



NEWSLETTER

MAY 1970

PRELIMINARY PROGRAMME SECOND INTERNATIONAL CODATA CONFERENCE

on
Generation, Collection, Evaluation and Dissemination of Numerical Data
for Science and Technology

St. Andrews, Scotland, 7 — 11 September, 1970

Conference Chairman: SIR GORDON SUTHERLAND

MONDAY, 7 September, 1970

Morning:

Chairman: SIR GORDON SUTHERLAND, Chairman of the
British National Data Committee

1. Chairman's Opening Remarks
2. The Progress of CODATA
3. Data Compilation and Evaluation Worldwide — An Analysis of the CODATA International Compendium of Numerical Data Projects
4. CODATA and the UNISIST Project (Joint ICSU-UNESCO Study on the Feasibility of a World Science Information System)
5. Recognition of Scientific and Technical Data as a National Resource and as a Currency for International Exchange

Evening:

1. Evaluation of Fundamental Constants
2. The Improvement of Presentation of Data in the Primary Literature

F. D. ROSSINI, President of CODATA, University of Notre Dame, Notre Dame, Ind., U.S.A.

M. LEWIS and C. SCHÄFER, CODATA Central Office, Frankfurt/Main, Germany — BRD

SCOTT ADAMS, ISCU Special Assistant for UNISIST, National Academy of Sciences, Washington, D.C., U.S.A.

T. S. AUSTIN, U.S. National Oceanographic Data Center, Washington, D.C., U.S.A.

E. R. COHEN, North American Rockwell Corp., Thousand Oaks, Calif., U.S.A.

Open Discussion for all Conferees.
Moderator: L. M. BRANSCOMB, National Bureau of Standards, Washington, D.C., U.S.A.

TUESDAY, 8 September, 1970

Morning:

1. Some Aspects of Computerized Type-setting of Importance to Data Centres
2. Visual and Other Non-printed Output Useful to Data Centres
3. Development of Scientific Information Centres for Nuclear Data
4. Title to be announced

Evening:

Several Computer Demonstrations

WEDNESDAY, 9 September, 1970

Morning:

1. Basic Principles to be Observed in Preparing Evaluated Data for Use in Industry
2. Results of a Feasibility Study for a National Materials Data Bank of the Federal Republic of Germany
3. Selected Thermodynamic Data on Organic Substances for the Petroleum and Chemical Industries in the U.S.A.
4. Some Aspects of Data in a Large Industrial Organization

Evening:

1. Problems of Compilation and Evaluation of Property Data of Substances and Materials
2. Aspects of Critical Evaluation of Nuclear Data Information
3. Data Compilation Activities in Japan — Infrared Chromatography, Gas Chromatography, Polarography, Molecular Weights of Polymers, Nuclear Data

THURSDAY, 10 September, 1970

Morning:

1. International Network for Generating, Collecting and Evaluating Thermodynamic Data, illustrated by the IUPAC Thermodynamic Tables Project
2. Panel Discussion on Transport Properties Data

Afternoon:

1. Are There Critically Evaluated Data in Geology?
2. Critically Evaluated Data in Biology
3. Problems of Indexing and Classification of Physical Properties
4. Discussion of the Programme of the Third International CODATA Conference

Evening:

Social Events

NOTE:

No Second Notice for the Conference will be distributed. Due to the great demand after the First Notice, the attendance limit was raised by the CODATA Bureau from 100 to 150, with preferred attendance of 130. Since the number of applicants already accepted is approaching this optimum figure, further applications will be considered only in exceptional cases.

C. J. DUNCAN, Computer Typesetting Research Project, The University, Newcastle, U.K.

Olga KENNARD, University Chemical Laboratory, Cambridge, U.K., and R. N. JONES, Division of Chemistry, National Research Council of Canada, Ottawa, Canada

I.P. SELINOV, Academy of Sciences of the U.S.S.R., Moscow, U.S.S.R.

Laboratoire de Thermodynamique et Physicochimie Métallurgiques (C.N.R.S.), Grenoble, France. Speaker to be announced

A. J. BARRETT, Engineering Sciences Data Unit, The Royal Aeronautical Society, London, U.K.

W. OBERENDER, Battelle Institute, Frankfurt/Main, Germany — BRD

B. ZWOLINSKI, Thermodynamics Research Center, Texas A & M University, College Station, Texas, U.S.A.

R. W. MCINTYRE, Rolls Royce, Ltd., Bristol, U.K.

T. V. GOLASHVILI, CODATA Central Office, Frankfurt/Main, Germany — BRD

J. J. SCHMIDT, International Atomic Energy Agency, Vienna, Austria

Y. MASHIKO, Japanese Government Chemical Industrial Research Institute, Tokyo, Japan

S. ANGUS, IUPAC Thermodynamic Tables Project Centre Imperial College, London, U.K.

Chairman: Y. S. TOULOUKIAN, Thermophysical Properties Research Center, Purdue University, West Lafayette, Ind. U.S.A.

A. HUBAUX, EURATOM, Ispra, Italy

R. ZWEMER, Federation of American Societies for Experimental Biology, Bethesda, Md., U.S.A.

C. SCHÄFER, CODATA Central Office, Frankfurt/Main, Germany — BRD

All Conferees

CODATA NATIONAL MEMBERSHIP

1. CANADA

Symposium on Computer Based Techniques for Storing and Retrieving Numerical Scientific Data

In association with the U.S. National Committee for CODATA and the CODATA Task Group on Computer Use, the Canadian National Committee for CODATA organized a one-day symposium on "Computer Based Techniques for Storing and Retrieving Numerical Scientific Data", which was held at the Sussex Drive Laboratories of the National Research Council of Canada (NRC), Ottawa, Canada, on 30 April, 1970. The Symposium was attended by around 100 scientists and computer experts from Canada, U.K., and U.S.A., and was chaired by Dr. R. Norman Jones, Division of Chemistry, NRC, who is the present Canadian National Member on CODATA.

Papers were presented by J. Hilsenrath, Office of Standard Reference Data, National Bureau of Standards, U.S.A., on "Status of teleprocessing as it relates to the interchange of numerical scientific data", by G. G. Johnson, Jr., Materials Research Laboratory, Pennsylvania State University, U.S.A., on "The computer identification of X-ray diffraction powder patterns", and by D. S. Erley, The Dow Chemical Company, Midland, Mich., U.S.A., on "The computer identification of infrared spectra".

Computer techniques for the generation, evaluation, processing, storage, and retrieval of numerical and graphical data were demonstrated as follows: FIRST-1 Program for the identification of infrared spectra (D.S. Erley); SCHINT Program for the identification of X-ray powder diffraction patterns (G.G. Johnson, Jr., and W.F. McClune, Joint Committee on Powder Diffraction Standards, Philadelphia, Pa., U.S.A.); segmented polynomial fitting of thermocouple tables — an example of data reduction (G.G. Kirby); on-line plotting of spectral data using a time-shared system (A. Savitzky, Perkin-Elmer Corp., Norwalk, Conn., U.S.A., and E.B. Wern, Time Share Peripherals Co., Wilton, Conn., U.S.A.); storage and retrieval of chemical structures and complex mathematical formulas; high speed printing techniques using Teletype 37 and Inktronic terminals; and other demonstrations of time-shared programs from the U.S. National Bureau of Standards (J. Hilsenrath, and C. Bates, G. Foye, L. Jagielo, and H. Weir, Teletype Corporation, Washington, D.C., and Skokie, Ill., U.S.A.); communication with a remote computer by Touchtone Telephone with direct voice response (D.S. Erley, and H.H. Mansch); demonstration of high speed alphanumeric and graphic printing using the Applicon electrolytic technique (R. Freeman, I. Moxham, and C. Patterson, Applicon Computer Systems, Ltd., Ottawa, Ontario, Canada); digital data recording of infrared spectra (R.N. Jones, M.A. MacKenzie, and A. Nadeau); and automatic measurement of single crystal X-ray intensity data (A.W. Hanson, Biochemistry Laboratories, NRC).

The Symposium dinner was followed by a talk by W.C. Brown, Division of Radio and Electrical Engineering, NRC, on "Integrating Information Systems by Computer".

The Secretary for International Relations of the NRC, and Ex officio Member of the Canadian National Committee for CODATA is now Dr. R. Martineau, who replaces Dr. J.D. Babbitt. Address: Secretary for International Relations, National Research Council of Canada, Sussex Drive, Ottawa 7, Canada.

2. GERMANY — BRD

On the initiative of the German National Committee for CODATA (Chairman: Prof. W. Klemm), a meeting was held at the Institut für Dokumentationswesen (IDW), Frankfurt/Main, Germany-BRD, on 24 April, 1970, in order to discuss feasibility and methods for the establishment of a logical and comprehensive classification of physical properties of substances

and materials. The primary aims of such a classification scheme are to provide a basis for the indexing of data tables, e.g., "Landolt-Börnstein", and for the development of a common format and arrangement for computer based information services, e.g., "Physikalische Berichte", and data banks.

Participants in the meeting included R. Abbel, IDW, H. Bauer, Zentralstelle für maschinelle Dokumentation (ZMD), Frankfurt/Main, E. Bretnütz, Physikalische Berichte, Braunschweig, G. Brühl, ZMD, A. M. and K.-H. Hellwege, Editors, Landolt-Börnstein, Institut für Technische Physik der Technischen Universität, Darmstadt, H. Kaiser, Institut für Spektrochemie, Dortmund, W. Klemm, Anorganisch-Chemisches Institut, Universität, Münster, M. Lewis, CODATA, W. Lippert, Gmelin-Institut, Frankfurt/Main, G. Loose, DECHEMA, Frankfurt/Main, W. Marthiensen, Physikalisches Institut, Universität, Frankfurt/Main, C. Schäfer, CODATA, K. Schneider, Director, ZMD, and W. Schramm, Internationale Dokumentationsgesellschaft für Chemie (IDC), Frankfurt/Main.

The value and application of the classification scheme to each of the interested organizations was discussed in detail, and it was decided that in view of its potential usefulness the scheme should be developed. It was further agreed that this work should be done over a period of two years by a qualified physicist, in conjunction with the Landolt-Börnstein organization, and financed by the IDW.

