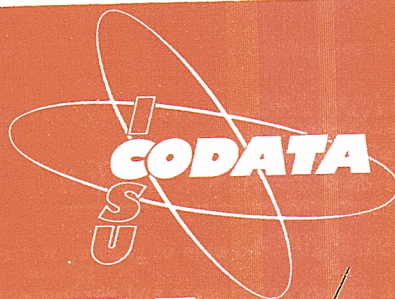


INTERNATIONAL COUNCIL OF SCIENTIFIC UNIONS
COMMITTEE ON DATA FOR SCIENCE AND TECHNOLOGY



17 CODATA / NEWSLETTER

FEBRUARY 1977

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

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

IMPORTANT ERRATUM

In CODATA Newsletter No. 16, on the left-hand side of page 6, in the article "New Prefixes for the SI System", there was an unfortunate and serious error and we are grateful to many readers for pointing this out.

The prefix denoting 10^{15} is peta (symbol P) and the prefix for 10^{18} is exa (symbol E).

We apologize to all our readers for any inconvenience that this error may have caused.

SOME 1977 CODATA MEETINGS

January 18-19, Asilomar, California, Task Group on Chemical Data for Industry
 February 18-19, Ottawa, Canada, Task Group on Methodology of Handling Space and Time Dependent Data
 March 21-22, New York City, New York, Task Group on Transport Properties
 April 18-19, London, England, Task Group on Presentation of Data in the Biosciences and Advisory Panel on the Biosciences
 June 28-29, Paris, France, CODATA 22nd Executive Committee Meeting
 August 19-20, Ronneby, Sweden, Task Group on Key Values for Thermodynamics

OTHER MEETINGS TO BE HELD IN 1977

The First International Conference of Scientific Editors, April 24-29, The Hebrew University of Jerusalem, Israel,
 For further information write to: Miriam Balaban, Chairman. Till March 25: P.O. Box 79, Pelham, NH 03076
 USA. After April 1: P.O.B. 4059, Jerusalem, Israel. Tel. 02.34405.
 Seventh Symposium on Thermophysical Properties, May 10-12, National Bureau of Standards, Gaithersburg, Maryland,
 USA. For further information contact: Dr. A. Cezairliyan, NBS, Washington, D.C. 20234, USA. Tel: (301)921-3687
 18th International Conference on Coordination Chemistry, July 17-22, IUCr/IUPAC, Sao Paulo, Brazil. For further
 information contact Dr. M. Williams, IUPAC Secretariat, 2-3 Pound Way, Cowley Centre, Oxford OX4 3YF, U.K.
 International Symposium on Macromolecular Chemistry, July 18-22, IUPAC, Dublin, Ireland. For further information
 contact Dr. M. Williams, IUPAC Secretariat, 2-3 Pound Way, Cowley Centre, Oxford OX4 3YF, U.K.
 Fifth International Conference on Thermal Analysis (ICTA), August 1-6, Kyoto, Japan. For further information write:
 The Secretariat, ICTA V, c/o Society of Calorimetry and Thermal Analysis, Japan, Daichi Kanamori Bldg.,
 1-5-31 Yushima, Bunkyo-ku, Tokyo 113, Japan.
 Fifth International Conference Thermodynamics, August 15-18, Ronneby, Sweden. For further information write:
 Fifth International Conference on Chemical Thermodynamics, Chemical Center, Lund University, P.O.B. 740,
 S-220 07 Lund, Sweden.
 1977 International Thermal Expansion Symposium, August 22-24, Gull Harbour, Canada. For further information write:
 Dr. I.D. Peggs, Atomic Energy of Canada Ltd., Pinawa, Manitoba R0E 1L0, Canada.
 15th International Thermal Conductivity Conference, August 24-26, Ottawa, Ontario, Canada. For further information
 write: Dr. V.V. Mirkovich, Chairman, Department of Energy, Mines and Resources, 405 Rochester Street,
 Ottawa, Ontario K1A 0G1, Canada.
 Vth International Conference on Vacuum Ultraviolet Radiation Physics, September 5-9, Montpellier, France. For
 further information write: Dr. M. Pouey, Executive Secretary, V.U.V.5, C.N.R.S., 1, Place A. Briand,
 92190 Meudon, France. Tel: 027.75.50 ext. 2170. Telex: LABOBEL 204135 F.
 Symposium on Data Analysis and Information, September 7-9, Rocquencourt, France. For further information write:
 Symposium Secretariat, External Relations Department, IRIA, Domaine de Voluceau - Rocquencourt, 78150
 Le Chesnay, France. Tel: 954.90.20 ext. 600. Telex: 600033 F.

CODATA'S FIFTH INTERNATIONAL CONFERENCE

HELD IN BOULDER, COLORADO, USA

JUNE 28 - JULY 1, 1976

CODATA, the Committee on Data for Science and Technology of the International Council of Scientific Unions (ICSU), has held biennial conferences since its establishment in 1966. CODATA was initially concerned with data in physics and chemistry only, but it has recently expanded its vista to encompass all sciences represented in ICSU, namely the biosciences, geosciences, and astronomical sciences. It has also turned its attention to data of importance to industry. Attended by about 250 people from 21 countries (including Australia, Austria, Belgium, Canada, Costa Rica, Federal Republic of Germany, France, German Democratic Republic, India, Israel, Italy, Japan, Luxembourg, Mexico, Norway, Poland, South Africa, Sweden, UK, USA, USSR), this was the first CODATA Conference to be held in the United States, previous ones having been held in the Federal Republic of Germany, United Kingdom, France, and USSR. Abstracts of the papers presented at Boulder have been published in CODATA Bulletin No. 18 (April 1976). (The full proceedings of the Plenary Sessions are presented in CODATA Bulletin No. 21.)

The activities of CODATA and other "data" oriented organizations represent a distinctive and growing sphere of information science, nurtured by the power of computer technology which has made it possible to attack massive problems of data evaluation, management and dissemination on something approaching a realistic scale ("data" in this context refer to factual measurements, observations and results, usually but not necessarily expressed quantitatively; excluded is the scientific literature per se, bibliographies, indexes, etc.). Aspects of data dealt with by the conference included general problems of data evaluation and analysis, data for technology, statistical techniques in the correlation and evaluation of data, data tagging and related activities, data on flavor and aroma, computer techniques in the handling and dissemination of data, national and international data programs, data needs for energy and environmental problems, data activities relevant to energy research and development, biological data banks and networking, biological data compilation and application, construction and indexing of files in the geosciences, data services in the astro- and geosciences, evaluation of data on thermophysical properties of fluids, computer techniques in numerical data handling, computer systems for numerical data handling, evaluation of thermochemical data, and evaluation of data on solid state properties. As emphasized by Lewis M. Branscomb, Chief Scientist, IBM, in his paper, the issue being addressed by CODATA is nothing less than maintenance of the observational foundations of science and technology, with the added contemporary pressure to provide for efficient and orderly response to societal problems of the day.

The Conference was held at the invitation of the National Academy of Sciences. The sincerest thanks of all participants are due to the chief host and to the many organizations and individuals who helped to make the

conference so rewarding and successful.

The General Assembly of CODATA was held immediately after the Conference while meetings of the CODATA Executive Committee both preceded and followed the Conference. Most of the CODATA Task Groups held meetings which were mainly devoted to planning CODATA's scientific activities for the period 1976-78.

The superb setting of the Conference -- the campus of the University of Colorado -- provided opportunities for well-earned, though all-too-brief periods of relaxation for the hardworking participants.

Two contrasting elements of the Conference activities are given in the following articles.

FUTURE OF CODATA*

Members of the Conference:

This is a Panel Discussion on the "Future of CODATA" as seen by the Members of the Original Bureau of CODATA.

There were seven of us: B. Vodar, of France; W. Klemm, of the German Federal Republic; M. Kotani, of Japan; G. Sutherland, of the U.K.; M.A. Styrikovich, of the U.S.S.R.; myself, of the U.S.A. and G. Waddington, of the National Research Council, U.S.A., as Executive Director for our first two years in Washington.

Most unfortunately, a conflicting engagement has kept Styrikovich away, and Kotani and Waddington could not come because of illness. So the remaining four of us constitute the Panel here.

To start the session, I will make some introductory background remarks to set the stage. Then statements will be made in order by Professors Sutherland, Vodar, Klemm, and myself. Following this, we hope there will be comments, questions, and suggestions by Members of the Conference. And at the end, I will try to summarize our conclusions, although this may not be necessary since the talks and discussions are being recorded on tape.

I now will make a series of general background statements, which are well known to most of you, on the problem of data for science and technology, putting them in what I consider a logical sequence. These statements will serve as a "jumping off" place for the discussion that follows:

1. The precision and accuracy of measurement has increased enormously in the past century, by factors of a million or more, all producing much new data.
2. Many new substances and systems are being generated each year, all producing much more new data.
3. The quantity of numerical data is thus increasing at a prodigious rate, said to be doubling or more every ten years.

* Remarks made by Prof. Frederick D. Rossini, first President of CODATA, during a Panel Discussion held on 1 July 1976 during the CODATA Conference in Boulder.

4. It is today essentially impossible for any one working scientist or engineer to review and critically appraise all of the original literature in his field.

5. The needs of about 98 percent of our scientific-technical community can be met by a system of review and critical appraisal of the original literature by qualified experts working essentially full-time to produce critical tables of standard reference data in each given field.

6. The numerical data of science and technology should be made available in whatever form is practically available today, including printed bound volumes, printed loose-leaf sheets, computer tapes, on-line retrieval, or whatever.

7. The review and critical appraisal of numerical scientific data constitutes an intellectual task of high order. Though such work can be greatly expedited by automatic machines and high-speed electronic computers, its efficient and effective performance requires skilled scientists.

8. To maintain the scientific quality and integrity of such compilations, the workers who produce these reviews and critical appraisals should have proper status and prestige in the scientific community, with corresponding remuneration.

9. The data of science and technology recognize no national or geographical boundaries. No country has a monopoly on intelligence.

10. The overall data problem is of such size that no one organization, and no one country, however large, can carry out all the reviews and critical appraisals necessary to serve all areas of science and technology.

11. The solution is to have many individual projects, each located somewhere in the world where there exists the intellectual expertise needed for the given work and the necessary financial support for the undertaking, with open avenues of communication.

12. Each country, or contiguous geographical area, needs appropriate national or geographical area coordination, as is already being done in a number of countries.

13. In addition, we need a system of international organization, which is now our CODATA organization.

14. The question then becomes, what is the best manner in which CODATA can perform the international coordination of many individual data-compiling projects and serve the data needs of the scientific-technical community of the world?

