



39 CODATA / NEWSLETTER

JANUARY 1987

"U.S. CODATA" Days

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A tripartite group of people with data concerns:

U.S. National Committee for CODATA (USNC-CODATA)

Integrated Data Users Workshop (IDUW)

National Governor's Association (NGA)

has organized a joint conference on integrating data for decision making on May 27-29, 1987, at the Shoreham Hotel, Washington, D.C., designated "Piecing the Puzzle Together."

The conference is oriented toward the theme of using information from multiple sources and developing analytic tools for improved decision making. It is the first conference of its kind to merge three independent meetings under this common theme. Concurrent sessions will be held by the three groups. Each group will work independently to enhance data compatibility and ease data integration for the future system needs of its members, but opening and closing plenary sessions will explore problems of current data incompatibility, approaches for integrating data from multiple sources, and cross-cutting issues such as data coordination.

In the concurrent sessions the CODATA program will concentrate on data bases containing scientific and engineering knowledge and its applications. The Data Users Workshop will emphasize the role of geographic information systems and other tools for data integration. The National Governors' Association program will examine such topics as State information management, the development of analytic tools, and federal/state issues affecting information availability and compatibility.

The program will include technical papers on conference topics, exhibits of information and data systems from public agencies and private sector firms, and poster presentations on data integration, analysis, or display.

More details will be provided in the April 1987 CODATA Newsletter. Approximately 300 participants are expected. A "proceedings" may be issued to document the conference.

Contact Lorraine Amico of NGA at (202) 624-5346 or Richard Hayes of NGA at (202) 624-5334 for exhibit, demonstration and poster information.

For additional program information, contact Lorraine Amico of NGA (at the Hall of States, 444 North Capital Street, Washington, D.C. 20001) or at (202) 624-5346. For registration and hotel information, contact Jan Dunlavey of NGA at (202) 624-5347.

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.

International Conference and Training Course on Geomathematics and Geostatistics

An International Conference and Training Course on Geomathematics and Geostatistics applied to space and time-dependent data will be held at the Technical University of Wrocław, Wrocław, Poland, June 1-6, 1987. The objectives of the Conference include an appraisal of the state of the art in using the advances made in the analysis of time and space-dependent data. Themes to be developed are resource appraisal, environmental surveillance, and land use planning.

The main themes of the conference are:

- Geostatistical models: validity, reliability and standards. (application of geostatistics model to the evaluation of mineral deposits)

- The practical aspects of using geostatistics in resources appraisal. (from experimental and observational values to models)

- Multivariable geostatistical analysis for estimating geological parameters. (statistical and geostatistical analysis for exploration)

- Relationship between data analysis, image analysis and resources appraisal. (development of integrated systems for multivariate analysis, use of image analysis in exploration and environmental sciences).

Although during the past twenty years major endeavors to gather and analyze geochemical, geophysical, atmospheric, remotely sensed, and natural resource data, and extensive facilities, some sponsored by CODATA, have been established to organize and disseminate these data, little coordinated international effort has focused on the analysis and interpretation of geoscience data. As a consequence, researchers in one country may remain unaware of developments in another, methodologies are rediscovered after great duplications of effort, and valuable techniques remain underutilized. More important differences in methodologies may lead to widely varying interpretations of the same global phenomena, with consequent international misunderstanding.

The Conference is intended to promote the exchange of ideas and concepts between leading geoscientists from the Eastern and Western blocks of Europe and from developing nations. It will provide scientists of all nations the opportunity to compare methodologies and to determine the comparative advantages of all. Moreover, it should result in better understanding of global processes and the nature of differences in interpretation.

Such a CODATA Conference provides not only an opportunity to bring scientists together, but provides a workshop ideal for discussing and interchanging ideas, for transferring methods to other geoscientists who have not been fully exposed to geostatistics or geomathematics, as well as comparing new techniques. It also provides a forum to compare, evaluate, and define standards in geodata processing involving problems common also to other disciplines.

The Scientific Program Committee includes A. Bylicki, J. Davis, P. Dowd, A.G. Fabbri, B. Namysłowska-Wilczynska, V. Nemec, D.A. Rodionov, J.J. Royer, R. Sinding-Larsen, and H. Thiergartner. It is sponsored by CODATA, IUGS, Unesco, and IAMG. Invited and contributed papers supplemented with discussions and training courses constitute the program. A proceedings volume will be published. Information and application for participation may be directed to: CODATA Conference, Centre de Recherches Petrographiques et Geochemiques, B.P. 20, 15 rue ND des Pauvres, 54501 Vandoeuvre-Les-Nancy Cedex, France. Telephone: 33 83 51 22 13. Telex: 960 431 F ADNANCY.

Organization of Data Dissemination Workshops

Much needed guidelines for the organization of short courses and workshops on the dissemination of data in science and technology have been addressed in a Unesco release by CODATA's Treasurer, Dr. David Watson of Cambridge University, after many years of experience in related activities.