3. POLAND

The Presidium of the Polish Academy of Sciences has now established the Polish National Committee for CODATA with the following membership:

Chairman: Prof. M. Nalecz, Corresponding Member of the Polish Academy of Sciences.

Secretary: Dr. T. Plebanski

Members: Prof. A. Bylicki

Dr. W. Klimecki

Prof. B. Paszkowski, Corresponding Member of the Polish Academy of Sciences

Prof. M. Suffczynski

Mr. H. Sztraj, Representative of the Governmental Committee on Science and Technology

Mr. H. Trebert

Dr. W. Zielenkiewicz

Correspondence should be addressed to: The Secretary, Polish National Committee on Data for Science and Technology, ul. Elektoralna 2, P. O. Box 10, Warsaw 1, Poland.

4. U. S. A.

The February 1970 membership of the U.S. National Committee for CODATA is as follows:

Chairman: Prof. F.D. Rossini,
Vice President for Research,
University of Notre Dame,
Notre Dame, Ind. 46556

Members: Prof. Robert B. Brode,
Department of Physics,
University of California,
Berkeley, Calif. 94720

Dr. Sydney P. Clark, Jr.,
Department of Geology,
Yale University,
New Haven, Conn. 06520

Dr. John W. Coltman, Director,
Mathematics and Radiation Research Laboratories,
Westinghouse Electric Corp.,
Pittsburgh, Penna. 15235

Dr. George E. Holbrook, Vice President,
E.I. duPont de Nemours and Co. Inc.,
Wilmington, Del. 19898

Prof. William Klemperer,
Department of Chemistry,
Harvard University,
Cambridge, Mass. 02138

Ex officio: Dr. Lewis M. Branscomb, Director,
National Bureau of Standards,
Washington, D.C. 20234

Prof. Harrison Brown, Foreign Secretary,
National Academy of Sciences,
2101 Constitution Avenue, N.W.,
Washington, D.C. 20418

5. U. S. S. R.

The Soviet National Committee for CODATA, Academy of Sciences of the U.S.S.R., Leninskiy Prospekt 14, Moscow, B-71, U.S.S.R., has recently been reorganized and expanded, and now has the following membership:

Bureau:

Chairman: Academician M. A. Styrikovich
Vice Chairman: Prof. L. V. Gurvich
Scientific Secretary: Dr. A. M. Belova
Members: Dr. B. V. Alexeyev
Corresponding Member
of the Academy, G. B. Bokiy
Prof. I. P. Selinov
Dr. V. I. Vedeneyev

Members:

Dr. V. T. Alexanyan	Prof. Ya. A. Kraftmakher
Prof. E. T. Denisov	Prof. V. A. Kusnezov
Prof. Ya. G. Dorfman	Prof. B. A. Mamyrin
Prof. L. P. Filippov	Dr. V. A. Medvedev
Corresponding Member of the Academy, Ya. I. Gerasimov	Prof. B. N. Oleynik
Academician V. P. Glushko	Dr. V. I. Pórov
Dr. T. V. Golashvili	Mr. G. A. Potemkin
Dr. S. V. Gorbatshevich	Dr. A. D. Povzner
Prof. N. I. Ionov	Prof. E. E. Shpilrain
Prof. B. M. Isayev	Dr. A. M. Sirota
Academician V. N. Kondratiev	Dr. V. V. Sytchev
	Prof. V. M. Tatevskiy

The Soviet National Committee prepared and arranged the First National Conference on Methods for the Estimation of the Reliability of Data in Science and Technology (4—6 February, 1969, in Moscow). More than 120 scientists, representing a wide circle of the institutes and laboratories of the Academy of Sciences of the U.S.S.R., of the Academies of Sciences of the Union Republics, of the Ministries, and of the governing bodies, participated in the Conference. Twenty-one scientific reports on methods of critical evaluation of numerical data were presented, seven of which were concerned with thermodynamic and thermophysical properties, five with nuclear properties, two with chemical kinetics, and one with fundamental constants. Three reports of a mathematical nature dealt with statistical methods of reducing excess information, and with problems of planning experiments with minimum experimental scatter.

A resolution taken at the Conference states: "The most effective way to solve the problem of reliable reference data in science and technology is to establish international reference tables of physical constants and of numerical data on properties of substances and chemical reactions. International co-operation in this field promises significant savings in finance, man-power and resources, and is a task of primary importance". The Conference authorized the Soviet National Committee to "promote through CODATA and other scientific organizations, international scientific co-operation in the generation, critical evaluation and distribution of numerical data". The Second National Conference on Methods for the Critical Evaluation of Numerical Data for Science and Technology is to be held in 1971.

The Soviet National Committee put forward a number of suggestions on the development of the State Service for Standards and Reference Data (GSSSD). These suggestions are based upon the belief that the scientific problems and means of classifying numerical data of properties of pure substances and chemical reactions have little in common with the task of classifying data of properties of industrial products and materials. Accordingly, the Committee recommended that the latter problem should be excluded from the tasks of GSSSD. The above suggestions are at present under consideration.

Four Soviet scientists have been recommended by the National Committee for membership on the CODATA Task Groups on Fundamental Constants and on Computer Use. The Committee has also continued to translate and distribute official and semi-official CODATA information. In particular, translation of the discussion at the First International CODATA Conference at Arnoldshain has served to increase the interest of the Soviet scientific community in the objectives and tasks of CODATA. Further, the Committee has been developing direct exchange of literature (tables, handbooks) free of charge with the National Committees of the other member countries of CODATA. Such an agreement has now been reached with the U.S. National Committee for CODATA.

The Soviet National Committee assigns great importance to the inclusion of points corresponding to the objectives of CODATA, into existing and planned intergovernmental agreements on scientific and technical co-operation between member countries of CODATA; the Committee is at present preparing a number of proposals on this matter.

Soviet Working Groups on Data for Chemical Kinetics

Within the Commission on Constants (Chairman: Academician V.N. Kondratiev) of the Kinetics Section, Scientific Council on Chemical Kinetics, Academy of Sciences of the U.S.S.R. the following eleven Working Groups have recently been established:

1. Exchange, combination, and disintegration reactions of simple molecules (Chairman: A.I. Porojkova)
2. Monomolecular reactions (V.I. Vedeneyev)
3. Reactions of radioactively contaminated particles (G. Karachevtsev)
4. Homolytic liquid-phase reactions (E.T. Denisov)
5. Heterolytic reactions (M.I. Vinnik)
6. Topochemical reactions (O.V. Krylov)
7. Reactions of solid inorganic compounds (Chairman to be appointed)
8. Reactions of solid organic compounds (Ya. S. Lebedev)
9. Polymerization reactions (A.A. Berlin)
10. Energy exchange processes (A.M. Tchajikin)
11. Theoretical group (E.E. Nikitin)

In addition to their task of co-ordinating research work in the field of quantitative chemical kinetics, the Working Groups have been assigned the responsibility for the compilation and critical evaluation of reaction rate data.

The work of the Commission on Constants and its Working Groups is intended to be carried out in co-ordination with that of the CODATA Task Group on Data for Chemical Kinetics, which was established in 1969 on the initiative of Academician V.N. Kondratiev.

CODATA UNION MEMBERSHIP

INTERNATIONAL UNION OF GEOLOGICAL SCIENCES (IUGS)

The new IUGS Member on CODATA is Dr. A. Hubaux, European Scientific Information Processing Centre (CETIS), Euratom, 21020 Ispra (Varese), Italy, who replaces Prof. M. Roubault. Dr. Hubaux is an active member of the IUGS Committee on Storage, Automatic Processing and Retrieval of Geological Data, COGEOGDATA (Chairman: Dr. S. C. Robinson, Geological Survey, 601 Booth Street, Ottawa 4, Canada; Secretary: Prof. A. A. Beus, Vavilova 49, KV 44, Moscow V-333, U.S.S.R.), and is Chairman of its Working Group on Reference Numbering and Coding.

In addition to the above Committee, the IUGS Subcommittee on Geochronology (Chairman: Dr. R. E. Folinsbee, University of Alberta, Edmonton, Alberta, Canada; Secretary: Prof. R. A. Burwash, Dept. of Geology, University of Alberta, Edmonton 7, Alberta, Canada), which co-ordinates absolute age determinations, and the Commission for the Geological Map of the World (Chairman: Mr. J. Marçais, 12, Rue de Bourgogne, Paris 7e, France; Secretary: Miss F. Delany, same address), which compiles regional geological data, operate within the sphere of interest of CODATA.

Among the 13 associations affiliated to IUGS, the following are of special interest to CODATA: International Mineralogical Association (Chairman: Prof. C. E. Tilley, Department of Mineralogy and Petrology, Cambridge University, U.K.; Secretary: Prof. A. Preisinger, Mineralogisches Institut, Universität, A-1010, Vienna, Austria), with its Commissions on Mineral Data (Chairman: Prof. H. Strunz, Institut für Mineralogie, Technische Universität, Berlin 12, Germany; Secretary: Dr. J. R. Butler, Mineralogy Society, 41 Queens' Gate, South Kensington, London, U.K.) and on New Minerals and Mineral Names (Chairman: Dr. M. Fleischer, U.S. Department of the Interior, Geological Survey, Washington, D.C., U.S.A.; Secretary: Prof. C. Guillemin, Bureau de Recherches Géologiques, Géophysiques et Minières, 74, Rue de la Fédération, Paris 15e, France), and the International Association for Mathematical Geology (Chairman: Prof. A. B. Vistelius, Laboratory of Mathematical Geology, Mathematical Institute of the Academy of Sciences of the U.S.S.R., Leningrad, U.S.S.R.; Secretary: Prof. R. A. Reymont, Paleontological Institute, Department of Historical Geology and Paleontology, Box 558, 751 22 Uppsala 1, Sweden).