15. CODATA, as an instrumentality of the International Council of Scientific Unions, has an obligation to serve all areas of science and technology, and to work down in depth in each such area in accordance with its importance and the intellectual and financial resources available for that area.

16. CODATA can provide communication and coordination among all data-compiling projects.

17. CODATA provides communication through four avenues:

- a. the Newsletter
- b. the Bulletin
- c. the Directory (formerly the Compendium)
- d. the International Conferences

18. CODATA provides coordination through Task Groups:

- a. general Task Groups, as Fundamental Constants, Computer Use, etc.
- b. special area Task Groups, as Key Values for Thermodynamics, Transport Properties, etc.

Now, then, two questions remain:

1. Is CODATA carrying out its present work properly and efficiently?
2. What work is not now being done by CODATA that it should be doing?

(Next Professor Rossini invited Professors Sutherland, Vodar, and Klemm to take the podium. The text of their statements will appear in the Conference Proceedings.) Prof. Rossini's concluding remarks were:

I want to suggest a practical undertaking for CODATA which will increase its visibility in the world of science and technology and increase its service to that community. This is to make available to the scientific-technical community of the world, in an efficient, expeditious, and economical manner, the products of the data compilations from the various countries of the world. There are two parts to the enterprise -- one is immediate and the other longer range.

1. As an immediate goal, CODATA should prepare a General Index for each area of science that has been sufficiently cultivated and well-harvested, and for which critically evaluated data are available. This General Index would give the following information for each area:

- a. The classes and ranges of substances and systems covered;
- b. The properties covered, with ranges of T and P;
- c. Where the data are produced, and by whom;
- d. In what forms the data are available;
- e. How one obtains the data; and
- f. What the costs of the data are.

2. As a longer range goal, CODATA should set up a CODATA Order Clearing Office, to receive and process orders for all data compilations which are requested in the CODATA System. I will illustrate what I have in mind by an example of what such a CODATA Order Clearing Office would do.

From the General Index mentioned above, I decide that I need a set of the data compilations from each of eight different projects, which projects happen to be located in five different countries. I send the appropriate amount of funds to the CODATA Order Clearing Office with my order for the eight compilations. The CODATA Order Clearing Office requests each of the eight projects

to send directly to me the desired compilations.

The CODATA Order Clearing Office retains an agreed-upon percentage of the funds as a service fee for its work, and credits each of the eight projects with its appropriate share of the funds. Financial settlement between CODATA and the projects can be made annually, semi-annually, or quarterly.

Orders of the kind I have described can be sent in by individual scientists or engineers, by University or Industry Libraries, by Business Organizations, and others.

Such a service would be of great benefit to the scientific-technical world community in expediting to them the available data compilations, and simplifying their manner of ordering and obtaining data compilations from a multitude of sources. Also, such a service provides a real-world link between each of the data-compiling projects and the CODATA Headquarters Office. Such a system can be made flexible in a number of ways, as for example, the establishment of national or area depots.

I recommend this two-part undertaking, which I first proposed about six years ago, as a work which will bring CODATA in direct contact with scientists and engineers and their institutions throughout the world, thus increasing the world visibility of CODATA and enhancing its capacity for service to the scientific-technical world community.

DATA RELEVANT TO FLAVOURS AND AROMAS:

THEORY AND EXPERIMENT *

The 3rd biennial International Conference of CODATA was held almost exactly four years ago in Le Creusot in the heart of Burgundy. Not unexpectedly the highlight of the conference -- at least of the social events -- was a banquet at which the splendid wines of the region flowed freely, almost too freely. The banquet, which took place in the nearby village of Les Couches was preceded by a colourful ceremony in a medieval chapel at which some 30 participants of the conference were made (honorary) Chevaliers or Officers de la Confrérie des Tastevins de St. Vincent and were invested with the insignia of their membership -- silver wine-tasting cups -- by La Reine du Beaujolais et du Maconnais, the Beauty Queen of the region. This impressive and enjoyable function was the brainchild of CODATA's then President, Professor Vodar and of Mme Vodar, herself a native of Burgundy. For the conception and the execution of this plan, Professor and Mme Vodar rightly earned the warm gratitude of all participants.

It is not altogether surprising and it is certainly significant that when earlier this year Professor Vodar was promoted from Chevalier to Officier de la Légion d'Honneur, the recommendation did not come from the Ministère de l'Education Nationale, or the Ministère de

*Remarks made by Prof. N. Kurti on the occasion of the wine tasting held during the CODATA Conference on 29th June 1976 at the National Center for Atmospheric Research, Boulder, Colorado.

l'Industrie et de la Recherche -- no, it was the Ministère pour la Qualité de la Vie which made the proposal. So, in the name of this assembled company, I want to offer our delighted congratulations to Professor Vodar, not only on this well-deserved honour but also on its being connected with the quality of life.

Over the last few years CODATA has expanded its activities and they now comprise the astro-, geo-, and bio-sciences. Some of us thought that we might go even further and include data of importance to the quality of life. Encouraged by the success of the extra-curricular activities at Le Creusot we concluded that a modest start might be made about data relevant to flavours and aromas, and that is how a parallel session on this subject came to be included in the conference programme. We were fortunate in securing the participation of Dr. Dinsmoor Webb and Dr. Ann Noble, both from the Department of Enology and Viticulture of the University of California at Davis, and are grateful to them for two learned yet amusing, enjoyable and refreshingly provocative lectures on the scientific aspects of the senses of taste and smell, mainly, but not exclusively, of relevance to the assessment and the enjoyment of wines. However, CODATA believes that theory and experiment are inseparable and it was obvious that the experimental aspects of flavours and aromas should also have a place in the programme, e.g. in the form of a wine-tasting. Unfortunately, the laws governing the transport of wines across the State boundaries of this great Republic introduced certain difficulties and made the original more ambitious plans impracticable. But thanks to the ingenuity and efforts of several people and organizations, we were able to mount this function.

Our thanks are due first and foremost to Professor Dinsmoor Webb, Chairman of the Department of Enology and Viticulture of the University of California at Davis. It was he who got the California Wine Institute interested in this venture and the Institute, in turn, convinced Almadén Vineyards that the participants at the CODATA Conference and their spouses would be worthy and appreciative recipients of samples of Californian wines. So, we are grateful to Almadén Vineyards for their generous hospitality and to the Director of the National Center for Atmospheric Research, Dr. Firor, for providing this spectacular setting. And last, but not least, our very warm thanks go to our ever-present, ever-helpful, untiring friend Neil Olien, the chief architect of this enjoyable and memorable function.

CODATA WELCOMES ITS ITS FIRST CO-OPTED MEMBER

At its 10th General Assembly in Boulder, Colorado, July 1976, CODATA voted to accept the ICSU Panel on World Data Centres as its first Co-opted Member in accordance with the revised constitutional statutes on Membership. The Panel on World Data Centres was established by ICSU in 1968 to provide scientific direction for the World Data Centre system on behalf of ICSU and the Unions and other ICSU bodies with an interest in the collection, archiving, and distribution of geophysical and solar data. Dr. Alan Shapley of NOAA has been designated as the WDC Delegate to CODATA.

EUSIDIC - SCIENTIFIC LITERATURE INFORMATION RETRIEVAL

EUSIDIC, the European Association of Scientific Information Dissemination Centres, was established in 1970 and now has a membership of 30 full members and some 60 associate members. Full members are organizations which either process questions for automated literature retrieval (current or retrospective awareness profiles) or produce data bases larger than 25 000 items per year. Only European organisations are eligible for full membership. Operation of EUSIDIC is through member meetings, annual conferences and Working Groups. The last Conference was held in Graz, Austria in December 1975. EUSIDIC maintains close contact with the parallel U.S. organization ASIDIC.

A recent EUSIDIC activity, organized by its Working Group R, is planned establishment of a European network of Scientific Information Referral Centres to be known as EUSIREF. Its main interest will be in bibliographical data bases and it will seek cooperation with CODATA concerning data bases containing mainly numerical data bases.

EUSIREF plans to operate through regional referral centers by providing documentary material on existing data bases and processing centres along with the necessary information on how to contact the selected services. Eleven European centers have already indicated their willingness to participate in the referral activities and to assign an employee to this task. A mechanism for information exchange between participating centers is being studied and the preparation of a data base on information resources available in Europe has been started. To date, two editions of Data Bases in Europe, containing information on some 400 data bases, mostly bibliographical, have been published by Aslib (the Association of Special Libraries and Information Bureaus) and EUSIDIC. For further information, contact Dr. H. Evers, ESA/SDS, European Space Agency, 8-10 rue Mario Nikis, 75015 Paris, France.

PHYSICAL PROPERTIES DATA SERVICE AT INSTITUTE OF CHEMICAL ENGINEERING

PPDS provides critically evaluated data on some 400 chemical compounds for chemical engineering designers. This data bank is available for direct computer access or batch mode operation. 180 compounds are hydrocarbons, 15 are inorganic and the remainder are organic compounds containing oxygen, nitrogen, hydrogen, chlorine, and sulphur. A service is operated by which compounds may be added on request.

Physical constants, e.g. T_m , p , T_b , p , heat of formation, critical properties, dipole moment, parachor, and flammability data are available together with 14 temperature dependent properties, viz. heat capacity, enthalpy, density, viscosity, thermal conductivity of the gas and liquid states and the vapor pressure, latent heat and surface tension of the liquid.

The quality of the data in the direct access bank might be described as suitable for engineering design work. A more sophisticated bank holds the Engineering Sci-

ences Data Unit (E.S.D.U.) correlations for vapor pressure, thermal conductivity and provides a best estimate of data point values derived from an equation with a maximum of eleven coefficients.

The service is supported by a grant from the U.K. Department of Industry but it is expected to be self-supporting after five years of operation.

PHYSICAL DATA ITEMS FROM ENGINEERING SCIENCES DATA UNIT (ESDU)

Seven volumes of loose-leaf Data Items are now available in this series. These deal with various properties of water; the vapor pressures of aliphatic, olefinic, and aromatic hydrocarbons; aliphatic alcohols and ketones; the thermodynamic properties of benzene and toluene and the thermal conductivity of similar series of compounds. For further information write to E.S.D.U., 251 Regent Street, London W1R 7AD, U.K.

IN MEMORIAM - ULRICH STILLE 1910-1976

Professor Ulrich Stille, a member of the Task Group on Fundamental Constants, died after a long illness on 7 March 1976 at the age of 66. Born on 23 January 1910 in Berlin, he was educated at the Technische Hochschule in Hannover and at the Universities of München and Göttingen, receiving his doctorate from the latter institution in 1933. His early studies were on the production and properties of ions, with particular interest to atmospheric electricity, excitation and ionization of active nitrogen, auroral afterglow and twilight fluorescence of atmospheric sodium. In 1948 he joined the Physikalische Technische Bundesanstalt and was its director from 1970 until his retirement in 1975. His book, Messen und Rechnen in der Physik (Vieweg, Braunschweig 1955), will serve as a memorial to his contribution to metrology.