The 73 page report reviews the recent dual roles of both CODATA and of Unesco in providing by collaboration such training endeavors. It proceeds with an analysis of curriculum design, including such subjects as data evaluation, dissemination, referral, and sources as well as the organization and activities of data centers with consideration of the special problems posed by certain types of data. Practical aspects concerning scheduling, lectures, and discussion sessions, site visits, projects, and handouts, together with the major aspects of planning, organization, administration, as well as selection of and assistance to the participating students are treated. Not neglected is the development of the course evaluation by the students and by others directly involved in the preparation of the course during, at the conclusion, and the potentially relevant post-course evaluation a year or more later.

Finally, there is an appended list of more than five or six hundred references to the eleven core areas (most of which have been mentioned in this review) together with those concerning broad scientific areas: earth and space sciences, physics, chemical structure and spectroscopy, thermodynamic and other physicochemical properties, crystallography, materials, and metallurgy, engineering, energy data, environmental data, and biosciences, including such CODATA materials as the Directory chapters and the guides for the presentation of data.

(More information on the report, "Guidelines for the Organization of Short Courses and Workshops on the Dissemination of Data in Science and Technology," by David G. Watson, will be found in the book section of the CODATA Newsletter #38).

Workshop on Needs for Fundamental Atomic Reference Data

A workshop organized for the Committee on Line Spectra of the Elements—Atomic Spectroscopy of the United States National Research Council by Alexander Scheeline, University of Illinois and Paul W.J.M. Boumans, Philips Research Laboratories, Eindhoven, Netherlands, is planned for June 19-21, 1987. Its purpose is the delineation of the current state of fundamental reference data as needed for the furtherance of analytical atomic spectroscopy, and to document what directions will be most useful in expanding the amount and availability of reference data in the near future. There will be three sessions covering reports on current status as revealed by a questionnaire distributed in 1986, needs of the applications community, and needs of the fundamental research community.

Invited speakers from North America and Europe will treat atomic reference data collection, evaluation, accessory dissemination, fundamental and perceived needs for reference data, data from the LANL vacuum interferometer, software for measuring wavelengths and intensities with recognition of spectral interferences, plasma diagnostics, and line selection in AES and other relevant topics.

All attendees are expected to participate actively in discussions which will be transcribed and published.

International Workshop on Materials Data Systems for Engineering

At the instigation of CODATA, an international Workshop on Materials Data Systems for Engineering was held at Schluchsee, Federal Republic of Germany, September 22-27, 1985. The convening of the Workshop and its design reflected several acknowledged shortcomings in presently available computerized materials databases for engineering:

- inadequate scope of coverage
- poor standardization in every aspect
- insufficient attention to user needs and facilities
- lack of international coordination and cooperation.

A 191 page book entitled "Materials Data Systems for Engineering" with further details on the recommendations is available from 712-Karlsruhe (see p. 7, CODATA Books).

The Workshop emphasized the critical importance of computer access to reliable data on the engineering properties of materials for economy, competitiveness, and rapid transfer of new technological developments. It was the particular intent of the Workshop to produce specific actionable projects and recommendations, especially those appropriate for international cooperative activity.

In the event, the Workshop defined fourteen Projects and eight Action Recommendations which are summarized in Chapter 17, cross-referenced for elaboration to the body of the report. Projects are activities of a continuing character for which certain individuals volunteered to lead the activity and other volunteers were recruited to begin work immediately to implement the Workshop findings. In the case of Action Recommendations, the plenary session directed that these be implemented by direct correspondence between the Workshop Chairman, Dr. G. Dathe, and responsible individuals in CODATA.

Because the supply and use of materials is international in scope, the computerization of materials information must reflect this, and hence the majority of the Projects and Action Recommendations imply international activity. Certain of these were selected by the Organizing Committee for oversight by CODATA through appropriate task groups and commissions, e.g., its Commission on Industrial Data:

● Initiate the organization of the managers of the world's most prominent and significant materials databases into an effective interacting group, the International Organization of Materials Database Managers (IOMADAM). The most important immediate tasks to which their attention should be directed are (in order of priority):

- Compile a listing of existing glossaries relevant to materials, as well as a listing of current programs and activities in materials terminology, effect harmonization of terms, and supply missing terms, definitions, symbols abbreviations, etc.
- Survey existing standards and the need for new standards in all aspects of materials database building.
- Prepare a manual of guidelines for database building.
- Establish a task group, "Computer Graphics-Data Capture and Presentation," to survey the state-of-the-art, identify hardware and software needs, and effect necessary standardization. (The CODATA General Assembly did indeed establish a task group under the name Materials Database Standards in July.)

(continued on page 5)

CODATA Calendar

1987

January

- 13-14 Scientific Program Committee Meeting, International Conference, Paris, France
- 15-17 31st CODATA Executive Committee Meeting Paris, France
- 18-19 Phase Equilibrium Data Task Group, Paris, France
- 19-20 CODATA Referral Database Task Group, Paris, France
- 23-27 Task Group on Coordination of Protein Sequence Data Banks, Nice, France

February

- 24-25 Technical Committee HDB, Washington, D.C.
- 28- Microbial Strain Data Network Task Mar.1 Group, Atlanta, Georgia, U.S.A.

