacek Cholinski, Andrzej Szafranski and Danuta Wyrzykowska-Stankiewicz.^p

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

^aAvailable from: Dr. J. Szoke, Secretary, CODATA Hungarian National Committee, Kozponti Fizikai Kutató Intézet, Piroška u.3, 1016 Budapest, Hungary (TEL: 36 1 369245. TELEX: 224722).

^bThis reference compilation provides tables of thermochemical (and thermophysical) data for over 3000 organic compounds. It is an expanded and revised second edition of the book by J.B. Pedley published by the University of Sussex in 1977. The first section contains standard enthalpies of formation of the compounds in molecular formula order calculated from experimental data (which are collected in a separate section). References to the original literature are provided together with an indication of the reliability of the data.

The necessary calculations have been performed using software capable of predicting the heats of formation of unknown compounds (CATCH). This important facility is described in the Appendix.

May 1986. Chapman & Hall, Promotion Department, 11 New Fetter Lane, London, U.K., EC4P 4EE. Hardback, 2nd Edition. 804 pages. ISBN 0 412 27100 1. £ 55.00.

^c1986. General Information Programme and UNISIST, Paris. 73 p. PGI-86/WS/11.

^dThe relevance of the title compounds encompasses solution chemistry, battery technology and environmental concern. This volume provides a complete compilation of solubility data published up to 1984, including all pertinent articles, together with critical evaluations of the data. Of interest to inorganic and analytical chemists, electrochemists, and those concerned with environmental quality. Solubility Data Series, Volume 23, 380 pages. Hardcover. ISBN 0 08 032497 5. 1986. \$100.00. Pergamon Press, Fairview Park, Elmsford, New York 10523, U.S.A.

^eContains critically evaluated solubility data for the gases of the title in a variety of solvent systems. The literature has been covered to 1983. The volume also highlights those areas of the subject where further experimental work is needed. Of interest to physical, analytical and environmental chemists, polymer scientists and gas technologists. Solubility Data Series, Volume 24, 447 pages. Hardcover. ISBN 0 08 029202 X. 1986. \$100.00. Pergamon Press, Fairview Park, Elmsford, New York 10523, U.S.A.

^fCovers binary amalgams of all metals, carbon, silicon and boron. Complete literature coverage extends through 1983. Phase diagrams have been included where they have been defined. The data have been critically evaluated, and may also be used to compute thermodynamic properties of the binary components. Of interest to metallurgists (particularly those using amalgam extractive metallurgy), electrochemists and analytical chemists (particularly users of amalgam electrodes), and physical and inorganic chemists. Solubility Data Series, Volume 25, 451 pages, 26 illustrations. Hardcover. ISBN 0 08 023921 8. August 1986. \$100.00. Pergamon Press, Fairview Park, Elmsford, New York 10523.

^gThis volume presents compilations and critical evaluations of reported solubility data for a wide range of compounds, including binary, ternary and more complex systems. The entire literature up to 1984 has been covered. Rigorous statistical procedures have been applied in the evaluations. For many of the ternary systems and some quaternary ones, computer-drawn phase diagrams are included (prepared to the same scale where possible to allow easy comparison). Of interest to physical, inorganic and analytical chemists, and those working in paper manufacture, fertilizer formulation and sugar refining. Solubility Data Series, Volume 26, 451 pages, 150 illustrations (approx). Hardcover. ISBN 0 08 032517 3. August 1986. \$100.00. Pergamon Press, Fairview Park, New York 10523.

^hChemical Data Series 30. Blackwell Scientific Publications, Oxford, 1985. 1020 pp.

ⁱChemical Data Series 31. Pergamon Press, Oxford, 1985. xviii + 161 pp.

^jA critical Review and Data Compilation. Chemical Data Series 32. Blackwell Scientific Publications, Oxford, 1985. 304 pp.

^kThe Handbook of Information Technology and Office Systems tackles the basic financial, engineering, political, and human problems inherent in modern IT systems-problems facing anyone implementing an IT project. A comprehensive tutorial section explains these problems in jargon-free language, discussing matters such as computing, semiconductors, information input, processing, storage and display, file handling, facsimile, telecommunication systems, speech recognition, cable, videotex, microforms, on-

line systems, and information/library science. The tutorial concludes with a look at human aspects, telecommunication monopolies and de-regulation, and the prospects for an information society. 1986. x + 996 pages. ISBN 0 444 87907 2. Price US\$95.00. Elsevier Science Publishing BV, Book Order Department, P.O. Box 211, 1000 AE Amsterdam, The Netherlands, or: Elsevier Science Publishing Co., Inc., P.O. Box 1663, Grand Central Station, New York, NY 10163.