Professor Stille was extremely active in international organizations concerned with standards in physics. He served on the IUPAP Commission on Atomic Masses and Fundamental Constants and the Commission on Symbols, Units and Nomenclature; at the time of his death, he was chairman of the latter commission. He was also active in IUPAC, ISO and CEI as well as directly with ICSU. He became a member of the International Committee on Weights and Measures (which serves as a board of directors of the BIPM) in 1970 and its vice-president in 1974.

His passing will be felt not only by his friends and associates, but by the entire community of metrology and standards.

E. Richard Cohen, Chairman
CODATA Task Group on
Fundamental Constants

FIRST CODATA/UNISIST TRAINING COURSES HELD IN ZAGREB — POLAND 1977 SITE

The CODATA Task Group on the Handling of Experimental Data (Chairman: Professor G.G. Johnson, Jr.; Members: Dr. J.J.B. van Eijk van Voorthuysen, Dr. Gerd Olofsson, and Professor J. Troe) completed its first international effort on this important activity at Varazhdin, Yugoslavia in August 1976.

Two five-day courses at the university level emphasizing physics and chemistry were organized locally, with the support of CODATA/UNISIST, by the University of Zagreb (Dr. Neva Silovic, Prof. Bozo Tezak, Dean Stephen Mikhalić), and attended by a total of 31 participants from 16 countries throughout the world. The main emphasis of these courses was:

- the importance of critically evaluated data;
- the treatment of experimental data, including design of experiments;
- model selection and evaluation, and the distinction between random and systematic errors;
- presentation of data in the primary literature, including discussion and criticism of actual papers;
- sources of evaluated data.

These courses were modeled after a similar course offered at Pennsylvania State University in 1973 and eighteen 4-day courses, organized by the American Association for the Advancement of Science, and offered at twelve sites within the United States in 1974/75 and 1975/76, all these courses being supported by the National Science Foundation of the U.S. From the experience of these courses the following attributes were common in all (both national and international) courses.

First - Team teaching was emphasized. Eight teachers were used in Yugoslavia while in the United States two members taught each statistics course. The teams at Varazhdin included major involvement by Dr. Dorian James (a nuclear scientist from the Atomic Energy Research Establishment at Harwell), Professor G.G. Johnson, Jr. (a crystallographer and computer scientist from Pennsylvania State University), Dr. Brian Joiner (from the Statistics Department of the University of Wisconsin and originator of the "Minitab" program), Prof. Dr. Branko Soucek (a world-renowned mini-computer expert from the University of Zagreb), Prof. Edgar F. Westrum, Jr. (a thermodynamicist from the University of Michigan and Secretary General of CODATA), together with contributions by three other lecturers from Zagreb (Professors Bozo Tezak, D. Shlaus, and N. Trinajstić).

Second - Actual experiments were performed during the period of the course emphasizing the control and design of experiments (i.e. pendulum and paper thickness measurements, while density and boiling experiments preceded several of the courses).

Third - A real-time computer facility was available with graphics capability for presentation of output for both participants' data and preselected data.

Fourth - Interaction, both during and after class hours,

among local personnel, guest speakers and participants was highly encouraged to break down any barriers which were present at the inception of these courses.

The results of these courses were educative for both the teachers and the participants. The participants appreciated many of the goals of the course and, without exception, were enthusiastic to return to their institutions to apply their newly obtained knowledge. Such national courses are understood to be scheduled in Yugoslavia and Sweden by the participants of this international course. The teachers were informed of the specific difficulties encountered in developing countries and how international organizations can help in such cases.

This course was not a one-time effort. In the summer of 1977 a second group of courses sponsored by CODATA/Unesco/UNISIST at university level and of a similar format, will be offered in Poland. Three 5-day courses are planned which will emphasize biosciences, engineering application, and physics and chemistry.

NBS ALLOY DATA CENTER SHIFTS EMPHASIS TO PHASE DIAGRAMS

A phase diagram appropriate to a particular material is often the most efficient way to provide an understanding of the structure of the material and information important to its scientific and technical applications. In recent years it has become increasingly clear that the need for reliable phase diagrams far exceeds their availability. A new program to provide reliable phase diagrams has been established by the NBS Alloy Data Center. The group plans to:

- compile and critically evaluate phase diagrams in specific areas. Work has already begun on metal-hydrogen systems of importance to hydrogen storage and hydrogen embrittlement;
- establish a computerized bibliographic file with on-line capabilities to aid other groups in evaluating phase diagrams;
- make data more accessible through development of an on-line system which uses graphic methods for handling numerical phase diagram data;
- coordinate the activities of other centers throughout the world to avoid costly and time-consuming duplication of effort, as well as identify areas of greatest need.

As part of the development of this program, a workshop on "Applications of Phase Diagrams in Metallurgy and Ceramics" was held at the National Bureau of Standards on January 10-12, 1977, to assess the current national and international status of phase diagram determinations and evaluations for alloys, ceramics, and semiconductors; to determine the needs and priorities for phase diagram determinations and evaluations; and to estimate the resources being used and potentially available for phase diagram determination. The workshop was highly successful, and attracted some 200 scientists from industry, academia, and many foreign countries. Proceedings of the symposium will be published by NBS through the U.S. Government Printing Office.

WORLD DATA REFERRAL CENTRE

In accordance with the Feasibility Study prepared by the CODATA Task Group on Accessibility and Dissemination of Data, CODATA is now working on the establishment of a World Data Referral Centre (WDRC). The Centre will seek to give guidance to data users on the availability and sources of the data they need. WDRC is intended to provide a worldwide focus on referral activities, and to improve all capabilities to answer scientific and technical questions, especially those involving data.

WDRC's functions and services will include:

- Collecting information concerning major resources of data and related scientific information on a worldwide basis and constructing a file of this material for convenient retrieval;
- Preparing and disseminating documents to assist local and national services to conduct data referrals;
- Provide advice to local and national services on problems of data referral;
- Performing data referrals on request from national and local services and, when necessary, from individual inquirers.

With the help of CODATA members in several countries it is now preparing a Master List of referral resources with emphasis on numerical data resources. When this list has been assembled, WDRC will begin actively to communicate with local, regional, and national referral organizations throughout the world. This should occur in late 1977.

Initially WDRC will be operated by CODATA and sponsored by Unesco-UNISIST, BNIST (Bureau National de l'Information Scientifique et Technique) and the EEC.

Publishers and editors interested in having their directories considered for inclusion on the Master List are requested to send a specimen copy to the CODATA Secretariat for consideration.



We have just learned that CODATA's dear friend and long time colleague, Dr. H. van Olphen, will be retiring to Holland after nearly 11 years with the Numerical Data Advisory Board of the National Academy of Sciences. "Closing the cycle, as in a biological process", says Van. We wish him all the best and will miss his good sense, sound science, and 'improvisations'!

NEW JOURNALS

FLUID PHASE EQUILIBRIA is a new international quarterly journal devoted to the multidisciplinary field of equilibria likely to obtain between two or more fluid phases. Theoretical as well as experimental studies are involved, together with their applications. The range of substances concerned is very wide, including electrolytes, non-electrolytes, fused salts, liquid metals and polymers. The multidisciplinary character of fluid phase equilibria studies can best be appraised when one realizes that such equilibria occur in practically all phases of engineering, as well as in geological phenomena, biological exchanges, ecology, etc. -The publishers are Elsevier Scientific Publishing Company, Jan van Galenstraat 335, P.O. Box 330, Amsterdam, The Netherlands. The subscription price is \$55.50 per year.

INTERDISCIPLINARY SCIENCE REVIEWS is not only a new journal, but a new kind of journal, inasmuch as its publishers (Messrs. Heyden & Sons) want to devote it to interdisciplinary (as distinct from multidisciplinary) topics, i.e. those subjects where two or more natural sciences or technologies interact. The basic philosophy behind this venture is that the future progress of science depends not only on information (this is provided to the scientific community in sufficient quantity) but equally on understanding, a much more elusive attainment and one whose realization can be greatly facilitated by resorting systematically to interdisciplinary techniques. To enhance still further the "fertilizing" aspect of this approach, the normal mode of expression of the new quarterly journal will consist of review articles, a good review being, in the words of Maurice Goldhaber, former Director of Brookhaven, "the moral equivalent of teaching". The contents of the first issue, dated April 1976, include articles on the ethical aspects of science and the importance of scientific research; the contribution of science to the economy; the probabilistic aspects of evolution; the aesthetics of engineering; an ethological study of the behaviour of laboratory rats; a review article on phytochemistry; a detailed account of the discovery of the Oklo natural Nuclear Reactors; and a review article on biotechnology, whose final illustration, in the shape of a Venn diagram, embodies the very notion of interdisciplinarity. -The subscription price for the four issues of 1976 is \$44 or £22 (£17 for the UK and Eire).

THE JOURNAL OF ENERGY is a new periodical published under the auspices of the Institute of Aeronautics and Astronautics (Editor-in-Chief: William H. Heiser). Starting January 1977, it will be devoted to all aspects of the production, transformation, conservation and usage of energy, in space and on Earth, with emphasis on advanced technologies. In addition to technical articles concerning the various energy-generating systems presently in use (nuclear, solar, chemical, wind) or under study (fusion, MHD, geothermal, ocean) and related matters (power conversion, storage, transmission), the Journal of Energy will also carry economic analyses, evaluations of systems performance, reports on process developments, as well as, of course, survey articles reviewing recent research.

NEW PUBLICATIONS

ASTRONOMY AND ASTROPHYSICS

- * ANNUAL REVIEW OF ASTRONOMY AND ASTROPHYSICS. Vol. 13 (1975, 577 pp, \$15, Annual Reviews: Palo Alto, Calif., ISBN 0-8243-0913-8), edited by Geoffrey R. Burbidge. - Contents: Computer simulations of stellar systems. Radio surveys and source counts. Neutrino processes in stellar interiors. Thermonuclear reaction rates, II. Chemical composition of extragalactic gaseous nebulae. Ultraviolet studies of the interstellar gas. On-line computer for telescope control and data handling. Young stellar objects and dark interstellar clouds. Stellar populations in galaxies. High-velocity neutral hydrogen. Unseen astrometric companions of stars. Equation of state at ultrahigh densities, II. Astrophysical processes near black holes. Instrumental technique in X-ray astronomy. On the pulsar emission mechanisms. Indexes.