March

- 11-13 WG on Environmental Data, Copenhagen, Denmark

April

- 15-20 Chemical Thermodynamic Tables Task Group, Moscow, U.S.S.R.
- 20-25 Geothermodynamic Data Task Group, Leningrad, U.S.S.R.
- 30- Hybridoma Data Bank Task Group, May 1 Paris, France

May

- 3-6 First CODATA Workshop on Nucleic Acid and Protein Sequence Data, Gaithersburg, Maryland, U.S.A.
- 27-29 Conference on Integrating Data for Decisionmaking: USNC CODATA, Integrated Users Workshop, National Governor's Association, Shoreham Hotel, Washington, DC, U.S.A.

June

- 1-6 Conference and Training Course on Geomathematics and Geostatistics, Wroclaw, Poland

September

- 6-8 Third CODATA/IUPAC Symposium on Phase Equilibrium, Budapest, Hungary
- 9-11 Third International IUPAC Workshop on Vapor-Liquid Equilibria, Budapest, Hungary

1988

March

- 3-5 32nd CODATA Executive Committee, Paris, France

July

- First International Symposium on Thermodynamics of Natural Processes, Strasbourg, France

September

- 26-29 11th International CODATA Conference, Karlsruhe, F.R.G.
- 30- CODATA General Assembly, Karlsruhe, F.R.G. Oct.1

NEA's Chemical Thermodynamic Database System

The OECD Nuclear Energy Agency (NEA) has undertaken the development of a CODATA-compatible chemical thermodynamic data base for a number of elements of interest to various areas of nuclear technology, especially to radioactive waste management research areas such as the safety analysis of nuclear waste repositories. The development of this data base involves not only a compilation of all relevant published thermodynamic data, but also a detailed critical review and, finally, the selection of a "best data set" which will be recommended. Each review is being performed by a group of four to five internationally acknowledged experts in chemical thermodynamics. Each expert team has at least one member who is CODATA liaison, to assure compatibility with the CODATA tables.

The first 10 elements to be reviewed are: uranium, neptunium, plutonium, americium, technetium, cesium, strontium, radium, iodine, and lead. The thermodynamic data being compiled and reviewed for each species include: the Gibbs energy and the enthalpy of formation, the entropy, as well as the heat capacity at constant pressure, together with precision indices and, if available, the temperature dependence. Emphasis is placed on data at 298.15 K, ambient pressure, and zero ionic strength.

Completion of the first review report, the uranium volume, is planned before the end of 1986. The uranium publication will be followed by one on technetium, and then by a neptunium volume. In agreement with CODATA, the NEA Thermochemical Data Base will be complementary to the CODATA Thermodynamic Tables.

In addition, an interface program is being developed which makes it possible to extract selected data from the thermodynamic data base and to convert them into a form readable by geochemical modeling codes, such as PHREEQE, MINEQL, and EQ3/6. The data can also be made available in a form compatible with other computer codes if there is user demand.

Further information on the NEA Thermochemical Data Base is available from: Dr. Hans Wanner, NEA Data Bank, OECD Nuclear Energy Agency, Bâtiment 45, F-91191 Gif-sur-Yvette Cedex (France), Tel. (1) 6908 4509, Telex: 690920F NEADATA.

First CODATA Workshop on Nucleic Acid and Protein Sequencing Data

Sponsored by CODATA and the Center for Advanced Research in Biotechnology (CARB) as well as additional co-sponsors, the workshop will take place on May 3-6, 1987, at the National Bureau of Standards, Gaithersburg, Maryland. In addition to posters and presentations on nucleic acid data, protein sequence data, and database management, the invited speakers and panel will concern crisis problems and solutions in database management, progress and needs in database structures, as well as global data interfacing, educational problems, and whether or not to publish. Database and technical demonstrations will also be provided.

The papers together with the decisions, recommendations of the panels and participant actions will be summarized in a proceedings volume.

Professor Rita R. Colwell is Chair of the Organizing Committee. For further program information contact Biotechnology Group, Idaho National Engineering Laboratory, P.O. Box 1625, Idaho Falls, ID 83415, Telephone (208) 526-1291, and for registration or general information, contact Kathy C. Stang, A345 Physics Building, National Bureau of Standards, Gaithersburg, MD 20899, telephone (301) 975-4513 or FTS 879-4513.

CODATA-France Day on Materials Databases

More than 200 participants audited the lively presentations and ensuing discussions of CODATA France's 20th November, 1986 "Journée d'étude" at La Défense, Paris, under the aegis of the Comité CODATA France.

Professor Bonnier (Grenoble, conceiver of THERMODATA) emphasized the importance and mutual interdependence of databases and researchers and stressed the importance of the a posteriori aspects of data validation and handling.