CODATA LIAISON REPRESENTATIVES

1. ICSU ABSTRACTING BOARD (ICSU AB)

The 1969 issues of two annual publications detailing the activities of the ICSU Scientific Unions and their Committees and Commissions will shortly be issued by the ICSU AB Secretariat, 17, rue Mirabeau, Paris 16e, France. The title *Tentative List of Publications of ICSU Scientific Unions, Special and Scientific Committees and Commissions of ICSU, Year 1969, and Corrections and Additions to the 1968 List* is self-explanatory. The second and larger publication (ca. 350 pages

in two volumes), entitled *Survey of the Activities of the ICSU Scientific Unions, Special and Scientific Committees and Commissions of ICSU in the Field of Scientific Information during the Year 1969*, presents information under the following headings: Name of Union, Commission, Committee, or Working Group; President/Chairman (name and address); Secretary (name and address); Members (names and countries); Date of Creation; Periodicity of Meetings; and Publication of Minutes of Meetings. A general description is given of the activities of each body, together with a summary of 1969 activities and a listing of 1969 publications. Particular attention is given to those bodies dealing with the following topics: notations, symbols, units, nomenclature, terminology, standards, bibliographies, abstracts, review articles, classification, and publication of data.

The purpose of the ICSU AB surveys is to make the activities of ICSU bodies in the field of scientific information more widely known in the scientific community, and to strengthen co-operation between those bodies working in similar fields.

2. INTERNATIONAL ATOMIC ENERGY AGENCY (IAEA)

Recent issues in the IAEA Technical Reports Series are of interest. The report STI/DOC/10/100 (US \$ 2.00), entitled "An International Neutron Data System", presents the findings of a Panel on Neutron Data Compilation organized by the IAEA upon a recommendation by the International Nuclear Data Committee (INDC) and held in Brookhaven, U.S.A., from 10–14 February, 1969. Current and future needs for nuclear data compilation are reviewed, together with the capability of the world's four principal neutron data centres (National Neutron Cross Section Center, Brookhaven, U.S.A., Information Centre on Nuclear Data, Obninsk, U.S.S.R., European Nuclear Energy Agency Neutron Data Compilation Centre, Saclay, France, and IAEA Nuclear Data Section, Vienna, Austria) to meet the requirements of experimental and theoretical neutron physicists, evaluators, reactor physicists, and other existing and potential users.

The Panel discussions were based upon 14 papers, now published as IAEA-111 "Neutron Data Compilation" (Available on microfiche, US \$ 0.65), which were submitted to the Panel by the neutron data centres, by experimenters as data centre users, and by evaluators as data centre users*.

IAEA publications may be ordered from booksellers, IAEA sales agents, or from:

Publishing Section,
International Atomic Energy Agency,
Kärntner Ring 11,
P.O. Box 590,
A-1011 Vienna, Austria

3. UNITED NATIONS EDUCATIONAL, SCIENTIFIC AND CULTURAL ORGANIZATION (UNESCO)

The most recent volume in the UNESCO series "Documentation and Terminology of Science" is now available under the title *World Guide to Technical Information and Documentation Services — Guide Mondial des Centres de Documentation et d'Information Techniques* (1969, 287 pages).

* For a comprehensive survey from the evaluator's viewpoint of the work of the Panel, the INDC and the IAEA, within the context of world-wide co-operation and co-ordination of neutron data compilation and evaluation, see J. J. Schmidt, "Neutron Nuclear Data Compilation and Evaluation — Past, Present and Future", page 3, CODATA Newsletter 3, December 1969.

The Guide lists selected centres (273) offering technical information and documentation services in 73 countries and territories. As in its companion volume *World Guide to Science Information and Documentation Services* published in 1965, only the principal centres, particularly those in developed countries, have been included, except in the case of countries where technical documentation is a comparatively recent activity, and relevant information is not available elsewhere. Readers requiring a complete list are referred to the international, national, and regional directories listed in the Guide.

The bilingual Guide (English-French) is arranged according to countries in alphabetical order, with a separate section listing selected international technical documentation centres. For each centre, the following information is given: name and address; history; staff; subject coverage; services, i.e., library, abstracting, bibliographies and literature searches, translations, and document reproduction; publications; and means of payment for services and publications. An alphabetical list of centres and a subject index are also provided.

UNESCO publications may be ordered from booksellers or from UNESCO national distributors throughout the world. Further information from: UNESCO, Distribution Division, Place de Fontenoy, 75-Paris 7e, France.

4. WORLD METEOROLOGICAL ORGANIZATION (WMO)

The World Meteorological Organization has recently issued World Weather Watch (WWW) Planning Report No. 28, entitled "Collection, Storage and Retrieval of Meteorological Data". Copies available from: WMO Secretariat, Case postale No. 1, CH-1211 Geneva 20, Switzerland.

The Report reviews the problems to be solved in the collection, storage and retrieval of meteorological data, and the work already done in this field by WMO and other interested organizations. The types of data which should be stored permanently, and specifically the data to be stored at the World (WMC), Regional (RMC), and National Meteorological Centres (NMC), are designated. Principles and methods for the collection (global telecommunication system), quality control (computerized checking), storage (computer, micro-film), retrieval (classification and catalogue systems), and distribution (magnetic tapes, print-out) of meteorological data are discussed. Specific proposals are made on the essential features of a world-wide system for the collection, storage and retrieval of data for meteorological research and other purposes. It is suggested that this system be introduced in two stages, the "interim system" to be implemented immediately and to be in operation by 1971, and the "ultimate system", representing the long-term goal. The Report concludes with suggestions for further studies by WMO.

The proposals in World Weather Watch Planning Report No. 28 were considered by the WMO Executive Committee at its twenty-first session in June, 1969. The Executive Committee decided to establish a Panel on Collection, Storage and Retrieval of Data for Research, to act as a focal point for all WMO activities in this field, and to consider the long-range goals of WMO with respect to the collection, storage and retrieval for research purposes of meteorological data and of data in those physical environmental sciences which are closely related to meteorology. Experts from several member countries of WMO, as well as from the Food and Agriculture Organization of the United Nations (FAO), the Intergovernmental Oceanographic Commission (IOC), ICSU and UNESCO have been invited to participate in the deliberations of the Panel, which held its first session in Geneva from 14-17 April, 1970.

Immediately preceding the first Panel session, an informal planning meeting of experts was convened (8-13 April, 1970) to plan the implementation of the interim system. Topics including collection and quality control, storage media, formatting for storage and retrieval, and classification for a world data catalogue of digital data were reviewed. The planning meeting, in which many of the experts from the Executive Committee Panel participated, was expected to provide valuable recommendations for consideration by the Panel.

CODATA TASK GROUPS

TASK GROUP ON COMPUTER USE

After serving as Chairman of the Task Group on Computer Use since its formation in 1967, Dr. Franz L. Alt, Deputy Director, Information Division, American Institute of Physics, New York, U.S.A., has been succeeded in this capacity by Prof. Gordon Black, Department of Computation, University of Manchester Institute of Science and Technology, Manchester, U.K., but now remains as a member of the Task Group. After the retirement of Mr. J. d'Olier, a new French member, Mr. M. H. Carru, National Centre for Telecommunications Research, Issy-les-Moulineaux, has been appointed to the Task Group.

The complete membership of the Task Group on Computer Use is now as follows:

Chairman: Prof. Gordon Black,
Department of Computation,
University of Manchester Institute of Science and Technology,
Sackville St.,
Manchester M60 1QD, U.K.

Secretary: Dr. R. Norman Jones,
Division of Pure Chemistry,
National Research Council of Canada,
Sussex Drive,
Ottawa 7, CANADA

Members: Dr. B. V. Alexeyev,
Computing Centre,
Academy of Sciences of the U.S.S.R.,
Moscow, U.S.S.R.

Dr. Franz L. Alt,
Deputy Director, Information Division,
American Institute of Physics,
New York, U.S.A.

Mr. M. H. Carru,
National Centre for Telecommunications Research,
Issy-les-Moulineaux, FRANCE

Dr. Olga Kennard,
University Chemical Laboratory,
Cambridge, U.K.

Dr. M. Kisawa,
Electrotechnical Laboratory,
Chiyodo-Ku, Tokyo, JAPAN

Dr. G. Ostertag,
Friedrich Uhde GmbH,
Bad Soden/Taunus, GERMANY-BRD

Mr. F. Schulte-Tigges,
Deutsches Rechenzentrum,
Darmstadt, GERMANY-BRD

Dr. R. L. Wigington,
Chemical Abstracts Service,
Columbus, Ohio, U.S.A.

Ex officio: Dr. Christoph Schäfer,
CODATA Central Office

Note: At the 9th CODATA Bureau Meeting held in Frankfurt/Main, Germany-BRD, on 16 and 17 March, 1970, it was agreed that the Executive Director of CODATA Central Office will be an Ex officio Member of all CODATA Task Groups, and that the President of CODATA has the right but not the duty to attend the meetings of all CODATA Task Groups.

ADVISORY COMMITTEES ON NUMERICAL DATA

in the National Academy of Sciences of the U.S.A.

The National Academy of Sciences of the United States has maintained a strong interest in critically evaluated numerical data since the production of the International Critical Tables for Science and Technology in the period 1920—1934. Over the years it has always had in its National Research Council a committee to provide appropriate leadership in numerical data matters in the U.S.A.

For some years before 1955, a Committee on Tables of Constants and Numerical Data discharged the Academy's responsibilities in this area. It provided guidance for the then Nuclear Data Project and the Chemical Kinetics Data Project, and related functions. These efforts were co-ordinated with those of the International Commission on Tables of Constants then supported by the International Union of Pure and Applied Chemistry.

In 1955 the Academy, because of the increasing need for co-ordination and stimulation in compilation matters in the U.S.A., authorized formation of the Office of Critical Tables to be guided by an Executive Committee, and an Advisory Board representing major scientific societies and governmental agencies in the U.S.A. The Office of Critical Tables was established in 1957 and continued its work until 1969, under the direction of Dr. Guy Waddington. When CODATA was formed in 1966, the Executive Committee of this Office took on another function and became the U.S. National Committee for CODATA.

In 1969, because of the growth of the National Standard Reference Data Program (NSRDP) at the National Bureau of Standards, and the emergence of CODATA as an international force, it was decided by the Academy to replace the Office of Critical Tables, with its Executive Committee and large Advisory Board, by a smaller unit.