ATOMIC AND MOLECULAR PROPERTIES

- HANDBOOK ON NUCLEAR ACTIVATION CROSS-SECTIONS. NEUTRON, PHOTON, AND CHARGED PARTICLE NUCLEAR REACTION CROSS-SECTION DATA. (1974, 558 pp, \$26, £10.80, 126 FF, 64 DM, IAEA, Vienna), edited by M. Brune and J.J. Schmidt. This handbook contains data on cross-sections for thermal, epithermal, and fast neutron induced nuclear reactions, as well as for reactions induced by charged particles and photons. Among the various applications considered, the main emphasis is on activation analysis, but radioisotope production and radiobiological protection are also considered. The information presented includes the following data: Neutron activation cross-sections at a neutron energy of 0.0253 eV (neutron velocity of 2200 m/s) are given for a large number of isotopes of interest in neutron activation analysis, the half-lives of the activities formed and the cross-sections for activation of isomeric and ground states. One chapter contains tables and graphs of cross-sections for (n,p), and (n, α), and (n,2n) reactions in the neutron energy region 1-37 MeV, and a compilation of graphs of excitation functions that can be measured by activation techniques. Another chapter reviews cross-sections averaged in a ^{235}U fission spectrum. It includes all integral measurements available in the literature up to April 1973 for (n,p), (n, α), (n,2n), and (n,n') reactions. One chapter contains a graphical compilation of excitation functions for charged-particle induced nuclear reactions in light elements at low projectile energies. The last chapter contains a compilation of about 60 photonuclear cross-sections of other types of reactions. Preference is given to monochromatic photon data where available. In all chapters the selection of data is generally weighted toward more recent measurements.

BIO-SCIENCES

- * ANALYSIS OF WATER (translated from French by IPST Staff Jerusalem, 1975, 926 pp, \$82.50, Halsted, Div. of Wiley, ISBN 0-470-72934-1) by Jean Rodier. Analysis of natural waters; residual waters; seawater. Bacteriological analysis. Biological analysis. Biological quality of fresh waters. Interpretation of results. Appendixes. Subject index.

CHEMICAL KINETICS

- * REACTION KINETICS IN THE LIQUID PHASE. (translated from Russian by R. Kondor. Translation edited by D. Slutzkin. IPST Program Jerusalem 1976, 362 pp, \$42.50, Halsted, Div. of Wiley, ISBN 0-7065-1516-1), by Entelis, S.G. and Tiger, R.P. Collision frequency and diffusion in liquid phase kinetics. Interaction between particles in solution. Solvation of ions and molecules in solution. The transition-state theory applied to liquid-phase reaction - physical models. The quantitative allowance for the effect of the medium by means of semiempirical correlation equations. Effect of the solvent on the dependence of the reactivity of compounds on their structure. Heterolytic reactions. Homolytic reactions. Polymerization and polycondensation reactions. Additional bibliography. Subject index. Note: the book presents critical results. The authors clearly define the applicability of each of the theories covered.

- * SYMPOSIUM ON CHEMICAL KINETICS DATA FOR THE UPPER AND LOWER ATMOSPHERE. PROCEEDINGS. Held at Warrenton, Virginia, Sept. 15-18, 1974. (1975, 656 pp, \$37.50, Wiley-Interscience, NY, ISBN 0-471-06784-9), edited by Sidney W. Benson. Contents, abridged: Chemical reactions in the atmosphere as studied by the method of instantaneous rates. Reactions of SH with atomic oxygen and hydrogen. The thermal structure and dynamics of the stratosphere. Rate constant measurements needed to improve a general kinetic mechanism for photochemical smog. Temperature dependence of the rate constants for reactions of ozone with some olefins. The reaction of ozone with hydrogen sulfide and its organic derivatives. Accuracy and precision of gas phase kinetics techniques. Reactions of hydroxyl radicals with alkanes. Current status of methods for the estimation of rate parameters. The photolysis of gaseous nitrous acid: a technique for obtaining kinetic data on atmospheric photo-oxidation reactions. The high temperature oxidation of methyl mercaptan (shock waves). The photostationary state in photochemical smog. Atmospheric aerosol formation by chemical reactions. A condensation nucleus size analyzer suitable for studying the kinetics of aerosol formation. Kinetics of homogeneous particle nucleation and growth. The influence of aerosols on the chemistry of the troposphere. Heterogeneous reactions of OH radicals. Subject index. Index of compounds.

CHEMISTRY

- * ANALYTICAL ASPECTS OF MERCURY AND OTHER HEAVY METALS IN THE ENVIRONMENT. (1975, 196 pp, \$19.50, Gordon and Breach, NY, ISBN 0-677-15890-4), edited by R.W. Frei and O. Hutzinger. Contents: Use of mercury in agriculture and its relationship to environmental pollution. The micro-determination of mercury and organomercury compounds in environmental materials. Mass spectra of some fungicidal organomercury compounds. Collections and determination of traces of lead. Determination of lead, cadmium, copper and zinc in biological materials by anodic stripping polarography. Determination of

traces of antimony by flameless atomic absorption spectroscopy. Determination of some transition metals by atomic absorption spectroscopy after extraction with pyridine-2-aldehyde 2-quinolyldrazone. The determination of trace transition elements in biological tissues using flameless atom reservoir atomic absorption. Activation and applications to environmental research. Articles originally appeared in the *International Journal of Environmental and Analytical Chemistry* and *Toxicological and Environmental Chemistry Reviews*.

- * CARBOHYDRATE CHEMISTRY. VOL. 8 (1976, 485 pp, \$66, Chemical Society, London, ISBN 0-85186-072-9) by J.S. Brimacombe, senior reporter. Contents, abridged: Free sugars. Glycosides. Ethers and anhydro-sugars. Esters. Miscellaneous nitrogen-containing compounds. Thio- and seleno-sugars. Unsaturated derivatives. Sugar acids and lactones. Nucleosides. NMR spectroscopy and conformational features of carbohydrates. Other physical methods. Separatory and analytical methods. Plant and algal polysaccharides. Enzymes. Chemical synthesis and modification of oligosaccharides, polysaccharides, glycoproteins, enzymes and glycolipids. Author index. Covers literature available between mid-January 1974 and mid-January 1975.

COMPUTER AIDED DATA BOOK OF VAPOR-LIQUID EQUILIBRIA. (1975, 944 pp, \$59.75/Dfl. 155, Elsevier Scientific Publishing) by M. Hirata, S. Ohe and K. Nagahama.

- * FAITH, KEYES, AND CLARK'S INDUSTRIAL CHEMICALS. 4TH ED. (1975, 904 pp, \$47.50, Wiley-Interscience, NY, ISBN 0-471-54964-9), by F.A. Lowenheim and M.K. Moran. Contents, abridged: Ammonia, aspirin, boric acid, caprolactam, chlorine, cresol, decyl. alcohols, ethanolamines, ethylene, hydrazine, lead alkyls, methyl ethyl ketone, nitric acid, penicillin, sodium, styrene, trichlorethylene. Company index. Subject index.

- * ENCYCLOPEDIA OF ELECTROCHEMISTRY OF THE ELEMENTS. VOL. 6. (1976, 341 pp, Dekker, NY, ISBN 0-8247-2506-9), edited by Allen J. Bard. Contents: Indium, scandium, yttrium and the lanthanides, aluminum, platinum, iridium, osmium, palladium, ruthenium, rhodium. Subject index. Comprehensive review of the electrochemical behavior of the elements.

JOURNAL OF PHYSICAL AND CHEMICAL REFERENCE DATA. VOL. 5. (1976, 1183 pp, \$90 for U.S., Canada and Mexico, \$94 other countries, special rates formembers ACS or AIP, American Chemical Society, Subscription Service, 1155 16th St., Washington, D.C. 20036), edited by D.R. Lide, Jr. Contents: Scaled Equation of State Parameters for Gases in the Critical Region; Microwave Spectra of Molecules of Astrophysical Interest, IX. Acetaldehyde; Microwave Spectra of Molecules of Astrophysical Interest, X. Isocyanic Acid; Diffusion in Copper and Copper Alloys, Part IV. Diffusion in Systems Involving Elements of Group VIII; A Critical Review of the Stark Widths and Shifts of Spectral Lines from Non-Hydrogenic Atoms (A Critical Review and Tabulation of Selected Data); Atlas of the Absorption Spectra

of Nitric Oxide (NO) between 1420 and 1250Å; Ideal Gas Thermodynamic Properties of Propanone and 2-Butanone; Refractive Index of Alkali Halides and Its Wavelength and Temperature Derivatives; Tables of Critically Evaluated Oscillator Strengths for the Lithium Isoelectronic Sequence; Ideal Gas Thermodynamic Properties of Six Chlorofluoromethanes; Survey of Superconductive Materials and Critical Evaluation of Selected Properties; Nuclear Spins and Moments; Nuclear Moments and Moment Ratios as Determined by Mössbauer spectroscopy; Rate Coefficients for Ion-Molecule Reactions. I. Ions Containing C and H; Microwave Spectra of Molecules of Astrophysical Interest. XI. Silicon Sulfide. Data compilation abstracts. Property Index. Author Index. Single copy and reprint orders accepted.

- * SCANDIUM: ITS OCCURRENCE, CHEMISTRY, PHYSICS, METALLURGY, BIOLOGY AND TECHNOLOGY. (1975, 598 pp, \$42.25, Academic Press, NY, ISBN 0-12-355850-6), edited by C.T. Horovitz et al. Survey of research, chemical, physical and technological properties, uses, biological significance and toxic effects of scandium. Large portion deals with the alloys and intermetallic compounds of scandium. Updated bibliographies, tabulated data, charts.

EARTH SCIENCES

BASIC TYPES OF PARTICLES OF LUNAR REGOLITH FROM LUNE (MARE FECUNDITATIS): ZAKLADNI TYPY CASTIC MESICNIHO REGOLITU Z LUNY 16. (In Czech; summaries in Russian and English, 184 pp, 38 Kcs, Academia, Prague), by A. Cimbáliková and M. Palivcová. Results are presented of a microscopic examination of unique rock material from the area of the lunar sea (Mare fecunditatis) differing in its characteristics from all other known rock materials. The sample of lunar regolith (weight 1.07 g) presented to the Czechoslovak Academy of Sciences by the Academy of Sciences of the USSR, was collected by the Soviet automatic lunar station Luna 16 in the area of the Mare fecunditatis in 1970.

GEOPHYSICAL DATA CENTERS: IMPACT OF DATA-INTENSIVE PROGRAMS. (1976, 32 pp, edited by Geophysical Data Panel. Carl H. Savit, Chairman. Available from Geophysics Research Board, National Research Council, 2101 Constitution Avenue, Washington, D.C. 20418.) Part I of this report sets forth and discusses the recommendations of the Panel. The operation of some typical World Data Centers and associated national data centers is described, and the impact of new data forms and quantities on them is considered. Part II contains the results of a survey of digital data quantities from past, ongoing and planned large-scale geophysics programs.