The notion of the confidentiality of a company's internal data and the creation of a six level hierarchy of users--and hence, of information proved important. Users of documentation for public dissemination only get a low level of details, marketing a bit more, and only at the highest level of accessibility did Daniel Vinard of St. Gobain Research indicate that all documents and fields were available.

Among the presentations on database development were a number of other distinguished French industrial, governmental, and academic experts. In addition, H. Krochel (The Netherlands) described material database developments in the European Community and J.R. Rumble (Gaithersburg, MD) those in the U.S.A.



Speaker at CODATA-France Day responds to participant questions.

International Federation for Information and Documentation (FID)

At the FID General Assembly held in Montreal on 12 September 1986, a number of important decisions were made which included the endorsement of the FID Strategic Plan, entitled Participation in Progress. This endorsement included a name change for FID from Federation Internationale de Documentation to Federation International pour l'Information et la Documentation (International Federation for Information and Documentation).

The FID Strategic Plan proposed five major programmes for FID work:

- improvements in the availability and applicability of information resources;
- achievement of maximum use of information services;
- development of tools for information work;
- increasing basic understanding of the properties of information; and
- professional development, especially education and training of documentalists.

In addition, the Strategic Plan called for the establishment of Special Interest Groups, a new category of Business Member and an increasingly important role for FID Affiliates on the FID Council.

CODATA Executive Committee Establishes Programs

A dozen members of the CODATA Executive Committee met January 15 and 16th at the Paris Secretariat and established new Task Groups and Working Groups. The new Task Group on Materials Database Standards, approved at the 15th General Assembly, at Ottawa, Canada, is chaired by Dr. A.J. Barrett, formerly of ESDU, U.K. The Executive Committee indicated that it would like this Task Group to make an assessment of potential users' needs, and provide an international coordination scheme. They also accepted the proposal for a Computer Graphics Task Group presented by E. Cerney subject to the modifications that the project be restricted to data capture and standardization for 32-bit microcomputers and exclude molecular graphics. It was recommended that the Task Group's end product be a specification. A chairman is to be named shortly.

Moreover a Working Group to prepare a Directory of Far-East Data Sources was unanimously established under the chairmanship of Professor J. Osugi. The proposal to establish a Geomedicine Working Group was declined by unanimous vote.

The Executive Committee unanimously approved the proposal on Improving Scientific and Technological Data Through Education submitted by Professors Kertes as amended by Professor D. Abir with the proviso that the Group reshape and rewrite the proposal, taking into account education of the end user of numerical data and numerical databases, that it investigate input into the traditional education process possibly through the use of data modules and textbooks, and that it look into the data modules already developed by Dr. Peter Signell. It was proposed that the title of the Group be amended to Teaching and Training.

A Biological Databases Working Group was established. The Chairman will be appointed by the President in consultation with the Executive Committee.

In order to better inform the officers and the Executive Committee of scientific progress, liaison assignments of Executive Committee members to task and working groups were initiated.

Dr. J.H. Westbrook reported on progress on the 100 page glossary of data-related terms. The CODATA Network (for electronic mail and conferencing) has expanded and grown and a 13-member Steering Committee for the CODATA Network was established as an advisory committee to the Executive Committee to act as an advisory body to the EC, to monitor the financial aspects, to make recommendations to put databases on DIALCOM and to consider policy matters. It is composed of Dr. D.G. Watson, Chairman, H. Behrens, J. Crease, B. Janicki, M. Krichevsky, B. Keil, and B. Molino. A. Bussard and D.R. Lide will be ex-officio members and L. Blaine, assisted by P. Glaeser and E. Ross, will be the Technical Adviser.



CODATA's President, David R. Lide, Jr. (left) and Secretary General, Alain E. Bussard, discuss task group progress.

The perennial matters of 1986 accounts, 1987 budgets, review of 1989 dues, and the review of the dues scheme were achieved or scheduled for decision.

Request for coopted membership in CODATA by the International Society of Soil Science will be treated by postal ballot.

A small ad hoc publications committee to devise a more effective, innovative format and dissemination program of CODATA literature was established.

Allocations for the support of a conference and training course on Geomathematics and Geostatistics (Wroclaw, Poland, June 1987), of a workshop on Atomic Data (Oxford, U.K., August 1987), and an International Symposium on Geothermodynamic Data (Strasbourg, July 1988) were authorized.

Following a presentation of the ICSU Global Change Program by the Executive Secretary of ICSU, the Executive Committee requested the President to advise ICSU that CODATA will be pleased to assist on data management aspects, a major component of the program.



CODATA's new Executive Committee in session (clockwise from left): A. Tsugita, H. Behrens, L. Gurvich, J. Crease, A. Bylicki (Vice-President), D. Abir, J.E. Dubois (Vice-President), D. R. Lide, Jr. (President), A. Bussard (Secretary General), P. Glaeser (Executive Secretary), D.G. Watson (Treasurer). Not shown: E.F. Westrum, Jr.. Excused: M. Carapezza and W.W. Hutchison.