The new unit has been named the Numerical Data Advisory Board (NDAB) and is supported by a small office staff, with Dr. H. van Olphen as Executive Secretary. Its primary purpose is to provide a focal point in the National Academy of Sciences - National Academy of Engineering - National Research

Council in all matters pertaining to the compilation and evaluation of numerical data for science and technology. Currently, this function is seen as having the following parts:

- 1) To provide advice on request to the Office of Standard Reference Data (OSRD) of the National Bureau of Standards concerning the National Standard Reference Data Program.
- 2) To provide liaison and appropriate co-ordination with data compilation activities located in the non-governmental sector of the U.S. scientific community.
- 3) To provide liaison between the U.S. scientific community and CODATA through the U.S. National Committee for CODATA.
- 4) To promote uniform practices in the use of internationally recommended symbols, units, nomenclature and physical constants in the publication of numerical data.

The advisory services to the Office of Standard Reference Data are provided at several levels. The Numerical Data Advisory Board itself from time to time reviews the status of the National Standard Reference Data Program and policy recommendations are made. Standing panels also meet at intervals to review work of the seven programme areas within the NSRDP framework and to provide advice on priorities. Finally, advice in narrow compilation areas is given by *ad hoc* panels of experts drawn from the country at large. This type of meeting is used particularly when new compilation areas are being considered for support by the OSRD.

The Numerical Data Advisory Board has representation from the following Divisions of the National Academy of Sciences - National Academy of Engineering - National Research Council: Division of Chemistry and Chemical Technology; Division of Earth Sciences; Division of Engineering; and the Division of Physical Sciences. The present membership is the same as that of the U.S. National Committee for CODATA (page 3), with the exception of Prof. Harrison Brown.

QUALITY SCREENING OF INFRARED SPECTRA — AN EXERCISE IN THE EVALUATION OF COMPLEX NUMERICAL DATA*

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INTRODUCTION

CODATA's mandate to code and evaluate the numerical data of science is of monumental scope, and it can be helpful to take an overall view of the project and develop some classifications of data types. Broad distinctions have already been made between two classes of data which we may call "basic" and "adaptive". Here, basic relates to properties of homogeneous materials or simple uniform mixtures; such properties are intrinsic to the gross physical and chemical composition of the materials; they are independent of the past history of the particular sample or of sampling errors. Adaptive properties are influenced by heat treatment, radiation exposure, climatic and geological conditions, or other environmental factors that have modified the particular sample in a permanent or semi-permanent manner. Many properties of industrially important materials, such as alloys and glasses, are in this second category and it is tempting to identify the basic category with the data of fundamental science and the adaptive category with industrial data. This is a trite and misleading distinction, because industry has as much reason for concern about the properties of pure materials as does fundamental science. It is true that

many of the products of industry have adaptive properties, but these must ultimately be related to the properties of the pure chemically defined constituents; this requires that the properties of the primary constituents be fully recorded and documented. The properties of a co-polymerized plastic depend on the conditions of polymerization, and we cannot expect to interpret and quantify the properties of the product without prior knowledge of the basic chemical properties of the constituent monomers on which the kinetics of the polymerization depend. The combustion characteristics of fuels and the viscosities of lubricants provide another example; these are complex functions of the constituent hydrocarbons and other components, and the petroleum industry has invested considerable capital in the generation of basic data on these primary substances.

In respect to this classification CODATA has so far addressed itself almost exclusively to the basic type.

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II. DATA CLASSIFICATION BY NUMERICAL TYPE

In this essay we shall examine another mode of classification which is based on the numerical form of the data; in these terms we can recognize three types:

- (a) Fundamental physical constants and numerically defined properties that do not depend on either the present or past environment of the sample.
- (b) More complex numerically defined properties; this group includes properties that are modified by the environment at the time of measurement or by factors with a strong topological content.
- (c) Complex quasi-numerical data dependent on many variables and commonly stored in graphical form.

Our main concern will be with (c), but there are some points about (a) and (b) that should first be noted.

(a) Fundamental Constants and Unique Numerical Properties

In this category are the fundamental numerical constants of nature and the physical properties of materials that are derived directly from them. Such a datum is represented by a single number in a specified unit system; it is independent of environmental variables such as temperature or pressure. Simple examples are the charge on the electron and the atomic weight of an isotope. The exact measurement of these properties is of crucial importance for science, and, because of this, international machinery has long existed to evaluate and standardize these constants. They account only for a minor part of the totality of scientific numerical data and their bulk storage and access present no technical problems.

(b) More Complex Numerically Defined Properties

This vast field contains all the varieties of physical characteristics of materials that can be conveniently expressed as discrete numbers or topological diagrams. Properties that vary with the temperature, pressure, concentration, and electric and magnetic field strength come under this heading, as also do properties, such as molecular structures, that depend on topological parameters. The evaluation, storage and retrieval of this class of scientific data is one of the major tasks confronting CODATA.

Physical properties dependent on a single variable can be recorded in a simple list. Data depending on two variables can be coded in a two-dimensional printed table, and data dependent on three variables can be recorded in a set of tables. Should the number of defining parameters exceed three, tabulation in a printed form becomes awkward and inefficient. Computer coding and storage are not embarrassed by such physical restrictions, and multi-dimensional storage systems can be generated and accessed without difficulty. Computer-based storage therefore has its major appeal, and greatest economic justification, in dealing with physical properties that are dependent on a large number of external conditions. It is to be anticipated that computer programs generated for the storage and retrieval of multi-variable dependent data will proliferate rapidly, and prompt action to systematize such coding procedures can be especially important. An extreme example is the coding and tabulation of the bond structures of organic compounds. The conventional methods of structure formulation, developed over the years by organic chemists, have acquired a strong topological content in order to represent spacially the multiple interactive dependence of the forces between the constituents atoms. Much effort is currently being expended in reducing such structural data to a linear sequence of coded symbols that can be conveniently stored in a computer and searched for whole or partial structures. Several complementary or competing systems for serially coding chemical structures are now operative and efforts should be made to stabilize such systems as soon as possible.

Bibliographical data storage has an archival character; it is continually accumulating and only rarely is it condensed by the

elimination of redundant material. For numerical data, however, interpolative algorithms can be established. These allow the computation of the numerical values of the system under conditions that need not correspond with previously measured ones; they also permit considerable compression of the data and simplify their transfer through communication networks. Computer programs that generate requested data by means of interpolative algorithms are more efficient than those that search through large banks of stored numerical data — computers do not store the values of logarithms and trigonometric functions, rather they generate the required values on demand from standard series functions. This is a technical area where CODATA could act effectively to promote the standardization of common interpolative formulas and compression programs for storing selected physical data.

(c) Complex Data Conventionally Stored in Graphical Form

Certain types of data that are dependent on a very large number of variables are conveniently stored in graphical form; traditionally this has been done in published atlases, and more recently these have been supplemented by microfilm strips and microfiche. Practically all spectral data fall in this category but it also includes phase diagrams, much geological and biological data and a range of transient data such as hydrograph charts and weather maps. There are several problems associated with the generation, evaluation, storage and access of this type of data. When the data banks are large, the search technique becomes extremely slow unless computer-based pattern recognition methods are introduced, and quality evaluation can be seriously hampered if, as often happens, some of the major variables are not known or known only imperfectly.

The infrared spectra of chemical substances are representative of this class of data. Over the past decade some experience has been accumulated concerning the problems of storage, evaluation and search techniques for infrared spectra and it can prove helpful to review this, since it illustrates some of the general problems involved.

III. THE EVALUATION OF INFRARED SPECTRA

An infrared spectrum of a substance in the liquid or solid state looks like a profile of a mountain pass with some 20–100 irregularly distributed peaks and valleys. The overall pattern of this spectrum provides a “signature” or “finger-print” of the material. With some reservations this spectrum can be accepted as uniquely characterizing the chemical structure.

So far about 100,000 infrared spectral charts have been catalogued. The majority reside in some half-dozen major atlases or collections based in several countries, and there exists one master index that has been programmed for computer search. A number of pattern recognition computer programs have been written to help in the identification of individual chemical substances by comparing their infrared spectra with those in the master file, or in sub-sets of it. The more efficient of the programs can search the files at a rate of about 1000 spectra per second, and some of them are now available commercially on a rental basis.

For the most part the spectra in these collections are not formally “evaluated” data: they separately reflect the judgement skill, and personal reputation of the spectroscopist who has measured each individual curve; they also reflect the continuous progress in the technique of measurement that has occurred over the twenty-year period during which the data have been accumulated.

In 1965, the National Standard Reference Data System of the U.S. National Bureau of Standards, acting in association with the American Society for Testing and Materials, was called upon to select curves suitable for publication from the large pool of infrared spectral data that had become available in the United States. This source material was of very varied quality and the responsibility for establishing a set of specifications to guide the evaluators was vested in the Coblenz Society. The

Society was established in 1950, and is composed of specialists in infrared spectroscopy in North America and elsewhere. In its reports*, the Coblenz Society recognized three categories of evaluated spectral data:

- I Critically Defined Physical Data
- II Research Quality Analytical Spectra
- III Approved Analytical Spectra

The first category took account of the fact that current technology does not permit the measurement of all the variables required to record an infrared spectrum with sufficient accuracy to make it acceptable as a physical constant in the sense of the experimental physicist. Specifications for Category I were outside of terms of reference of the Coblenz Society's mandate. They were, and remain for the present, technically unattainable, but the creation of this high level category serves to place the remaining two categories in their proper perspective in relation to other kinds of numerical scientific data.

The specifications written for Category II pertain principally to new data generated since the publication of the report, and they call for the use of modern commercially available infrared spectrometers in the hands of skilled operators. These specifications represent a quality of data that is frankly a compromise between the idealism of an academic spectroscopist and the economic realities of the industrial research laboratory. Spectra of this quality are not likely to be generated in the course of the ordinary routine operation of an analytical laboratory, but they are within the instrumental capability and competence of most well-equipped spectroscopy laboratories. Several laboratories in North America are at present collaborating in a technical and cost evaluation program to generate data of this quality. The Coblenz Society is also organizing "consulting clinics" to aid in this program. These clinics will be operated at designated scientific meetings. Research groups will be able, by prior appointment, to consult at the clinics with specialists whom the Society will make available for this purpose; instruments to demonstrate the techniques will also be on hand.