- * INTERPRETATION OF ENVIRONMENTAL ISOTOPE AND HYDROCHEMICAL DATA IN GROUNDWATER HYDROLOGY. (1976, 228 pp, \$14, IAEA, Vienna, ISBN 92-0-141076-X). Proceedings of an Advisory Group Meeting held in Vienna, Austria from 27-31 January 1975. Of interest to hydrologists, hydrogeologists, hydrochemists and isotope specialists, engineers, soil physicists, mineralogists, and meteorologists. Aspects of the interpretation of environmental isotope and hydrochemical data in ground water hydrology are discussed. Interdisciplinary case-study and methodology demonstrated.

STUDY OF METEOROLOGICAL DATA PROCESSING METHODS. (1972, 104 pp, prepared by Ground Facility for a Geostationary Meteorological Satellite System (GFGMS), European Space Research Organization (presently European Space Agency, Paris). The report reviews the potential applications of observations obtained from a geostationary meteorological satellite. The data processing tasks that must be accomplished by a supporting Ground Facility in preparing the various classes of input data for operational use by the Meteorological Services are listed. Much of the report is devoted to a discussion of the handling of IR and visible data generated by a spin-scan radiometer. Emphasis is placed on the description of those data processing methods currently in use, their probable development, and estimation of the magnitude of the associated computer work load at the Ground Facility.

HANDBOOKS

ELECTROCHEMICAL DATA. A HANDBOOK FOR ELECTROCHEMISTS IN INDUSTRY AND UNIVERSITIES. (1975, 340 pp, \$38.50/Dfl. 100, Elsevier Scientific Publishing, Amsterdam, Oxford, NY), edited by D. Dobos. This book provides a comprehensive source of ready information for chemists, physical chemists, and electrochemists engaged in industrial practice, dealing with a variety of problems that may emerge in day-to-day work. The wide range of tabulated data includes specific and equivalent conductivities, ionic immobilities, transport numbers, diffusion coefficients, thermodynamic data for ions in electrolyte solutions, relaxation times, and relative permittivities of inorganic salts and mixtures and a few organic mixtures, as well as equilibrium values, activity coefficients, solubility products, and pH values of organic and inorganic acids, bases and salts. The book also includes tables of data on indicator ranges, measurement of pH, buffer solutions, approximate pH values for different materials, standard mixtures for dielectrometric investigations, electrode potentials, and characteristics of galvanic cells, accumulators, and coulometers. It also includes tables of deposition potentials, decomposition potentials, polarographic half-wave potentials, and electrokinetic data and isoelectric points. All data are given in SI units, and, where considered useful, also in traditional units.

- * HANDBOOK OF IRON METEORITES; THEIR HISTORY, DISTRIBUTION, COMPOSITION AND STRUCTURE. Volumes 1-3. (1976, 243 pp, 577 pp, and 598 pp respectively, \$140 set, ISBN 0-520-029348, Univ. of California Press, Berkeley) by Vagn F. Buchwald. Contents Vol. 1: The minor bodies of the solar system, physics of the fall, on multiple falls, end point height and sound phenomena, meteorite craters, statistical and historical notes, shapes and surface characteristics, classification, chemical composition, the minerals and structural components of iron meteorites, the primary structures of iron meteorites, meteorite ages. 8 appendices, 37 tables, 200 photographs; Vol. 2: A guide to the use of this handbook, iron meteorites: Abakan - Mejilones; Vol. 3: Iron meteorites: Merceditas-Zerhamra supplement, index. Definitive handbook on the subject.

- * METALS HANDBOOK. 8TH ED. VOL. 10: FAILURE ANALYSIS AND PREVENTION. (1975, 604 pp, \$47.50, American Society for Metals, Metals Park, Ohio), edited by American Society for Metals. Contents: engineering aspects of failure and failure analysis. Failures from various mechanisms and related environmental factors, analysis and prevention of service failures: products of principal metalworking processes: manufactured components and assemblies. Index. Reference tables

- * METALS REFERENCE BOOK. 5TH ED. (1976, 1566 pp, \$105, Butterworths, Woburn, Mass., ISBN 0-408-706279), edited by Colin J. Smithells. Contents: First aid. Introductory tables, general physical and chemical constants, X-ray crystallography, crystallography, crystal chemistry, metallurgically important minerals, thermochemical data, physical properties of molten salts, metallography, equilibrium diagrams, gas-metal systems, diffusion in metals, general physical properties, elastic properties, radiating properties of metals, electron emission, electrical properties, steels and alloys with special magnetic properties, mechanical testing, mechanical properties of metals and alloys, hard metals, lubricants, friction and wear, casting alloys and foundry data, refractory materials, fuels, controlled atmospheres for heat treatment, masers and lasers, guide to the corrosion resistance of metals, electroplating and metal finishing, welding, solders and brazing alloys. Index.

ZIRCONIUM: PHYSICO-CHEMICAL PROPERTIES OF ITS COMPOUNDS AND ALLOYS: ATOMIC ENERGY REVIEW SPECIAL ISSUE NO. 6. (1976, 268 pp, \$16, IAEA, Vienna, ISBN 92-0-149276-6), edited by O. Kubaschewski. Critical evaluation and documentation of thermodynamic properties, densities, crystallographic structures, equilibrium diagrams and diffusion rates in the condensed states.

MATHEMATICAL METHODS AND COMPUTER PROGRAMS

A COMBINED LEAST SUMS AND LEAST SQUARES APPROACH TO THE EVALUATION OF THERMODYNAMIC DATA NETWORKS. (NBS Publication No. NBSIR 76-1147, 1976, 37 pp, \$4, NTIS, Springfield, Va. 22151) by D. Garvin, V.B. Parker, D.D. Wagman, and W.H. Evans. A description is given of a system for computer-based evaluation of interrelated thermodynamic measurements of enthalpies of reaction, equilibria and entropies. This system is an extension of the CATCH program developed by J.B. Pedley, University of Sussex. In the new system linear least sums and least squares techniques are used to solve networks of thermodynamic equations to obtain the enthalpies, free energies of formation and the entropies of chemical substances. The least sums technique is shown to be useful in assessing the consistency of the data. A method combining least sums and least squares solutions, provides a weighted solution that reproduces closely the solutions that are obtained by a detailed analysis of the data using the customary sequential procedure. The results from tests on four large networks involving compounds of B, U, Rb and salts of Sn, Pb, Cd and Hg are discussed.

METHODS IN COMPUTATIONAL PHYSICS; ADVANCES IN RESEARCH AND APPLICATIONS. VOL. 15: VIBRATIONAL PROPERTIES OF SOLIDS. (1976, 429 pp, \$43.50, Academic Press, NY, ISBN 0-12-460-815-9), edited by Gideon Gilat. Computation methodology for analyzing data generated through research experiments in lattice dynamics.

MICROCOMPUTER DICTIONARY AND GUIDE. (1976, 704 pp, \$17.95; CALCULATOR USER'S GUIDE AND DICTIONARY (1976, 428 pp, \$9.95, Matrix Publishers, Inc., 207 Kenyon Rd, Champaign, IL 61820).

NUMERICAL METHODS USED IN ATMOSPHERIC MODELS. (1976, 64 pp, GARP Publication Series No. 17, WMO, Case Postale No. 5, Geneva 20).

PHAS20, A PROGRAM FOR SIMULTANEOUS MULTIPLE REGRESSION OF A MATHEMATICAL MODEL TO THERMOCHEMICAL DATA. (1974, 162 pp, \$5, U.S. Geological Survey -GD-74-018, available from NTIS, Springfield, VA 22151), by John L. Haas, Jr. PHAS20 performs simultaneous multiple regression of a mathematical model for the functional relations among the thermodynamic quantities to experimental data for a group of chemically related species. The thermodynamic quantities included are heat capacity, entropy, enthalpy, free energy, equilibrium constant, electrochemical potential, and relative heat content. Without further adjustment, PHAS20 will fit the model to 70 sets of data containing a total of 1200 observations on 20 species.

A PROGRAM FOR STORING OCEANOGRAPHIC DATA ON MAGNETIC TAPE (1975, 50 pp, available from National Research Laboratory, Washington, DC 20375) by M.L. Blodgett and J.V. Massingill. A program has been written for the storage of navigation, bathymetry, and magnetics data on magnetic tape in BCD form. This eliminates the problem of storing vast amounts of data collected on computer cards by oceanographic and geophysical cruises. This program uses a slightly modified format recommended by the National Research Council of the National Academy of Sciences. The program was written in Fortran IV for use on the CDC 3800; however the program can be converted to run on other systems with little difficulty.

MECHANICAL AND ENGINEERING DATA

CRITICAL SURVEY OF DATA SOURCES: CERAMICS. NBS special publication 396-2, \$1.25, and CRITICAL SURVEY OF DATA SOURCES: CORROSION OF METALS. NBS special publication 396-3, \$1.30. Available from the Supt. of Documents, U.S. Govt. Printing Office, Washington, DC 20402. The second and third in a series of reference guides for users of ceramics and metals identify the best data sources for both products according to scope, assets and deficiencies. Both directories list important handbooks and technical compilations, information centers, technical societies and trade associations. Materials and property indexes and useful references are also included.

ENCYCLOPÉDIE DES GAZ - GAS ENCYCLOPEDIA. (1976, 1150 pp, 942 FF, L'Air Liquide, 75 Quai d'Orsay, 75321 Paris Cedex 07, France). This is a compilation of the main properties and uses of 138 more or less current gases, one half of which are inorganic gases, the other half being made up of carbon-containing molecules. After a lengthy introduction devoted to the physical properties of gases and the particular problems encountered in gas metrology, the compilation proper takes up the

1100 other pages. Each gas is the subject of a monography, the length of which corresponds to the overall importance of the gas in science. The main physical and thermodynamic properties are given either as data tables or as sets of characteristic curves. The biological properties, technological uses and guidelines for the safe handling of each gas are also given.

MATERIALS INFORMATION PROGRAMS. (1977, 271 pp, \$3.35, NBS Special Publication 463, available from Supt. of Documents, US Govt Printing Office, Washington, D.C. 20402, SD No. C13 10:463), edited by S.A. Rossmassler. Proceedings of a conference which took place in April 1974 on an interagency review of Federal Agency activities on Technical information about materials.

NOMENCLATURE, SYMBOLS, UNITS, STANDARDS AND CONSTANTS

QUANTITIES, UNITS AND SYMBOLS. (1975, 54 pp, £1.05, The Royal Society, London).