Engineering Materials (continued from page 3)

- Institute liaison and advisory activities as follows:
 - Establish liaison with ICSTI on the subjects of security, copyright and transborder data-flow.
 - Establish liaison with CEC, UK, UNESCO and other directory projects especially as regards materials data sources.
 - Advise the Editor-in-chief of the CODATA Directory of the priority needs for materials-related Directory chapters.

The remaining recommendations of this Workshop are to be brought to the attention of other international bodies, including Unesco, ICSTI, UITA, FACE, IBF, WFEO, UNIDO, ISO, OECD, COMECON, and CEC-CIDST.

(Adapted as a contents review from the Executive Summary)

Thermodynamic Data for Biochemistry

A monograph, edited by H.-J. Hinz, provides a marked enhancement and interpretation of thermodynamic contributions to biological sciences and technology. The present compilation probably owes much to international co-operation of IUB, IUPAB, IUPAC, and CODATA, as well as devoted engagement and authoritative expertise provided by authors and referees.

Certainly, the enhanced trend in the biological sciences towards quantitative characterization of processes has promoted an increased use of thermodynamic reasoning not only from the recognized power of thermodynamics to predict the direction of chemical change, but also from the realization that knowledge of quantitative thermodynamic parameters provides a deeper understanding of many biochemical problems. This treatise is concerned primarily with building up a reliable data base, particu-

larly of biothermodynamic and related quantities, such as partial specific volumes and compressibilities, which will help scientists in basic and applied research to choose correct data from a special field that may not be their own. Most chapters reflect this emphasis on data provision. To provide the expert user deserved information on the basic methodology of data acquisition and on the criteria of data selection, tables are preceded by a critical evaluation of the techniques as well as a survey of the pertinent studies in the corresponding areas. The surveys are usually self-consistent and provide references to further sources of data that, though important, are not covered in the present volume. Unification of nomenclature problems demonstrates the ambiguity that arises where the same quantity is referred to by different symbols and underlines the desirability for still further steps toward unified nomenclature to facilitate identification and proper use of data. The first steps are being made in a forthcoming suggestion for nomenclature to be approved by IUB, IUPAB, and IUPAC. (Further details about the book appear on page 7 of this Newsletter.)

Footnotes for Books

on page 7

^aContains papers presented at the IFSA Conference in Hawaii, plus selected surveys invited for inclusion. Contributions include current research on the ideas of approximate reasoning through the use of fuzzy sets, featuring historical overviews, state-of-the-art surveys, long research papers, short notes, and some interesting applications to current problems. CRC Press Inc., 2000 Corporate Blvd. N.W., Boca Raton, FL, U.S.A. 3-volume set, Catalog no. 6294JG....Prepub. U.S. \$450.00/Outside U.S. \$520.00.

^bca. 304 pp., 7 x 10 inches (1987) ISBN-0-8493-6296-2.

^cca. 272 pp., 7 x 10 inches (1987) ISBN-0-8493-6297-0.

^dca. 304 pp., 7 x 10 inches (1987) ISBN-0-8493-6298-9.

^eA Collection of Selected Papers from the 2nd International IUPAC Workshop on Vapor-Liquid Equilibria in 1-Alkanol + n-Alkane Mixtures, Paris, France, 5-7 September 1985 and the 2nd International Symposium on Critical Evaluation and Prediction of Phase Equilibria in Multi-component Systems, Paris, France, 11-13 September 1985. This book covers the proceedings of the two meetings in Paris which were organized under the framework of CODATA and IUPAC projects. The measurement, correlation, prediction, computer handling and dissemination of phase equilibrium data was the unifying theme of these conferences.

In the first part of the volume papers deal with consistent representation of the equation of state, phase equilibrium and calorimetric data of various 1-alkanol-n-alkane mixtures. The second part of the work focuses on evaluation of phase equilibrium data of mixtures. This part discusses recommended methods for measurement, critical evaluation, prediction and computer handling of vapor-liquid, liquid-liquid and solid-liquid equilibrium data in multi-component systems.

Studies in Modern Thermodynamics, 6. Edited by H.V. Kehiaian. Institut de Topologie et de Dynamique des Systemes, Université Paris VII-CNRS, Paris, France and H. Renon, Ecole des Mines, Paris, France. Reprinted from Fluid Phase Equilibria, Vol. 27. xiv + 502 pp. 1986. US \$133.25/DFI.360.00. Elsevier Science Publishers, P.O. Box 211, 1000 AE Amsterdam, The Netherlands, and Elsevier Science Publishing Co., Inc. P.O. Box 1663, Grand Central Station, New York, NY 10163. ISBN 0-444-42652-3.