^lIn the present publication the results of the updating of the summaries of the previous "Guide" concerned with Mass Spectral Data are presented and discussed. The authors have tried to make this publication as accurate and comprehensive as possible. 14 pages. Available from: Dr. R.W.A. Oliver, Director, Biological Materials Research Unit, University of Salford, Salford, U.K. M5 4WT.

^mFor information write: Technical Database Services, Inc., 10 Columbus Circle, New York, New York 10019.

ⁿData Analysis - BBN Software Products has introduced RS/1, a data-analysis package for scientists and engineers designed for the new IBM RT PC. The package includes graphics, data management, statistics, curve fitting, modeling, simple English commands and a powerful programming language. BBN Software Products, 10 Fawcett Street, Cambridge, Massachusetts 02238.

^oProblem Solving - C. Abaci has released a version of The Scientific Desk for the new IBM RT PC. The package contains a number of functions and subroutines for mathematical and statistical calculations. The programs incorporate examples, tutorials and documentation and are menu driven. C. Abaci, 207 St. Mary's Street, Raleigh, North Carolina 27605.

^pThermodynamical Data for Technology Series A. Polish Academy of Sciences, Institute of Physical Chemistry. PWN-Polish Scientific Publishers, Warsaw 1986. \$30. Available from the CODATA Secretariat, 51, Boulevard de Montmorency, 75016 Paris, France.

CODATA Conference Reveals New Developments in Scientific Databases

The 10th International CODATA Conference, held in Ottawa, Canada, July 14-17, 1986, brought together nearly 300 experts in the evaluation and dissemination of numerical databases in all fields of science and technology. The central theme of the Conference, "Computer Handling and Dissemination of Data" was exemplified in sessions devoted to data validation by statistical techniques, to general approaches for database design, and to options for computer-based dissemination of data to the scientific community.

Specialized sessions reviewed the state of the art of data management in fields such as materials properties, molecular biology, geophysics and mapping, and thermodynamics. Demonstrations were offered of over 20 numerical or factual databases covering various topics in chemistry, physics, biology, and the geosciences. Poster sessions provided additional information on the activities of Task Groups and Union Members of CODATA.

Highlights of the developments presented include:

Demonstration of on-line retrieval of data on hybridomas and monoclonal antibodies from the CODATA/IUIS Hybridoma Data Bank

Description of plans for an on-line version of the Beilstein Handbook of Organic Chemistry

Announcement of the new 1986 CODATA Recommended Values of the Fundamental Physical Constants

Presentation of an overview of scientific databases in the People's Republic of China

Report of the results of a CODATA project on multisatellite thematic mapping in Tanzania

Description of new approaches to a relational database structure for properties of engineering materials

Consideration of expert systems for use in data evaluation and retrieval

Advances in the modeling and three-dimensional display of protein structures

Report on radiological data collection in the aquatic environment after the Chernobyl accident.

The Conference emphasized common features of data management and database design in the various scientific disciplines. A strong theme throughout the Conference was the growing database management capabilities of microcomputers and the prospect for dissemination of databases in PC-compatible formats for use by individual scientists. Many prototype databases of this type were demonstrated.

The Proceedings of the 10th International CODATA Conference will be published early in 1987 by North Holland Publishing Company. Further information on the Conference and General Assembly, as well as CODATA publications and other activities, can be obtained from the CODATA Secretariat, 51 Boulevard de Montmorency, 75016 Paris (Telephone: 1-4525-0496) or the Office of Standard Reference Data, National Bureau of Standards, Gaithersburg, MD 20899 (Telephone: 301-975-2200).

1986 Fundamental Physical Constants

The summary of the values of the fundamental physical constants presented on the first page will be provided in greater detail later this year as a CODATA Bulletin and subsequently in an extended definite publication in a scientific journal. These decades of deliberations leading to these selections have been made by the CODATA Task Group on Fundamental Constants chaired by T. J. Quinn and eight members: E.R. Cohen, B. Kramer, B.A. Mamyrin, M. Morimura, B.N. Oleinik, B.W. Petley, H. Preston-Thomas, B.N. Taylor.

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