SOLID STATE PROPERTIES

* ADVANCES IN LIQUID CRYSTALS. VOL. I. (1975, 320 pp, \$31.50, Academic Press, NY, ISBN 0-12-025001-2), edited by Glenn H. Brown. Contents: Composition, properties and structures of liquid crystalline phases in systems of amphiphilic compounds. Order and structure of liquid crystals. Mesomorphic properties of block copolymers. Plastic crystals, liquid crystals, and the melting phenomenon - the importance of order. Defects in liquid crystals. Subject index.

CRYSTAL STRUCTURE TRANSFORMATION IN INORGANIC SULFATES, PHOSPHATES, PERCHLORATES, AND CHROMATES. (NSRDS-NBS 56, 1975, order by SD Catalog No. C13.48:56 from Supt. of Documents, U.S. Govt. Printing Office, Washington, D.C. 20402), edited by C.N.R. Rao and P. Prakash. Literature dealing with the crystal structure transformations of simple inorganic sulfates, phosphates, perchlorates, and chromates has been critically reviewed. Data on thermodynamic, crystallographic, spectroscopic, dielectric, and other properties are given. The most extensive discussion deals with the sulfates; data on the other substances is in tabular form only. Experimental techniques used to obtain the data are indicated and comments on the data made where necessary. All pertinent references up to 1974 are listed.

* CRYSTALLOGRAPHY AND CRYSTAL CHEMISTRY OF MATERIALS WITH LAYERED STRUCTURES. (1976, 368 pp, \$39, D. Reidel, Hingham, Mass, ISBN 90-277-0586-0), edited by F. Lévy. Contents: Growth and the crystal characteristics of dichalcogenides having layered structures of ternary chalcogenides with alkali and transition metals. Structural aspects of non-stoichiometry in materials with layered structures. Physical and chemical properties of phyllosilicates. Polytypism and stacking faults in crystals with layered structure. Thermal behavior of stacking faults. Name index, subject index, formula index. For crystallographers and researchers in solid state physics and chemistry.

PHYSICS AND CHEMISTRY OF MATERIALS WITH LAYERED STRUCTURES. VOL. 1 - PREPARATION AND CRYSTAL GROWTH OF MATERIALS WITH LAYERED STRUCTURES. (1976, 200 pp, \$26/Dfl 65, ISBN 90-277-0638-7, Reidel Publishing Co., Dordrecht, Boston) edited by R.M.A. Lieth. Reviews the current application of preparative methods and crystal growth techniques in the investigation of inorganic materials with a layered structure. Contents: Elements. Halides. Hydroxides. Di-chalcogenides of the transition metals. Chalcogenides of the Group III-metals. Chalcogenides of the Group IV-metals.

PHYSICS AND CHEMISTRY OF MATERIALS WITH LAYERED STRUCTURES. VOL. 4 - OPTICAL AND ELECTRICAL PROPERTIES. (1976, 455 pp, \$49/Dfl 135, Reidel Publishing Co., Dordrecht, Boston, ISBN 90-277-0676-X), edited by P.A. Lee. Contents: Optical properties of layer compounds. Some aspects of modulation spectroscopy in layer materials. Optical properties, electronic structure and photoconductivity of arsenic chalcogenide layer crystals. Photoemission studies of materials with layered structures. Transport properties of layered semiconductors. Transport properties of layered structure metals. Experimental aspects of superconductivity in layered structures. Structural and magnetic properties of layered chalcogenides of the transition elements.

THERMAL CONDUCTION IN SOLIDS. (1976, 186 pp, £9.75, Clarendon Press: Oxford University) by R. Berman. Describes the physics of the processes involved in thermal conduction in solids in a detailed but uncomplicated way, illustrated by experimental results on insulating crystals, non-crystalline solids, metals, alloys and semiconductors.

SPECTRA COLLECTIONS

* ABSORPTION SPECTRA IN THE INFRARED REGION. VOL. 2. (1976, 318 pp, \$34, Butterworths, Woburn, Mass., ISBN 0408-10610-7), edited by L. Láng. A compilation of 311 absorption spectra valuable for all physical science collections. Subject, author and formula indexes included.

* ATLAS OF INFRARED SPECTROSCOPY OF CLAY MINERALS AND THEIR ADMIXTURES. (1976, 396 pp, \$63.50, Elsevier, Amsterdam, ISBN 0-444-41187-9) by H.W. van der Marel and H. Beutelspacher. Extensive collection of infrared spectra of clay minerals.

DIATOMIC MOLECULES. A CRITICAL BIBLIOGRAPHY OF SPECTROSCOPIC DATA. (1973, 2 volumes, 890 pp, 150 FF, 1975, 2 volumes, 796 pp, 150 FF, Editions du CNRS, Paris), edited by R.F. Barrow. These four volumes, in a series to be published at irregular intervals, consist of a series of critical abstracts arranged molecule by molecule. Each of the 2093 references includes bibliographic information, a note of the experimental technique, if any, used, and a list of the properties, if any, measured, as well as the abstract. These volumes are published as books, but printed on one side only and so arranged that entries may be transferred to standard reference cards for convenience. The 1973 volumes carry the data to the end of 1970 and the 1975 volumes through 1974. It makes no claims for completeness or for uniformity of treatment.

* FLAME EMISSION AND ATOMIC ABSORPTION SPECTROMETRY. VOL. 3. ELEMENTS AND MATRICES. (1975, 674 pp, \$49.50, Dekker, NY, ISBN 0-8247-1137-8). edited by John A. Dean and T.C. Rains. Contents: Lithium, sodium, potassium, rubidium, and cesium. Magnesium, calcium, strontium, and barium. Copper, silver, gold, zinc, cadmium, and mercury. Beryllium, boron, aluminum, gallium, indium, and thallium. The rare earth elements. Titanium, zirconium, hafnium, niobium, tantalum, silicon, and germanium. Vanadium, chromium, manganese, molybdenum, and tungsten. Tin, lead, antimony, and bismuth. Arsenic, selenium, and tellurium. Iron, cobalt, and nickel. Ruthenium, rhodium, palladium, osmium, iridium, platinum, and rhenium. Halogens. Helium, neon, argon, krypton and xenon. Carbon, nitrogen, oxygen, phosphorus and sulfur. Agronomic applications. Biological fluids. Food analysis. Petroleum products. Glass. Portland cement and kits raw components. Ferrous metals and alloys. Application of atomic absorption spectrometry in geochemistry. Water. Air pollution. Nonferrous metals and alloys. Appendix. Index.

* INFRARED SPECTRA OF SURFACE COMPOUNDS. (translated from Russian by N. Kaner. Translation edited by D. Slutzkin, IST Program of Jerusalem, 1975, 384 pp, \$37.50, Halsted, Div. of Wiley, ISBN 0-470-48905-7), by A.V. Kiselev and V.I. Lygin. Note: The book covers theoretical concepts, technology and state of research in application of infrared spectroscopy to investigations of surface processes in various compounds. For specialists in the academic world and industrial laboratories in the fields of adsorption, catalysis, polymer chemistry and various types of chromatographic analyses. Subject index. Updated bibliographies, diagrams, tabulated data.

* MOLECULAR SPECTROSCOPY. VOL. 3. (1975, 588 pp, 66, Chemical Society, London, ISBN 0-85186-526-7), R.F. Barrow, D.A. Long and D.J. Millen, senior reporters. Contents: Microwave spectroscopy. Force-constant calculations in molecules. Experimental resonance Raman spectroscopy. Matrix isolation. Rotation and vibration-rotation Raman and infrared spectra of gases. Raman spectra of solids. The electronic spectra of triatomic molecules and the Renner-Teller effect. 2794 citations cover the period 1973 and early 1974. Author index.

SELECTED ¹³C NUCLEAR MAGNETIC RESONANCE SPECTRAL DATA. API Research Project 44, Supp. Vol. G-5, (Oct. 1976, 97 pp). Contents: Alkylbenzene, C₈; pinenes, C₁₀; cyclohepta[a]naphthalenes, C₂₀, C₂₁, C₂₅; aliphatic and cyclic ketones, C₅, C₆, C₈; chlorinated and brominated hydrocarbons, C₁, C₃-C₉, C₁₂, C₁₄, C₁₉; chloroether, C₃; chloro- and bromoacids, esters, alcohols, and ketones, C₃-C₅, C₈, C₁₁, C₁₄, C₁₅; alkyl-, cyclo-, and aryl amines, C₃-C₁₂; nitroalkane, C₃; amides, C₂-C₄; cyano compds., C₅, C₉; morpholine, C₄; bromoanilines and quinoline, C₆, C₈, C₉; chlorotoluene, C₇; acetonil phosphonate, C₅; and tetrabutylammonium tetrafluoroborate, C₁₆, alkyl phthalate, C₁₀; aldehyde, C₁₀; naphthyl cyclohexanol, C₁₈; cholestanone and bromocholestanones, C₂₇.

* STRUCTURAL STUDIES OF MACROMOLECULES BY SPECTROSCOPIC METHODS. (1976, 339 pp, \$37, Wiley-Interscience, NY, ISBN 0-471-43120-6), edited by K.J. Ivin.

TOPICS IN CARBON-13 NMR SPECTROSCOPY.

(1976, 485 pp, \$27.50, Wiley-Interscience, NY, ISBN 0-471-53169-3), edited by G.C. Levy. Contents: Conformation and structure of peptides. Carbon-13 NMR spectroscopy of naturally occurring substances. C-13 NMR biosynthetic studies. C-13 NMR studies of biopolymers. C-13 NMR studies of organometallic and transition metal complex compounds. Organic structure assignments using C-13 spin-relaxation data. The computer in Fourier transform NMR. Theory of indirect nuclear spin-spin coupling constants with applications to C-13 NMR. Index.

THERMODYNAMIC PROPERTIES

CHEMICAL EQUILIBRIA IN CARBON-HYDROGEN-OXYGEN SYSTEMS. (ENERGY LABORATORY; VOL. 1)

(1976, 110 pp, \$9.95, MIT Press, Cambridge, ISBN 0-262-02121-8), by R.E. Baron, J.H. Porter and O.H. Hammond, Jr. Contents: Thermodynamic basis and assumptions. C-H-O system. Tables. Composition vs. temperature plots. Composition vs. pressure plots. Composition vs. IN(H/O) plots. C-H-N-O system. Tables. The adiabatic reactor case. Tables. Composition vs. temperature plots. Note: Provides tables and graphs which will permit rapid estimation of the equilibrium compositions of the gas phase (i.e. for C-H-O systems) under a variety of reaction conditions. Appendixes.