^fEight State of the Art Reports are published during each calendar year and Pergamon Infotech's continuing programme of conferences, seminars, courses and publications ensures that Report editors are in close contact with all the mainstream computing developments. The 1986 Series of Reports continues the stylish, easy-to-read format, and the technical level of content remains high. The standard sections of each Report have been designed for ease of reading and reference while still remaining authoritative. Invited Papers are specially commissioned to give a wide-angle view of the state of the art as seen by world experts. Analysis identifies the issues by gathering together all other relevant information and creating a dialogue which gives an original insight into information processing developments. In the Bibliography, each key item of relevant literature is reviewed and annotated with full reference to the source and publisher's name and address. Single copies at DM990, \$495. Series 14 Complete, DM6000, \$3000. Pergamon Infotech Limited, Berkshire House, Queen Street, Maidenhead, Berkshire, U.K. SL6 1NF. Telephone: 0628 39101; International +44 628 39101; Telex: 847319 INFO G.

^gThis essential reference compilation consists of tables of thermochemical data for over 3000 organic compounds.

The need for accurate thermochemical data is continually increasing. In industry the accurate prediction of the

thermodynamic feasibility of producing useful materials is of great importance while proving progressively more important in the biological sciences. At the same time traditional usage in pure chemical research continues.

This reference is a greatly 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 heats of formation of the compounds in molecular formula order. These have been calculated from experimental data which are collected in a separate section. Full 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. 804 pp., 1986. Ls55.00. Chapman and Hall Ltd., Promotion Department, 11 New Fetter Lane, London, England EC4P 4EE.

^hThe carbon-13 NMR chemical shift data for over 600 compounds are combined into thirteen tables by chemical class and subclasses. The classes presented are: Ketones, Aldehydes, Acids, Esters, Thiocarbonates and Thioesters, Carboxylic Acid Salts, Carboxylic Acid halides, Amides, Anhydrides, Imides, Ureas, Carbamates and Chloroformates. 1986. Sadtler Research Laboratories, 3316 Spring Garden Street, Philadelphia, PA 19104, (U.S.A.) Tel. (215)382-7800. TWX 710-670-1186 Cable SADTLABS.

ⁱThe 48-hour ELECTRONIC ANSWER MAN is a novel on-line service designed to give information seekers the name, address and telephone number of a free expert who can solve their information problem. The service costs as little as \$6.00 per hour connect charge. Contact Information USA, Inc. for more details at 301-657-1200.

^jA directory of free and fee-based databases and files available from the U.S. Federal Government. \$125. Information USA, 4701 Willard Ave., Suite 1707, Chevy Chase, MD 20815, Tel. 301-657-1200.

^kSadtler Research Laboratories has published a new three volume, desk reference collection of infrared spectra of polymer additives. Over 1500 spectra are featured: Volume 1, Polymerization Materials, contains 460 compounds; Volume 2, Protective Materials, contains 590 compounds; and Volume 3, Processing and Auxiliary Materials, contains 500 compounds.

The purpose of these handbooks is to provide a convenient and practical reference source for polymer chemists and technologists. Each volume contains the infrared spectra, physical and chemical data and other supporting information for the polymer additives grouped by principal function and arranged within each group by chemical class. 1986. Sadtler Research Laboratories, 3316 Spring Garden Street, Philadelphia, PA 19104, Tel. (215)382-7800. TWX 710-670-1186 Cable SADTLABS.

^lThis survey of existing factual databases (those containing numbers, graphs, etc.) in physics, chemistry, and materials sciences has been completed. Identifies over 200 databases of which 175 are available publicly and 50 are either produced or distributed by groups affiliated with the Department of Energy (DOE). A description of characteristics of factual databases is also given. It provides an in-depth look at the present status of databases in the areas of chemistry, physics, and materials to help the Department of Energy and its Office of Scientific and Technical Information as they make plans for meeting the needs of the energy research community.

The authors have attempted to identify and classify all of those publicly available, either as part of an on-line data service or as a self-contained file that can be used on another computer. In addition, they have surveyed some

DOE-supported laboratories to determine the level of their activity in building such databases, either to help solve a particular problem or to facilitate transferring information to other groups. Moreover, the unique characteristics of scientific and technical (S&T) databases are enumerated and discussed in detail. Factual databases differ significantly from bibliographic, financial, and full-text databases, a fact that has major implications, as outlined, in computerizing S&T data. Report DOE/TC/40017-1 (DE87001518) (Distribution Category UC-13). Prepared by: Office of Standard Reference Data, National Bureau of Standards, Gaithersburg, MD 20899, U.S.A., October 1986, and Submitted to Office of Scientific and Technical Information, United States Department of Energy, Oak Ridge, Tennessee 37830, U.S.A.. Code price: Printed Copy A15, Microfiche A01. Available from the National Technical Information Service, U.S. Department of Commerce, Springfield, Virginia 22161, U.S.A.

^mxvi + 456 pp. 1986. \$142. Springer-Verlag New York, Inc., 175 Fifth Ave., New York, N.Y. 10010. ISBN 3-540-16368-9, ISBN 0-387-16368-9, QP517.T48T47 1986 574.19'283 86-1812.