The third category of Approved Analytical Spectra comprises a more relaxed set of technical specifications that provide a continuing flow of evaluated spectra into the bulk collections. Experience recently gained by the Coblenz Society, while screening the first 2000 "evaluated" spectra, has shown that rejection from the Approved Analytical Spectra category stems more often from a failure to meet criteria for the verification of the correct chemical structure than from the technical insufficiency of the spectrum itself. Poor quality data is bad, but data of a technically high quality referenced to the wrong chemical structure can be calamitous. These spectra will pass into the data bank as a flagged sub-set, and in course of time such evaluated data may gradually replace the older unevaluated curves.

The evaluation program established by the Coblenz Society had a limited objective and was set up to perform a specific task. During the past year the specifications for Research Quality Analytical Spectra discussed above have formed the basis of a broader international study initiated by Commission I.5 of IUPAC (Molecular Structure and Spectroscopy). The IUPAC Commission has retained most of the technical aspects of the Coblenz Society's specifications unchanged, and prepared for international use a set of "Tentative Specifications for the Measurement and Evaluation of Infrared Spectra for Documentation Purposes"**. These tentative proposals include a recommendation that "To be acceptable for documentation purposes as an evaluated spectrum each curve would need to be approved by a national or international agency designated by

CODATA or by one of its participating International Unions for this purpose". Such an organization is referred to in the specifications as "the evaluating agency" and is assigned discretionary powers in the interpretation of a number of the technical aspects of the evaluation process.

IV. GENERAL IMPLICATIONS

Considered as an experimental case history, this account of a largely *ad hoc* attempt to bring some order into a currently confused, but sharply delineated area of the overall data problem serves to illustrate several points.

First, there is the problem of establishing technical standards so that the accepted data are of an approved quality and warrant the designation "evaluated". Such evaluation requires the establishment of authorized "evaluating agencies" and this will considerably increase the cost of generating evaluated as opposed to unevaluated data. The quality level to be established for acceptable data must also be carefully considered. If maintenance of the highest quality were made the sole basis of the screening process, then the project may easily be priced out of the market. This may be true in the literal financial sense and also more figuratively since there will always exist some inverse ratio between the quality of data generated and its quantity; if the rate of output of evaluated data becomes too slow the pressures to publish unevaluated data will increase and the purpose of evaluation will be defeated. In many areas it will be advantageous to formulate several different levels of quality evaluation each appropriate to a different functional use. It is preferable that these quality criteria be sharply differentiated so that any isolated datum can be clearly categorized. In computers we can store data of varied quality en masse and search the whole data bank at designated quality levels by appropriate instructional coding.

CODATA cannot be expected to undertake the establishment of such quality specifications, each of which calls for its own type of specialized knowledge, but this expertise will generally be found within the membership of the participating Unions. A CODATA Liaison Unit within each Union would provide an appropriate channel of communication between the specialists in a particular discipline and the accumulating experience of the overall problem within CODATA. In the larger Unions this communication might function most effectively at the level of the individual Commissions. Commission I.5 of IUPAC did in fact establish a Sub-Commission (I.5.2.) on The Storage and Retrieval of Spectral Data in 1963, and it is this Sub-Commission that was instrumental in promoting the tentative specifications on infrared spectra discussed above. The chain of communication should also extend from the main body of CODATA to the Task Group on Computer Use, which should be able to tap the expert knowledge of specialists in programming and in visual, graphical and typographical display techniques to help in the selection of storage and retrieval systems most appropriate for each type of data. A panel of mathematicians and numerical analysts should also be available to advise on data compression and interpolation techniques where these might be used effectively to increase the efficiency of the data storage system.

The operation of such an evaluation system will need funding and is probably best performed by national organizations, especially in those countries where the volume of data is large. It needs to be emphasized that in the smaller countries individual workers are liable to encounter great difficulties in obtaining financial support for the publication of numerical data. To circumvent this, it is sometimes deemed propitious to incorporate such data into a review type article, in which case the publication of the paper is justified in terms of the interpretive analysis of the data rather than on their intrinsic merit. The fact that an individual worker could demonstrate that his data meet specifications set by CODATA should strengthen his case for financial support to publish the data on their own merit by establishing that they achieve an objectively defined quality standard.

* *Anal. Chem.* 38 (1966), 27A; *Coblenz Soc. News Letter* No. 41 (1969)

** *IUPAC Information Bulletin* No. 34 (1969), 23—30

CONFERENCES

INTERNATIONAL

An **INTERNATIONAL CONFERENCE ON PRECISION MEASUREMENT AND FUNDAMENTAL CONSTANTS**, organized by the U.S. National Bureau of Standards (NBS), is to be held at the NBS headquarters, Gaithersburg, Maryland, U.S.A., from 3—7 August, 1970. Sponsors of the Conference include the Committee on Data for Science and Technology, the International Union of Pure and Applied Physics, the International Committee of Weights and Measures, the International Bureau of Weights and Measures, the Committee on Fundamental Constants of the U.S. National Academy of Sciences - National Research Council, and NBS.

The aim of the Conference is to discuss modern techniques and current theoretical developments of precision measurement, which provide a basis for future adjustments in the values of the fundamental constants. Among the topics to be covered are research developments in the precise measurement of the established basic standards, particularly length, time, and electrical standards. The fundamental constants, for example, the velocity of light in vacuum, the Rydberg constant, the proton moment, and the gravitational constant, will also be included, in addition to associated experimental and theoretical problems.

Prof. F. D. Rossini, President of CODATA, and Dr. E. Richard Cohen, Chairman of the CODATA Task Group on Fundamental Constants; who are also members of the Conference Executive Committee, will represent CODATA at the Conference.

Proceedings of the Conference will be published by NBS, with papers presented in English, French, or German. For further information contact: Dr. Ernest Ambler, Room A 363, Building 221, National Bureau of Standards, Washington, D.C. 20234, U.S.A.

The International Atomic Energy Agency (IAEA) is sponsoring the **SECOND INTERNATIONAL CONFERENCE ON NUCLEAR DATA FOR REACTORS** to be held at the Technical University of Helsinki, Otaniemi, Helsinki, Finland, from 15—19 June, 1970. The aim of the Conference is to bring together physicists who are specialists in nuclear data, especially those which involve neutrons, and scientists concerned with the use of such data, particularly for reactors.

Provisional programme topics and speakers include: General Status of Nuclear Data Requirements (Invited papers: J. J. Schmidt, IAEA, Vienna, Austria, "General status of nuclear data requirements"; P. Greebler, B. A. Hutchins, C. L. Cowan, General Electric Co., Sunnyvale, California, U.S.A., "Implications of nuclear data uncertainties to reactor design and operation"; D. D. Clayton, Rice University, Houston, Texas, U.S.A., "Importance and needs for neutron nuclear data to astrophysics"; Special papers: Yu. F. Chernilin, I. V. Kurchatov Institute of Atomic Energy, Moscow, U.S.S.R., "Nuclear data requirements for controlled thermonuclear devices"; J. Lynn, AERE Harwell, Didcot, Berkshire, U.K., "Progress in understanding neutron interactions with nuclei"; Cross Sections and Techniques for High Precision Neutron Nuclear Data Measurements (Invited paper: A. J. Deruytter, Euratom, Geel, Belgium, "Status of experiment and evaluation for high precision neutron nuclear data measurements"); Nuclear Data in the Thermal and Resonance Energy Regions: $A > 220$ (Invited paper: G. D. James, AERE Harwell, Didcot, Berkshire, U.K., "Cross sections of the heavy nuclei in the resonance region"), and $A < 220$ (Invited paper: J. S. Story, Fast Reactor Physics Division, Winfrith, Dorset, U.K., "Evaluation"); Nuclear Data Above the Resonance Energy Regions: $A > 220$ (Invited papers: W. P. Poenitz, Argonne National Laboratory, Illinois, U.S.A., "Recent experimental data of heavy nuclei"; W. G. Davey, Argonne National Laboratory, "Status of important heavy element nuclear data above the resonance region"), and $A < 220$ (Invited paper: V. Benzi, CNEN, Centro di Calcolo,

Bologna, Italy, "Evaluation"); Relationships of Microscopic and Integral Data; Evaluation Problems and Methods (Special paper: S. Pearlstein, NNCSC, Brookhaven, Upton, New York, U.S.A., "Progress in international nuclear data compilation and exchange — a report of the four neutron data centres and Summary Panel).

The Scientific Secretaries of the Conference are Mr. Konsi and Dr. Hjärne, Division of Research and Laboratories, IAEA; the Administrative Secretary is Mr. H. Storhaug, Division Scientific and Technical Information, IAEA.

The Proceedings of the Conference will be published by IAEA; those of the First International Conference on Nuclear Data for Reactors, Paris, October 1966, are available in two volumes at a price of U.S. \$ 12.00 — £ 4.4.8. (Volume I) and U.S. \$ 9.00 — £ 3.3.6. (Volume II).

A recent IAEA meeting also of interest is the **SYMPOSIUM ON THE HANDLING OF NUCLEAR SCIENCE INFORMATION**, which was held in Vienna from 16—20 February 1970, and attended by more than 160 delegates from 31 countries and 11 international organizations. Among the papers presented at the Symposium, that by A. Spemol, Central Bureau for Nuclear Measurements, Euratom, Geel, Belgium, entitled "Comments on the Evaluation of Nuclear Data, a Determination of the Values and their Accuracy" is of particular interest. The Proceedings of the Symposium are scheduled for publication in June, 1970, at a price of approximately U.S. \$ 16.

Orders and enquiries regarding Proceedings of IAEA meetings should be forwarded to: Publishing Section, International Atomic Energy Agency, P.O. Box 590, Kärntner Ring 1 A-1011 Vienna, Austria, or to the IAEA national sales agent and booksellers.

Colloquium No. 9 of the International Astronomical Union (IAU), entitled "**THE IAU SYSTEM OF ASTRONOMICAL CONSTANTS**", will be held in Heidelberg, Germany-BRD from 12—15 August, 1970.

The primary purpose of the Colloquium is to provide a basis for subsequent formal proposal by IAU Commission 4 (Ephemerides) for the adoption or otherwise of new values of the astronomical constants that were left unchanged when the IAU system was adopted in 1964. The principal constants concerned are the precessional constants and the planetary masses.