LIQUID AND SOLID HELIUM. Europhysics Topical Conference on Liquid and Solid Helium, Technion, Israel Institute of Technology, 1974. (1975, 410 pp, \$32, Israel Universities Press, Jerusalem, dist. by Halsted, Div. of Wiley, ISBN 0-470-51095-1), edited by C.G. Kuper, S.G. Lipson and M. Revzen. Survey of advances and present research on thermodynamics, structure and nuclear characteristics of liquid and solid helium.

SELECTED THERMOCHEMICAL DATA COMPATIBLE WITH THE CODATA RECOMMENDATIONS. (1976, 34 pp, \$4, NBS Report NBSIR 75-968), by V.B. Parker, D.D. Wagman, and D. Garvin. Selected thermochemical properties data at 298.15K are given for 384 substances.

SELECTED VALUES OF PROPERTIES OF HYDROCARBONS AND RELATED COMPOUNDS. API Research Project 44, Supp. Vol. A-73, October 1975, 119 pp, TRC, Texas A&M, College Station, Texas). Physical properties for alkylbenzo[*a*]phenanthrenes, C₁₈-C₂₂, alkyltriphenylenes, C₁₈-C₂₂, alkylpyrenes, C₁₆-C₂₀; vapor pressures and boiling points at 0.004 to 1500 mmHg for alkyltriphenylenes, C₁₈-C₂₂, alkylpyrenes, C₁₆-C₂₀; enthalpy of formation for alkanes, C₆, C₇, C₈; ideal gas standard state thermodynamic functions for *n*-alkanes, C₁-C₂₀; condensed phase thermodynamic functions for alkanes, C₆, C₇, C₉.

SOLID-LIQUID PHASE EQUILIBRIA. (1976, 360 pp, Elsevier, Amsterdam), by Jaroslav Nývlt. A comprehensive survey of phase equilibria in condensed systems. Descriptions are given of measurement, methods and various modes used for the elaboration of experimental data by means of semiempirical and theoretical procedures. Text is completed with numerous tables and programs for computers.

THERMODYNAMIC AND THERMOPHYSICAL PROPERTIES

OF COMBUSTION PRODUCTS. (Termodinamicheskie i teplofizicheskie svoystva produktov sgoraniya).

VOL. II - OXYGEN BASED PROPELLANTS (Topliva na osnove kisloroda), translated from Russian (Moscow, 1972, translation 1975, 505 pp, \$12.75 (\$15.25 foreign) NTIS, Springfield, VA 22161 as TT 74-50032), edited by V.P. Glushko. This volume contains the thermodynamic and thermophysical properties of the combustion products of four composite propellants (hydrogen, kerosene, unsymmetrical hydrazine, and ammonia as fuel with oxygen as the oxidizer). All of the data reported were obtained by the authors by calculation using the methods and programs described in Volume I of the series (see Newsletter 15).

VOL. III - OXYGEN AND AIR-BASED PROPELLANTS.

(Topliva na osnove kisloroda i vozdukh), translated from Russian (Moscow, 1973, translation 1975, 632 pp, \$16.25 (\$18.75 foreign), NTIS No. TT 75-50007), edited by V.P. Glushko. This volume of the series give information on the thermodynamic and thermophysical properties of the combustion products of eleven propellants. One group includes two component liquids based on oxygen as the oxidizer. These are: liquid oxygen with pentaborane, with a mixture of pentaborane and kerosene, and with beryllium hydride. A second group refers to three-component propellants: liquid oxygen with liquid hydrogen and beryllium in a variety of proportions. The third group consists of propellant compositions with air as the oxidizer. These include: air plus liquid hydrogen, air plus kerosene, air plus 95% ethanol, and air plus natural gas. The list of the properties determined by calculation is the same as in Volumes I and II.

THERMOPHYSICAL PROPERTIES OF MATTER, VOL. 12.

THERMAL EXPANSION: METALLIC ELEMENTS AND

ALLOYS. (1975, xxv + 1348 + App., \$80, IFI/Plenum, New York, Washington), by Y.S. Touloukian, R.K. Kirby, R.E. Taylor and P.D. Desai. This volume of the TPRC Data Series presents data on the percent thermal linear expansion coefficients for almost all metallic materials for which data are known to exist. The volume comprises three major sections: the front text on theory, estimation, and measurement, the main body of numerical data, and the material index. The text is intended to be merely complementary to the main body of data which is the primary purpose of this volume. The materials covered include 64 elements, 94 intermetallic compounds, 125 binary alloy systems, and 70 groups of multiple alloys. Of the 353 materials, systems, and groups covered, the data for 246 have been critically evaluated, analyzed, and synthesized, and recommended reference values or provisional values have been generated and are presented together with the original experimental data.

THERMOPHYSICAL PROPERTIES OF MATTER AND SUBSTANCES. Translation of Volumes I-IV, edited by V.A. Rabinovich. Translations may be ordered from the National Technical Information Service, Springfield, VA 22161, USA, using the TT-numbers provided.

VOL I - THERMOPHYSICAL PROPERTIES OF GASES AND LIQUIDS (original 1968, translation 1970, 207 pp, \$7.75 (\$10.25 foreign), No. TT 69-55091).

VOL II - THERMOPHYSICAL PROPERTIES OF MATTER AND SUBSTANCES. (original 1970, translation 1974, 384 pp, \$10.75 (\$13.25 foreign), No. TT-72-5001). Contents: air and its components; hydrogen and monatomic gases; hydrocarbons and their derivatives; carbon dioxide; metals and their components; and mixtures, solutions,

and materials. Critically evaluated data are given for the thermodynamic properties of parahydrogen at temperatures and pressures of 14 to 1500 K and 0.5 to 5000 bars; and of the rare gases (except helium) at saturation. Viscosity coefficients of rarified normal hydrogen at temperatures of 10 to 1273 K, of parahydrogen at 15 to 100 K and 6 to 10 atmospheres, and of liquid normal and parahydrogen at the saturation line are evaluated, as are those of the rare gases at temperatures of 25 to 1300 K. Evaluated data on the molal volumes and volatility of nitrogen at temperatures and pressures of 0 to 400 C and 3000 to 12 000 atmospheres; specific volumes of methane; density of normal hexane; thermodynamic functions of fluorinated benzenes; coefficient of thermal conductivity of carbon dioxide in the near critical region; and coefficient of thermal expansion of mercury.

VOL III - THERMOPHYSICAL PROPERTIES OF MATTER AND SUBSTANCES (original 1971, translation 1975, 207 pp, \$7.75 (\$10.25 foreign), No. TT-73-52029. This volume includes articles on the thermodynamic properties of gases such as para- and normal hydrogen, neon, argon and krypton, and carbon dioxide. Topics covered are unified equation of state, heat conductivity, compressibility, phase transitions, viscosity, coefficient of thermal conductivity, enthalpy, and molar volumes. Studies on the thermodynamic properties of water, and the velocity of sound and adiabatic coefficient of compressibility of aqueous solutions of electrolytes at high pressures. Unified equation of state valid in the temperature and reduced density ranges of 14 to 5000 K and 0 to 2.8 is formulated for normal hydrogen, and values of the density, compressibility, isobaric and isochoric specific heat, velocity of sound, and Joule-Thompson coefficient calculated from it. Known experimental works on thermal conductivity of normal H are summarized and critically analyzed to give recommended values of the coefficient of thermal conductivity in the rarified state at temperatures of 10 to 1300 K. New type of equation for the calculation of thermal conductivity of gaseous and liquid Ar is presented and results calculated at temperatures and pressures of 90 to 620 K and 28 to 690 bars compared with those of variety of experimental works. Recommended values of the coefficients of thermal conductivity of Ar, Ne, Kr, and Xe from the triple point to 1300 K at atmospheric pressure are given from an analysis of experimental results of various authors.

VOL IV - THERMOPHYSICAL PROPERTIES OF MATTER AND SUBSTANCES (original 1971, translation 1975, 173 pp, \$7.50 (\$10.00 foreign), No. TT-73-52029. This volume includes articles presenting the results of studies of freons.

VOL X - THERMOPHYSICAL PROPERTIES OF MATTER AND SUBSTANCES (TEPLOFIZICHESKIE SVOISTVA VESHCHESTV I MATERIALOV) (in Russian, 1976, 271 pp, 88 kopecks, available from "Znak Pocheta" Izdatelstvo Standartov, Novopresnenskiy Per. 3, Moscow D-557), edited by V.A. Rabinovich. This volume presents a collection of papers entitled: composition of a unified equation of state using the computer, determination of thermodynamic functions of gases by PVT-measurements using simulation techniques on a computer, equation of state for molecular solid H, thermodynamic properties of crystalline parahydrogen, viscosity of parahydrogen, thermodynamic properties of H and He at high pressures (to 10 000 bars), thermal properties of N in wide range of temperatures and pressure (1 to 300 bars), experimental studies on the compressibility of Kr in the gaseous state at low temperatures, use of adiabatic calorimetry for the determination of specific heats and their derivatives in Type I transitions, study of thermodynamic prop-

erties of binary solutions of He, Ar, Ne, Kr, and Xe: analysis of experimental data, study of thermodynamic properties of binary systems in the vicinity of the equilibrium curve, on the thermodynamic properties of the C₂H₆-CO₂ system: P,V,T,N data and the system's thermodynamic functions, measurement of transfer coefficient of liquids and liquid mixtures by optical methods, experimental study of H₂O viscosity in the vicinity of the critical point, study of the dynamic viscosity of trifluorobromomethane (F₃BrC) and method and apparatus for the study of specific heats and heat of phase transition for condensed phases in the range 300-1573 K.

VAPOUR-LIQUID CRITICAL PROPERTIES. (1975, 48 pp, £10, Information Services, National Physical Laboratory, Teddington, Middlesex, UK) by D. Ambrose and R. Townsend. Experimental data on vapour-liquid critical properties of pure liquids and a few well-defined mixtures. 141 non organic compounds, 444 organic compounds.

MISCELLANEOUS

* BASIC INSTRUMENTATION LECTURE NOTES AND STUDY GUIDE; MEASUREMENT FUNDAMENTALS. 2nd ed. (1976, 303 pp, Instrument Society of America, Pittsburgh), edited by Ralph L. Moore. Contents: Introduction to measurement fundamentals. Pressure measurement, level measurement, weight measurement, density measurement, flow measurement, temperature measurement, heat flux measurement sensor types, humidity and moisture measurement, physical and chemical measurements. Note: An invaluable ready reference for quick look-up of nine different basic instrument applications. Excellent diagram and descriptive accompanying outline for each of the 216 instrument variations.

DATA BASE DIRECTIONS. THE NEXT STEPS. (NBS-SP 451, 1976, 175 pp, \$2.40, Sup. of Doc., US Govt. Printing Office, Washington, D.C., SD Cat. No. C13. 10:451), edited by John L. Berg. Information about data-base technology a manager needs in order to make prudent decisions about using new technology.