ⁿxxi + 852 pp. 1986. \$65 AICHE members; \$90 others. American Institute of Chemical Engineers, 345 East 47th St., New York, N.Y. 10017.

^oxxiv + 1069 pp. 1986. \$98. Noyes Publications, Mill Rd. at Grand Ave., Park Ridge, N.J. 07656.

^pAugust, 1985. Sponsored by National Bureau of Standards and U.S. Army DARCOM. NBS Special Publication 702. U.S. Government Printing Office, Washington, D.C., 20402.

^qDecember 1984. National Bureau of Standards Publication 685. Sponsored by: Design Institute for Physical Property Data Project 811. American Institute of Chemical Engineers. New York, N.Y.

^r1896 pp., 2 volumes, hardcover. Supplement Number 1 to Volume 14, 1985. The JANAF Thermochemical Tables, Third Edition, is a two-volume supplement of the Journal of Physical and Chemical Reference Data. These tables have been widely used data sources in science and engineering since the first version appeared 25 years ago. This Third Edition combines four supplements printed in 1974, 1975, 1978, and 1982—with revised and updated material from the Second Edition (in 1971)—and a number of previously unpublished tables. Thus, the tables for thermodynamic properties of more than 1800 substances have been brought together into a single publication. All tables have been expressed in SI units and the notation has been made consistent with current international recommendations and is a definitive reference source for thermodynamic properties of inorganic materials over a wide temperature range. Cloth: U.S. and Canada, \$130. All other countries, \$156. American Chemical Society, Marketing Communications Department, 1155 Sixteenth Street, NW, Washington, DC 20036. ISBN 0-88318-473-7.

^s(Supplement Number 1 to Volume 13) 288 pp. 1984. Cloth: U.S. and Canada, \$40. All other countries, \$48. ISBN 0-88318-447-8.

^t451 pp. 1986. Ls64.00. (hardback) Pergamon Press, IUPAC, Headington Hill Hall, Oxford OX3 0BW, UK. Fairview Park, Elmsford, New York, 10523, USA. ISBN 0-08-023921-8.

^u451 pp. Ls64.00. (hardback) Pergamon Press. IUPAC. Headington Hill Hall, Oxford OX3 0BW, UK. Fairview Park, Elmsford, New York, 10523, USA. ISBN 0-08-032517-3.

New CODATA Publications

Methodology for Multisatellite Thematic Mapping. (A Report of the CODATA Task Group on Multisatellite Thematic Mapping) Bulletin 62, October 1986.

Materials Data Systems for Engineering. (A CODATA Workshop, Schluchsee 1985) Editors, J.H. Westbrook (Editor in Chief), H. Behrens, G. Dathe, and S. Iwata.^Q

The 1986 Adjustment of the Fundamental Physical Constants. A Report of the CODATA Task Group on Fundamental Constants. By E. Richard Cohen and Barry N. Taylor. CODATA Bulletin 63, November 1986.[#]

^{*vi} + 85 pp. Number 62, October 1986. Individual copies available for U.S. \$15 from Pergamon Press, Ltd., Headington Hill Hall, Oxford, OX3 0BW, U.K. Fairview Park, Elmsford, New York 10523, U.S.A.

^{#iv} + 32 pp. Number 63, November 1986. (See footnote ^{*})

^Q Printed in F.R.G. in English. Paperback. 191 pp. Complimentary copies may be obtained from ISBN 3-

88127-100-7. Fach-informations-zentrum. Energie, Physik Mathematik, GmbH., Karlsruhe. 7514 Eggenstein-Leopoldshafen 2, Federal Republic of Germany. Telephone: 07247/82-4600, -4601. Telex: 724710=FIZKA; Über Telex: 17724710+. Telefax 07247/824639.

Books and Computer Services *

Analysis of Fuzzy Information. By James C. Bezdek.^a

Federal Database Finder. Second Edition. Information USA^J

◦ Vol. I: Mathematics and Logic.^{a,b}

Infrared Spectra Atlas of Polymer Additives.^k

◦ Vol. II: Artificial Intelligence and Decision System.^{a,c}

Scientific and Technical Factual Databases for Energy Research and Development. Characteristics and Status for Physics, Chemistry, and Materials. By J. Rumble, J. Sauerwein, and S. Pennell.^l

◦ Vol. III: Applications in Engineering and Science.^{a,d}

Measurement, Evaluation and Prediction of Phase Equilibria. Edited by H.V. Kehiaian and H. Renon.^e

Thermodynamic Data for Biochemistry and Biotechnology. Edited by Hans-Jurgen Hinz.^m

State of the Art Reports. Series 14 (1986) Pergamon Infotech.^l

Handbook of Aqueous Electrolyte Thermodynamics. By Joseph F. Zermaitis, Jr., et al.ⁿ

◦ IBM - Small and Medium Systems. Edited by R.C. Burgess.ⁱ

Hazardous Chemicals Data Book. Edited by G. Weiss.^o

◦ Software Reliability. Edited by A. Bendell and P. Mellor.ⁱ

Standards and Metadata Requirements for Computerization of Selected Mechanical Properties of Metallic Materials. By Jack H. Westbrook.^p