Participation in the Colloquium is by invitation only, but written contributions are welcome. A report on the proceedings of the Colloquium will be published. Information on purpose, programme, participation, preprints, and proceedings from Dr. G. A. Wilkins, H. M. Nautical Almanac Office, Royal Greenwich Observatory, Herstmonceux Castle, Hailsham, Sussex, England; on local arrangements from: Prof. W. Frick, IAU Colloquium No. 9, Astronomisches Rechen-Institut, Mönchhofstrasse 12—14, 6900 Heidelberg 1, Germany-BRD.

IMEKO V, the Fifth Congress of the International Measurement Confederation (IMEKO), will be held from 25—30 May 1970, at the Versailles Congress Palace, Versailles, France. Both the Congress and the Fourth International MESUCOR Exhibition which follows are being organized by the French Member Organization of IMEKO, the Association Française pour la Cybernétique Economique et Technique (AFCEET) Centre Dauphine, Place de Tassigny, Paris 16e, France.

The scientific programme is divided into "Current Topics measurement and instrument problems of great current significance which are treated in introductory survey lectures, section meetings, and "Round Table" discussions, and "General Section" meetings, in which more general questions concerning theory, standards, and special advances in measurement and application are discussed. Round Table discussion topics of particular interest are "metrological basis of gas chromatography and evaluation of accuracy of measuring data from composition of mixtures", "manufacturing approaches to increase the reliability and accuracy of measuring devices

"data reduction and information processing of biological data", "evaluation of instruments and its results", and "what accuracy of measurement is really needed, how shall this accuracy be defined?". In a General Section entitled "Novel Standards for Basic and Derived Units", advances in theory and measurement techniques for standards (microwave attenuation, fundamental capacitance, secondary temperature, physical constants, radio-frequency, SI units) and constants will be discussed.

The Congress Proceedings will be published as *ACTA IMEKO* by the IMEKO Secretariat, P.O.B. 457, Budapest, 5, Hungary.

The International Measurement Confederation was established in 1961, in order to "promote the international exchange of scientific and technical information relating to developments in measuring techniques, instrument design and manufacture, and in the application of instrumentation in scientific research and in industry". Membership in the Confederation comprises scientific and technical societies in 18 countries.

— NATIONAL

A SYMPOSIUM ON THE EVALUATION OF THE THERMODYNAMIC PROPERTIES OF FLUIDS was held in Warrenton, Virginia, U.S.A., from 5—7 November, 1969, under the auspices of the Numerical Data Advisory Board of the National Academy of Sciences - National Research Council (see page 7) and the NBS Office of Standard Reference Data.

The Symposium was attended by more than 75 scientists from the U.K. and U.S.A., who are active or interested in the generation and evaluation of thermodynamic property data. Speakers and topics included: S. Angus, Director, IUPAC Thermodynamic Tables Project Centre, U.K., "World Wide Data Evaluation Efforts"; R. C. Downing, E.I. du Pont de Nemours, U.S.A., "Industrial Needs"; J. F. Masi, U.S. Air Force, "Needs of a Government Agency"; H. M. Roder, NBS, "Fluid Properties, The Case for High Quality Evaluation"; J. M. H. Levelt Sengers, NBS, "Correlation of Thermodynamic Data in the Critical Region"; J. R. Macdonald, Texas Instruments, Inc., U.S.A., "Error Analysis and Model Determination"; J. H. Keenan, MIT, U.S.A., "A Single Fundamental Equation for Vapor and Liquid Water"; M. Klein, NBS, "On the Determination of the Intermolecular Function for Macroscopic Properties"; and L. M. Branscomb, Director, NBS, "A Standard for Reference Data".

Panels were also held in order to discuss the needs, resources, and current programmes in the following areas: atmospheric gases (Panel Chairman: V. J. Johnson, NBS); hydrocarbons (P. T. Eubank, Texas A & M University, U.S.A.); refrigerants (J. J. Martin, University of Michigan, U.S.A.); polar gases (T. S. Storvick, University of Missouri, U.S.A.); and mixtures (L. N. Canjar, University of Detroit, U.S.A.). Publication of the panel discussions is planned by NBS; availability will be announced in the *NSRDS News* and the *Bulletin of Thermodynamics and Thermochemistry*.

NEW JOURNALS

THERMOCHIMICA ACTA

The first issue of a new bi-monthly journal, entitled *Thermochimica Acta*, was published by the Elsevier Publishing Company in March, 1970. Subscription price per annual volume (six issues) Dfl. 81.00 + Dfl. 5.40 postage (U.S. \$ 22.50 + U.S. \$ 1.50, £ 9.8.0 + 13 s.).

The journal includes original research reports and critical and comprehensive reviews of studies in the fields of high temperature chemical thermodynamics, thermochemistry of high temperature reactions and thermoanalytical chemistry. The main fields of science covered are inorganic, organic, polymer, physical and analytical chemistry and biochemistry; in addition, the chemical research areas of metallurgy, materials science, ceramics, physics, geochemistry, soil science, geology, and other applied sciences are included. Techniques given particular

attention are static calorimetry of all types, dynamic calorimetry, including differential scanning and specific heat calorimetry, and pyrolytic and thermoanalytical techniques, such as thermogravimetric and differential thermal analysis.

Manuscripts in English, French or German should be submitted to Prof. W. W. Wendlandt, Editor-in-Chief, *Thermochimica Acta*, Department of Chemistry, University of Houston, Cullen Boulevard, Houston, Texas 77004, U.S.A. Papers in French or German should be accompanied by summaries in the language of the paper, and in English.

Further information and free sample copy from: Elsevier Publishing Company, P.O. Box 211, Amsterdam, The Netherlands.

HIGH TEMPERATURE SCIENCE

Academic Press is to publish a new journal, *High Temperature Science*, which will include reports on new and original research in the fields of high-temperature chemistry, physics, materials science, and related areas.

The journal will be devoted specifically to thermodynamic and structural studies of high temperature systems by mass spectrometric, optical, X-ray and electron diffraction, electrochemical, and other techniques; phase diagrams; flame and explosion phenomena; electric arc chemistry and physics; molten salt properties; new synthetic methods; high temperature, high pressure phenomena; novel approaches to the generation, measurement, and control of high temperatures; exploding wires; imaging techniques; special modifications of devices and techniques for use at high temperatures; shock waves; solid state studies; energy conversion processes; materials science; and related theoretical developments in thermodynamics, kinetics, quantum mechanics, and statistical mechanics.

Contributions in English should be submitted in triplicate to the Editor, Prof. John L. Margrave, Department of Chemistry, Rice University, Houston, Texas 77001, U.S.A.

Subscription information from: Academic Press, Inc., 111 Fifth Avenue, New York, N. Y. 10003, U.S.A.

PHYSICA STATUS SOLIDI (a) — applied research

The monthly journal *Physica Status Solidi* has been supplemented by a second monthly series starting in January, 1970, and entitled *Physica Status Solidi (a) — applied research*. The original journal will continue to cover topical results from pure fundamental solid state research with 450—500 pages per monthly issue (six volumes per year). The new series comprises 240—260 pages per monthly issue (three volumes per year), and contains review articles, original papers, and short notes on aspects of both the application and experimental techniques of fundamental solid state research.

A second index volume, *Subject and Author Index, Volume 16 to 30, 1966 to 1968*, is also now available, and will be sent free of charge to new subscribers to *Physica Status Solidi (a) — applied research*.

Subscription price for each volume (900—950 pages) of each journal series is M 120,—, or U.S. \$ 32.50, excluding overseas postage.

Further information from: Academic Press Inc. (London) Ltd., Berkeley Square House, Berkeley Square, London W1X 6BA, England (for U.K., British Commonwealth, Japan, India, Africa); Academic Press, Inc., 111 Fifth Avenue, New York, N.Y. 10003, U.S.A. (United States, Central and South America); Akademie-Verlag GmbH, Leipziger Strasse 3—4, 108 Berlin, German Democratic Republic (all other countries).

JOURNAL OF MAGNETIC RESONANCE

A new bimonthly periodical, entitled *Journal of Magnetic Resonance*, has been published by Academic Press, Inc.,

New York, U.S.A., under the editorship of Wallace S. Brey, Jr., University of Florida, Gainesville, Fla. 32601, U.S.A.

Coverage includes both nuclear and electron magnetic resonance, and extends to related fields such as quadrupole resonance, cyclotron resonance, the Mössbauer effect, and magnetic properties of the solid state. Interpretive correlations of data and discussions of the relation of structure to magnetic resonance parameters are also within the scope of the journal.

JOURNAL OF APPLIED SPECTROSCOPY

The new Soviet journal, *Zhurnal Prikladnoi Spektroskopii*, published by the Academy of Sciences of the U.S.S.R. and edited by B. I. Stepanov, is being published in English under the title *Journal of Applied Spectroscopy* by The Faraday Press, Inc., 84 Fifth Avenue, New York, N.Y. 10011, U.S.A. Advisory Editor is J. P. Suchet, Centre National de Recherches Scientifiques (C.N.R.S.), 15 Quai Anatole France, 75 - Paris 7e, France.

The journal covers the applications of spectroscopy in chemistry, physics, metallurgy, and biology, and includes reports on topics such as the theory and application of lasers, chemical spectroscopy, luminescence, spectral techniques and equipment, spectral properties of optical materials, and the application of optical methods to crystals and semiconductors.

Annual subscription price (12 issues) is US \$ 150.00.

ISO BULLETIN

The first issue of the new *ISO Bulletin* was published in January, 1970, by the International Organization for Standardization (ISO) Central Secretariat, 1, rue de Varembe, 1211 Geneva 20, Switzerland.

The *ISO Bulletin*, published in both English and French, replaces the *ISO Journal*, and supplements the *ISO Newsletter*, which is primarily an information source for other news media.

The aim of the *Bulletin* is to provide "a monthly commentary of interest and use to a wide range of readers — in fact, not only those already familiar with standardization, but also people as yet unaware of its influence on their lives". In future, the calendar of ISO meetings, together with amendments to the Memento, will be announced in the *ISO Bulletin*.

NNCSC NEWSLETTER

The National Neutron Cross Section Center (NNCSC), Brookhaven National Laboratory, Upton, New York 11973, U.S.A., issued the first of its bi-monthly *Newsletters* in March, 1970.