DATA BASES IN EUROPE. 2nd Edition. (1976, 58 pp, £6, Aslib, 3 Belgrave Sq., London SW1X 8PL.), edited by Alex Tomberg.

DIRECTORY OF ENERGY INFORMATION CENTERS IN THE WORLD (1976, 299 pp, 230 FF, \$55, £28, IFCE, 3 rue Henri Heine, 75016 Paris, ISBN 2-85933-001-1), edited for the World Energy Conference by the Centre de Documentation de l'Institut Français des Combustibles et de l'Energie under the supervision of Mme. A. David. Bilingual-English and French. Lists 230 organisations from 47 countries. The following information is given for each centre: name and address, fields covered, documentary sources, availability, users concerned, services provided, use of computer. In one chapter the centers are grouped by country and in another by the type of information supplied. A final chapter on "Statistical Publications on Energy by International Organisations" brings together statistical publications by international organisation and by source of energy.

* Grateful acknowledgement for the reprint of this review is given to New Technical Books, The New York Public Library, Fifth Avenue and 42nd Street, New York, NY 10018, USA.

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REPORT OF THE FIRST MEETING OF CODATA TASK GROUP ON DATA FOR THE CHEMICAL INDUSTRY.....

The CODATA Task Group on Data for the Chemical Industry held its first meeting in Asilomar, California in January 1977 under the chairmanship of Dr. Arnold Bondi. The following recommendations grew out of the animated discussions which took place:

1. The industrial users of physical property correlations present at this conference complained about the inadequate testing of newly published correlations by their authors. Hence this Task Group considers its first task to prepare a "Guide for the Presentation of Physical Property Estimation Procedures in the Literature", similar to the CODATA "Guides for the Presentation of Physico-Chemical Data in the Literature". That guide should produce a testing method for new estimation procedures, as well as a standardized presentation format for the benefit of the prospective users. The recommended testing method should include statistical evaluation of the goodness of fit to the data of the group of compounds to which the correlation is supposed to apply (standard deviations, and coefficient of determination) as well as of the uniqueness of the coefficients, as measured by evidence for autocorrelation (such as Durban-Watson coefficients), and finally a proof of the significance of the proposed coefficients (F-test) and their reliability (T-test, or standard deviation of the regression coefficients).

2. As an interim measure the Task Group recommends that engineers use the latest version of the API-Technical Data Book Petroleum for the look-up and estimation of the physical properties of hydrocarbons, and the third edition of "The Properties of Gases and Liquids", by R.C. Reid, J.M. Prausnitz and T.K. Sherwood for the estimation of the physical properties of non-hydrocarbons.

3. For the longer range definition of the Task Group's priority rankings of physical properties, we intend to survey user's needs for improved reliability of correlations in specific areas by means of a questionnaire. It will be addressed to the participants and invitees of the present Engineering Foundation Conference.

While the Terms of Reference of the Task Group exclude vapor-liquid equilibrium from their purview, the questionnaire will contain questions on this subject as well, primarily in order to increase the industrial recipient's interest in answering the questionnaire. But it will be pointed out that the replies to that V/L Equil. question will be transmitted to the second CODATA Task Group which is intended to tackle that particular program.

4. Those substance classes have been broadly identified by the Task Group which are expected to become increasingly important in the chemical industry and which cannot be covered by existing property estimation methods because there have never been enough property data to start from. A description of these substance classes is printed below as a first guide to physical chemists who want to contribute to our art by measuring the

thermodynamic properties of the proposed substances over a wide temperature range.

5. The Task Group will ask the new editor of the Bulletin of Thermodynamics and Thermochemistry to include in his Bulletins a survey of on-going projects in the area of physical property estimation. That listing would fill a very important communications gap of the "property correlators community". At present many people throughout the world may work simultaneously on the same correlation objective in complete ignorance of each other.

Preliminary Recommendation on the Selection of Pure Compounds

Recommendations on the Selection of Pure Compounds for the determination of physical properties, especially the thermodynamic properties (heat capacity from cryogenic temperatures to just below the atmospheric boiling point, vapor pressure over a wide temperature range, and the typical inspection properties) by the CODATA Task Group on Data for the Chemical Industry.

The recommended selection principles are:

1. The compound(s) should be key compounds for the development or amplification of correlations of physical properties with molecular structure in molecular structure areas not now represented in the data base for such work.
2. Preferably these key compounds should be members of compound families which occur in industrially important processes as process stream components, whether as intermediates, products or by-products. Today the economic significance of such process stream components may reside as much in their environmental impact even at low concentrations as in their intrinsic commercial value when produced in massive amounts.
3. The value of physical property correlations in the areas of "minor" process stream components may often be to assess the validity of the single point property data references in the literature which can (mis)guide regulating agency and company action alike.
4. Specifically we recommend the following chemical families for the selection of key compounds:
 - a) Hetero cyclics and polynuclear aromatics, preferably as mono alkyl substituted, because the unsubstituted parent of a series is rarely suitable for property correlations, as well as being commonly too high melting to give the most important liquid phase properties.
 - b) Difunctional and multifunctional compounds, especially of the class possessing different polar groups on the same molecule. Assuming that no polar groups are selected which react chemically with each other, one needs to know at what distance in the molecule one can treat the two or more groups as independent (for purposes of property estimation) and the nature and magnitude of group interactions at shorter distances.

For the latter case the selection rule (2) may well be relaxed in favor of the choice of bifunctional key compound on methodological grounds. So much spectroscopic and physical property work has been done in support of chemical reactivity studies on bifunctional group interactions, especially on aromatic and olefinic backbones, that much could be gained by building on existing knowledge of group interactions, and choose key compounds for physical property measurements from that class of well studied substances.

A. Bondi
January 1977

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Springer-Verlag, Berlin, Heidelberg, New York, 1969, 295 pp, DM 48.—. Us \$ 20.—, FF 120.—.

The "CODATA Compendium" provides a comprehensive world-wide survey and analysis of the organisation, coverage, services and publications of the existing data analysis centres in the physical and chemical sciences. In addition to its usefulness as a directory, the book provides a "key" or index to the substance-property content of the published data compilations. A descriptive brochure is available on request.

Proceedings : Third International CODATA Conference ; Le Creusot, France, 26 – 30 June, 1972

CODATA, Frankfurt Main, F.R.G., Aug. 1973, 100 pp, 297 x 210 mm, DM 30.—, US \$ 15.—, FF 75.—.

CODATA Newsletter

No 1 (Oct. 1968), 12 pp ; No 2 (Aug. 1969), 12 pp ; No 3 (Dec. 1969), 8 pp ; No 4 (May 1970), 16 pp ; No 5 (Dec. 1970), 28 pp ; No 6 (June 1971), 20 pp ; No 7 (Dec. 1971), 20 pp ; No 8 (May 1972), 16 pp ; No 9 (Dec. 1972), 12 pp ; No 10 (June 1973), 12 pp ; No 11 (March 1974), 20 pp ; No 12 (Aug. 1974), 24 pp ; No 13 (Sept. 1974), 20 pp ; No 14 (June 1975), 12 pp ; No 15 (Nov. 1975), 16 pp ; No 16 (Mar. 1976) 16 pp.

CODATA Bulletin : Annual subscription : US \$ 20 or 100 French Francs.

No 1 (Oct. 1969), 12 pp, *Automated Information Handling in Data Centers*, US \$ 1.50, superseded by Bulletin No 4.

Nos 2, 5, 6, 7 and 10, superseded by Bulletin No 17.

No 3 (Dec. 1971), 28 pp, *A Catalog of Compilation and Data Evaluation Activities in Chemical Kinetics, Photochemistry and Radiation Chemistry*, US \$ 3.50.

(Report of the CODATA Task Group on Data for Chemical Kinetics).

No 4 (Dec. 1971), 12 pp, *Automated Information Handling in Data Centers*, US \$ 1.50 2nd Edition.

(Report of the CODATA Task Group on Computer Use, Nov. 1971).

No 8 (Nov. 1972), 32 pp, *Geological Data Files : Survey of International Activity*, US \$ 3.50.

(Report of COGEOCODATA, Committee on Storage, Automatic Processing and Retrieval of Geological Data of the International Union of Geological Sciences (IUGS).

No 9 (Dec. 1973), 6 pp, *Guide for the Presentation in the Primary Literature of Numerical Data Derived from Experiments*, US \$ 1.50.

(Report of the CODATA Task Group on Presentation of Data in the Primary Literature, Sept. 1973).

No 11 (Dec. 1973), 8 pp, *Recommended Consistent Values of the Fundamental Physical Constants, 1973*

(Report of the CODATA Task Group on Fundamental Constants, August 1973).

No 12 (Sept. 1974), 12 pp, *Energy Data Accessing and/or Retrieval*, US \$ 1.50.

(Report on Data Tagging, compiled by a Panel of Experts at the Energy R & D Data Workshop held at Gaithersburg, Md, May 6-7, 1974).

No 13 (Dec. 74), 8 pp, *The Presentation of Chemical Kinetics Data in the Primary Literature*, US \$ 1.50.

(Report of the CODATA Task Group on Data for Chemical Kinetics).

No 14 (Feb. 1975), 180 pp, *Proceedings of the Fourth International CODATA Conference on the Generation, Compilation, Evaluation and Dissemination of Data for Science and Technology* (Tsakhcadzor, U.S.S.R., June 1974), US \$ 17.00.

No 15 (March 1975), 32 pp, *Man-Machine Communication in Scientific Data Handling*, US \$ 5.00.

(Proceedings of the Symposium sponsored by the CODATA Task Group on Computer Use, Freiburg im Breisgau, F.R.G., July 1973).

No 16 (October 1975), 32 pp, *Study on the Problems of Accessibility and Dissemination of Data for Science and Technology*

(Report of the CODATA Task Group on Accessibility and Dissemination of Data), US \$ 5.00.

No 17 (Jan. 1976), 12 pp, *Key Values for Thermodynamics, 1975*, US \$ 5.00.

(Report of the CODATA Task Group on Key Values for Thermodynamics).

No 18 (April 1976), 44 pp, *Abstracts - Fifth International CODATA Conference*, US \$ 5.00.

No 19 (June 1976), 22 pp, *Flagging and Tagging Data*, US \$ 5.00.

(Report of the ICSU AB/CODATA Joint Working Group).

No 20 (Sept. 1976), 16 pp, *Recommendations for Measurement and Presentation of Biochemical Equilibrium Data*, US \$ 5.00.

(Report of the ICSU Interunion Commission on Biothermodynamics).

No 21 (Oct. 1976), 122 pp, *Proceedings of the Plenary Sessions Fifth International*

CODATA Conference, US \$ 10.00.

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