◦ Communications Standards. Edited by A.V. Stokes.^f

Compiled Thermodynamic Data Sources for Aqueous and Biochemical Systems: An Annotated Bibliography (1930-1983). By Robert N. Goldberg.^q

◦ Phototyping. Edited by M.E. Lipp.^f

JANAF Thermochemical Tables. Third Edition. By M.W. Chase, Jr., C.A. Davies, J.R. Downey, Jr., D.J. Frurip, R.A. McDonald, and A.N. Syverud.^r

◦ Relational Databases. Edited by D.A. Bell.^f

◦ Micro/Mainframe Links. Edited by S. Zographos.^f

Heat Capacities and Entropies of Organic Compounds in the Condensed Phase. By E.S. Domalski, W.H. Evans, and E.D. Hearing.^s

◦ Information Management. Edited by P. Griffiths.^f

◦ Technology-Based Training. Edited by P. Finch and M. Labinger.ⁱ

Solubility Data Series, Vol. 25: Metals in Mercury. Edited by A.S. Kertes.^t

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

Solubility Data Series, Vol. 26: Sulfites, Selenites and Tellurites. Edited by A.S. Kertes.^u

IR and NMR Spectral Data-Structure Correlations for the Carbonyl Group. By R. A. Nyquist.^h

Electronic Answer Man. Information USA, Inc.ⁱ

*Further details on content, identification, price, source, etc. for above items (if available) are referenced on page 6.

Multicomponent System and VLE Symposium/Workshop

The Third CODATA Symposium on Critical Evaluation and Prediction of Phase Equilibria in Multicomponent Systems will be held in Budapest, Hungary, September 6-8, 1987. The related Third International IUPAC Workshop on Vapor-Liquid Equilibria in 1-Alkanol + n-Alkane Mixtures will be held the 9-11th in conjunction with this meeting. These sessions are a continuation of the meeting in Zaborow, Poland, in May 1984 and the Thermo Festival in Paris, France, in September 1985. (See book section.)

The scope parallels that of the preceding conferences; state-of-the-art reviews, case studies, short oral lectures, posters, and presentations on microcomputers will be welcome.

Detailed information on scientific program, etc., will be given in the second circular. This and other information may be obtained from: IUPAC/CODATA Conferences, Chikany Gabor, Budapesti Muszaki Egyetem, Vegyipari Muveletek Tan-szek, H-1521 Budapest, Hungary. Telex: 225931 Muegy H.

Thermophysical Properties

The 11th European Conference on Thermophysical Properties will be held 13-16 June, 1988, at the University of Umea, Sweden, featuring heat capacity, thermal expansion, thermal conductivity, etc., especially on solids. More information may be obtained from: Professor Gunnar Backstrom, Department of Physics, S-901 87 UMEA, Sweden.

International Conference on Thermodynamics of Aqueous Systems

This conference -- May 10-14, 1987, Airlie House, Warrenton, Virginia -- involves experiment, theory, correlation, estimation, compilations, computer evaluation of equilibria, industrial applications, and new directions. It 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.

For registration, contact:

Ms. Mary Pat Healy, DIPPR-AIChE.,
345 East 47th Street, New York, NY
10017. Tel.: (212) 705-7332.

Materials Data Code of Practice

A Code of Practice for use in the Demonstrator Programme on Materials Databanks has been devised by the Commission of the European Communities. This Code of Practice specifies a number of common databank features at four different levels, i.e. access level, host operation level, data system operation level and data system content level, which will be implemented by databanks participating in the Demonstrator Programme. The Code of Practice may provide more comprehensive standard databank features for use in European system services in the future, guidelines, and orientation for existing or developing engineering materials data information systems.

Mathematical Geology

12-16 October 1987: 16th Annual Geochautauqua on Mathematical Methods in Geology to be held in conjunction with Mining Pribram Symposium at Pribram, Czechoslovakia. Sponsored by International Association for Mathematical Geology, Czechoslovak Scientific and Technical Society and Mathematical Geologists of the U.S. For information contact: V. Nemec, Geoindustría, Geologická 2, 152 00 Praha 5-Barrandov, Czechoslovakia; Phone (42-2) 590228 or (42-2) 7811801.

Newsnotes

Dr. Harrison Brown died on 8 December 1986 at the age of 69. He was President of ICSU 1974-76 and was a prime mover in the deliberations that led to the creation of CODATA at the ICSU General Assembly in 1966.

We have been informed that **Dr. Maurice Menache** died in October 1986. He was CODATA Delegate from IUGG from 1978-83, a physical oceanographer, concerned with the determination of the absolute density of standard mean ocean water, and Chairman of the IAPSO Working Group. He was a quiet, soft spoken--but firm--advocate of the definition of symbols, units, and nomenclature, a splendid gentleman, and a Perigordian gourmet!

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