In addition to items of general interest to producers, evaluators, and users of nuclear cross section data, this new publication includes information on additions to the data files and publications of the NNCSC after 1 January, 1970. This information is extracted using computer techniques from the three computerized data libraries at the NNCSC: the Evaluated Nuclear Data Files (ENDF/A and ENDF/B), and the experimental Cross Section Information Storage and Retrieval System (CSISRS). New input to CSISRS is listed under the headings: element, isotope, cross section type, energy range, number of data points, reference, date of release, and authors' names; additions to ENDF are similarly described, but are also quoted with a "Material Number", which uniquely identifies a data set. If necessary, notes are added for clarification.

Copies of the data listed in the *NNCSC Newsletter* may be requested from the NNCSC (U.S.A. and Canada), or the ENEA Neutron Data Compilation Centre, B. P. No. 9, 91 — Gif-sur-Yvette, France (OECD member countries), or the Nuclear Data Section, International Atomic Energy Agency, Kärntner Ring 11, A-1010 Vienna, Austria (All other countries). Only CSISRS data are available from the IAEA, but by special agreement, users in Australia, India, and Israel can request ENDF data from the NNCSC.

NEW PUBLICATIONS

NUCLEAR PROPERTIES

Systematization of Particles — Atoms, Nuclei, Elements, a collection of articles, by D. N. Trifonov, J. Selinov, K. P. Stanokovich, and V. G. Lapchinskij, Atomizdat Publishing House, Moscow, 1969, 158 pp, 31 k.

Basic Characteristics of Isotopes of Heavy Elements, by V. I. Gorbachev, Yu. S. Zamyatin, and A. A. Lbov, Atomizdat Publishing House, Moscow, 1970, 126 pp, 97 k.

This recent Soviet handbook is an extensive compilation (1 tables, 79 drawings) of physical properties and constants of heavy elements from atomic number 90 to 104, and of nuclear properties of the isotopes of these elements. Information is also given on radio-active disintegration, and methods for accumulation of the transplutonium elements. A comprehensive bibliography of 635 references is provided. The handbook will be of interest to all scientists and technologists working in the fields of atomic and nuclear physics and engineering.

ATOMIC AND MOLECULAR PROPERTIES

NSRDS — NBS — 22, *Atomic Transition Probabilities. Critical Data Compilation, Volume II, Elements Sodium through Calcium**, by W. L. Wiese, M. W. Smith, and B. I. Miles (306 pp, \$ 4.50), is a recent publication in the NSRDS series of the U.S. National Bureau of Standards (NBS), the second volume in a continuing series of compilations critically evaluated atomic transition probabilities. This compilation contains approximately 5000 transition probabilities for the elements with atomic numbers between 11 (sodium) and 20 (calcium).

The data for each element and for each stage of ionization are presented in separate tables, with estimated accuracy indicated. For each ion, the transitions are generally arranged according to multiplets, supermultiplets, transition arrays, and increasing quantum number. Allowed and forbidden transitions are listed separately. For each line, the transition probability for spontaneous emission, the absorption oscillator strength, and the line strength are given, together with spectroscopic designation, wavelength, statistical weights, and energy level of the upper and lower states.

Brief introductions to the tables for each ion discuss the justification for the choice of the recommended data and for the accuracy rating. A general introduction to the compilation includes a detailed discussion of the critical factors relevant to each major experimental and theoretical method, a general critical assessment of the widely-used Coulomb approximation and a number of illustrative examples for the exploitation of regularities or systematic trends among oscillator strengths. The first volume, NSRDS — NBS — 4, *Atomic Transition Probabilities (A Critical Data Compilation), Volume I, Hydrogen through Neon**, by W. L. Wiese, M. W. Smith, and B. I. Glennon (B. M. Miles) (1966, 169 pp, \$ 2.50), follows the same organization and approach as Volume II, and contains about 4000 critically evaluated transition probabilities for allowed and forbidden lines of the lightest ten elements. (For a complete description of the NBS Atomic Transition Probabilities Data Center, see CODATA *International Compendium of Numerical Data Projects*, 3.2.2.).

NSRDS — NBS — 29, *Photon Cross Sections, Attenuation Coefficients, and Energy Absorption Coefficients From 10 keV to 100 GeV**, by J. H. Hubbell (\$ 0.75), is another recent publication in the NSRDS series. This compilation up-dates and extends previous NBS tabulations in this field (see CODATA *International Compendium of Numerical Data Projects*, 3.1.18., 3.2.47.), and reviews the literature on theoretical and experimental studies up to 1968.

New information taken into account in this analysis includes recent advances in: photoeffect calculations; double Compton and radiative corrections to Compton scattering; radiative corrections to nuclear-field pair production; electron-field pair production calculations near threshold; calculations of coherent (Rayleigh) and incoherent (Compton) scattering; and additional experimental data.

Cross sections for the predominant processes (photoelectric absorption, Compton scattering, and pair production), and the attenuation coefficient between 10 keV and 100 GeV are tabulated for 23 elements (between ^1H and ^{92}U) and for 13 compounds and mixtures. In addition, energy absorption coefficients consistent with these data are given for air, water, and 18 elements from 10 keV to 10 MeV, and for air, water, and 7 elements from 10 MeV to 100 MeV. Information on other processes, such as photomeson and photonuclear interactions, is summarized.

Computer Compilation of Molecular Weights and Percentage Compositions for Organic Compounds, by M. J. S. Dewar, University of Texas, U.S.A., and R. Jones, I.C.I. Petrochemical and Polymer Laboratory, U. K., Pergamon Press, 1969, 476 pp, US \$ 32.00, £ 12.

The tables, including data for over 100,000 formulae, comprise the computer output from a programme which calculates the molecular weights and percentage compositions of organic compounds allowed by the valency laws. The elements bromine, chlorine, fluorine, iodine, nitrogen, oxygen, and phosphorus are included with a maximum limit of 30 carbon, 2 halogen and phosphorus, 5 nitrogen, and 9 oxygen atoms.

NBS Special Publication 306, *Bibliography on the Analyses of Optical Atomic Spectra — Section 4: ^{57}La — ^{71}Lu , ^{89}Ac — ^{99}Es* (56 pp, \$ 0.55), by Charlotte E. Moore, formerly supervisor of the NBS Atomic Energy Levels Data and Information Center (CODATA International Compendium of Numerical Data Projects, 3.2.1.).

SPECTRA

Infrared Band Handbook, Revised Edition, edited by Herman A. Szymanski, Alliance College, Pennsylvania, U.S.A., and Ronald E. Rickson, Chemistry Department, University of Montana, U.S.A., Plenum Publishing Corporation, 227 West 17th Street, New York, N.Y. 10011, U.S.A., ca. 1350 pp, 1970, in preparation.

UV Atlas of Organic Compounds, Volume 5

The fifth and final volume of the *UV Atlas of Organic Compounds/UV Atlas organischer Verbindungen* was published in September, 1969, by the Butterworth Group, 88 Kingsway, London, W.C.2, England, and Verlag Chemie GmbH, Pappelallee 3, Weinheim/Bergstr., Germany - BRD. The Atlas is produced within "Documentation of Molecular Spectroscopy", in collaboration with the Photoelectric Spectrometry Group, London, England, and the Institut für Spektrochemie und angewandte Spektroskopie, Dortmund, Germany - BRD, (CODATA International Compendium of Numerical Data Projects, 3.2.34.). The *UV Atlas of Organic Compounds* now comprises a collection of selected ultraviolet absorption spectra of approximately 1000 compounds containing typical chromophoric groups. The spectra are supplemented by tables showing the effects of substituents and solvents, by explanatory text in English and German, and by alphabetical and cumulative formula indexes.

The *UV Atlas* is available from the publishers at £ 9.2.3. or DM 80,— (US \$ 21.86) per volume, and £ 45.11.3 or DM 400,— (US \$ 109.30) per five-volume set. In the U.S.A., Central and South America available from Plenum Publishing Corporation, 227 West 17th Street, New York, N. Y. 10011, U.S.A., at US \$ 27.50 per volume or US \$ 115.00 per set.

Atlas of Mass Spectral Data

A comprehensive new compilation of mass spectral data, together with the first in a series of up-dating journals, has

recently been published by John Wiley and Sons, Ltd., England. The data were originally compiled under the supervision of Professors E. Stenhagen and S. Abrahamsson, Institute of Biochemistry, University of Göteborg, Sweden, for use in science information centre at the University.

The *Atlas of Mass Spectral Data*, edited by E. Stenhagen, S. Abrahamsson and F. W. McLafferty, Department of Chemistry, Cornell University, Ithaca, New York, U.S.A., contains three volumes (2572 pp) data for the mass spectra of 683 organic compounds, organized by molecular weight (16.0313–702.7981). The contents of each volume follow an identical format and include the following information: formulae and abbreviations; source or supplier of mass spectra; atomic weight table; natural abundance of isotopes; the use of computers in low resolution mass spectrometry; tabular data; and register of elemental compositions.

To supplement and up-date the *Atlas*, a new journal, *Archive of Mass Spectral Data*, is to be issued on a quarterly basis. The four issues of Volume I will comprise 784 pages containing additional or revised data for 372 compounds, in the same format as those in the *Atlas*. The data given in both the *Atlas* and the *Archives* are also available on magnetic tape.

The three volumes of the *Atlas of Mass Spectral Data* are not sold separately and are priced together at US \$ 150.00 — £ 7. (magnetic tape, US \$ 1000 — £ 417). Subscription price for the *Archives of Mass Spectral Data* is US \$ 52 — £ 23. Additional information from:

John Wiley and Sons, Ltd., Baffins Lane, Chichester, Sussex, England.

Spectral Data of Natural Products, Volume 1, by K. Yamaguchi, Research Laboratories, Torii and Co. Ltd., Tokyo, Japan (XIV + 750 pp, Dfl. 175.00, £ 21, US \$ 56.00), was published in May, 1970, by the Elsevier Publishing Company, P. O. Box 211, Amsterdam, The Netherlands.

This first volume includes compounds, the structures of which were elucidated before 1963, while Volume II will cover those structures determined during 1964 and 1965. In each volume the natural products are classified by their structural type into the following 20 groups: hydrocarbons and derivatives; carboxylic acids; amino acids; acid amides; carbohydrates, uronic acids, and related compounds; glycosides; triterpenoids; steroids; steroidal sapogenins; cardenolides; diterpenoids; sesquiterpenes; isoprenoids and non-terpenic essential oil; pyrethroids; constituents of male-fern and hop-corn; phenolic substances; quinones; lignoids; carotenoids; and alkaloids.

The structure, available physical constants, and absorption spectral data (infrared, ultraviolet, mass, nuclear magnetic resonance) of each compound are presented, together with their natural origin and relevant literature references.

SOLID STATE PROPERTIES

NBS Monograph 25, Section 7, *Standard X-Ray Diffraction Powder Patterns**, by Howard E. Swanson, Howard F. McMurdy, Marlene C. Morris, and Eloise H. Evans (190 pp, \$ 1.50), is the latest in a series of publications containing information on X-ray diffraction powder patterns. In this section, standard X-ray diffraction powder patterns are presented for 81 substances. Of these patterns, 45 were determined experimentally, while 36 were calculated.

The compilation, evaluation, and experimental work at NBS are part of a continuing programme to extend and up-date the "Powder Diffraction File", a compilation of X-ray data from many sources. This activity is carried out under the auspices of the Joint Committee on Powder Diffraction Standards, which is composed of representatives of the sponsoring organizations, the American Society for Testing and Materials, the American Crystallographic Association, the British Institute of Physics, and the National Association of Corrosion Engineers, U.S.A.

The experimental X-ray powder diffraction patterns in the present NBS publications were obtained with a Geiger or proportional counter X-ray diffractometer, using samples of high

purity. All "d" values were assigned Miller indices, determined by comparison with computed interplanar spacings and from consideration of space group extinctions. The densities and lattice constants were calculated, and the refractive indices measured wherever possible. The calculated X-ray patterns were computed from published crystal structure data. Both peak height and integrated intensities are given for the calculated patterns.

For full information on the organization and publications of the "Powder Diffraction File", and also details of earlier related NBS publications (NBS Circular 539, *Standard X-Ray Diffraction Powder Patterns*, Volumes 1-10, and NBS Monograph 25, *Standard X-Ray Diffraction Powder Patterns*, Volumes 1-6) refer to section 3.3.3. of the CODATA *International Compendium of Numerical Data Projects*.

Landolt - Börnstein, *Numerical Data and Functional Relationships in Science and Technology*, New Series, Group III, Crystal and Solid State Physics, Volume 4, Part a, *Magnetic and Connected Properties of Some Oxides and Related Compounds*, by J. B. Goodenough, W. Gräper, F. Holtzberg, D. L. Huber, R. A. Lefever, J. M. Longo, I. M. McGuire, and S. Methfessel, Editors, K.-H. Hellwege and A. M. Hellwege, Springer-Verlag, Heidelberger Platz 3, 1 Berlin 33, Germany - BRD, or 175 Fifth Avenue, New York, N. Y. 10010, U.S.A., 1970, 385 pp, DM 218,—, US \$ 60.00.

The magnetic properties of the following compounds are tabulated: iron oxides and iron-metal-oxygen compound systems (except ferrites, garnets, and perovskites), compounds with lanthanide and actinide elements of special structural types (except garnets and perovskites), perovskites, and garnets.

Details of the organization and publications, both Sixth Edition and New Series, of Landolt-Börnstein are given in section 2.1. of the CODATA *International Compendium of Numerical Data Projects*.

Crystal Chemical Classification of Minerals, by A. S. Povarennykh, Institute of Geological Sciences, Academy of Sciences of the Ukrainian S.S.R., translated from Russian by J. E. S. Bradley, Plenum Publishing Corporation, 227 West 17th Street, New York, N. Y. 10011, U.S.A., 1970, ca. 600 pp, US \$ 40.00.

THERMODYNAMIC PROPERTIES

NSRDS — NBS — 30, *High Temperature Properties and Decomposition of Inorganic Salts, Part 2. Carbonates** (\$ 0.45, SD Catalog No. C 13.48:30), by K. H. Stern and E. L. Weise, is another recent publication in the NSRDS series, and the second volume in a series detailing thermodynamic and kinetic data relevant to the high-temperature behaviour of important classes of inorganic salts.

The series will be restricted for the present to anhydrous salts which contain monatomic cations, and oxyanions containing one element besides oxygen, e. g., sulphates, carbonates, nitrogen-oxygen, and halogen-oxygen anions. Through critical reviews of the literature, the following three types of information are correlated for each salt: the reactions by which salts decompose in various temperature ranges; thermodynamic functions for these reactions, e. g., Gibbs energies, free-energy functions, equilibrium constants, and partial pressures; and kinetic parameters such as rate constants, activation energies, and mechanisms.

NSRDS — NBS — 7, *High Temperature Properties and Decomposition of Inorganic Salts, Part I. Sulfates** (\$ 0.35, SD Catalog No. C 13.48:7), by the same authors, covered the relevant literature and data for 60 sulphate compounds.

Phase Diagrams for Ceramists; 1969 Supplement, by E. M. Levin, C. R. Robbins, and H. F. McMurdie, American Ceramic Society, Inc., 4055 N. High Street, Columbus, Ohio 43214, U.S.A., 1969, 625 pp, US \$ 30.00.

This compilation of 2083 phase diagrams supplements and updates the 1964 edition of *Phase Diagrams for Ceramists*

(CODATA *International Compendium of Numerical Data Projects*, 3.4.12.). A selected "best" diagram is given for each system in the following areas: metal-oxygen systems, including those containing valence changes; metal oxide systems; systems with oxygen-containing radicals; systems containing halides only; systems containing halides with other substances; systems containing cyanides, sulphides, etc.; and systems containing water.

Chemical Thermodynamics of Organic Compounds

A comprehensive survey (882 pp) of selected thermodynamic data of organic compounds, entitled *The Chemical Thermodynamics of Organic Compounds* by D. R. Stull, Thermal Research Laboratory, Dow Chemical Company, Midland, Michigan 48640, U.S.A., E. F. Westrum, Jr., Department of Chemistry, University of Michigan, Ann Arbor, Michigan 48104, U.S.A., and G. O. Sinke, Dow Chemical Company, was published in August, 1969, by John Wiley and Sons, Ltd., Baffins Lane, Chichester, Sussex, England, at a price of US \$ 29.95 — £ 14.1.

After a consideration of basic thermodynamic principles, thermal and thermochemical properties in the ideal gaseous state from 298 to 1000 K are given for the elements, selected inorganic compounds, hydrocarbon compounds, compounds of carbon, hydrogen and oxygen, nitrogen compounds, halogen compounds, and organic sulphur compounds. Selected values of the enthalpy of formation and entropy of organic compounds at 298 K are also tabulated. An extensive bibliography of 1656 references covers the literature up to January, 1966.

Tables of Thermophysical Properties of Water and Water Vapour, by M. P. Vukalovich, S. L. Ryvkin, and A. A. Alexandrov, State Service for Standard and Reference Data (GSSSD), and the Soviet Co-ordinating Committee on the Properties of Steam, Academy of Sciences of the U.S.S.R., Moscow, U.S.S.R., Publishing House for State Standards, Moscow, 1969, 407 pp, 3 r. 50 k.

This compilation comprises data on the thermodynamic and transport properties of water and steam, in accordance with the *International Skeleton Tables of 1963*, approved at the Sixth International Conference on the Properties of Steam, 1963, (see CODATA *International Compendium of Numerical Data Projects*, 3.4.16.). All equations used to calculate the data are quoted.

Tables of thermodynamic properties are given for temperatures up to 800°C and pressures up to 1000 bars. Viscosity data are given for temperatures and pressures up to 700°C and 800 bars respectively, while thermal conductivity data and Prandtl numbers are quoted for a similar temperature range, but for pressures up to 500 bars only. Enthalpy-entropy (Mollier, h, s) and enthalpy-temperature (h, T) diagrams are also included.

TRANSPORT AND THERMOPHYSICAL PROPERTIES

Thermophysical Properties Research Center (TPRC) Data Series, edited by Y. S. Touloukian, Director, Thermophysical Properties Research Center, Purdue University Research Park, 2595 Yeager Road, West Lafayette, Indiana 47906, U.S.A., and C. Y. Ho, Head, Data Tables Division, Thermophysical Properties Research Center.

The first ten volumes of the first edition of this comprehensive compilation of evaluated data on the thermophysical properties of matter are scheduled for publication in 1970 by Plenum Publishing Corporation, 227 West 17th Street, New York, N. Y. 10011, U.S.A. Volumes 11, and 12 and 13 are planned for completion in respectively 1971 and 1972. The titles and estimated number of pages of the 13 volumes are as follows:

- Volume 1. Thermal Conductivity, Metallic Elements and Alloys (1600 pp),
- Volume 2. Thermal Conductivity, Nonmetallic Solids (1300 pp),
- Volume 3. Thermal Conductivity, Nonmetallic Liquids and Gases (700 pp),

- Volume 4. Specific Heat, Metallic Elements and Alloys (820 pp),
- Volume 5. Specific Heat, Nonmetallic Solids (1730 pp),
- Volume 6. Specific Heat, Nonmetallic Liquids and Gases (380 pp),
- Volume 7. Thermal Radiative Properties, Metallic Elements and Alloys (1650 pp),
- Volume 8. Thermal Radiative Properties, Nonmetallic Solids (880 pp),
- Volume 9. Thermal Radiative Properties, Coatings (1690 pp),
- Volume 10. Thermal Diffusivity (500 pp),
- Volume 11. Viscosity (400 pp),
- Volume 12. Thermal Expansion, Metallic Elements and Alloys (1000 pp),
- Volume 13. Thermal Expansion, Nonmetallic Solids (1000 pp).

For a complete description of the Thermophysical Properties Research Center and previous TPRC publications, refer to section 3.4.20., CODATA *International Compendium of Numerical Data Projects*.

Thermophysical Properties of Alkali Metals, by E. E. Shpilrain, K. A. Yakimovich, E. E. Totskij, D. L. Timrot, and V. A. Fomin, editor, V. A. Kirillin, Publishing House for State Standards, Moscow, 1970, 486pp, 2r. 9k.

This recent publication presents a detailed analysis of the existing experimental and theoretical data on the thermophysical properties of the alkali metals (Li, Na, K, Rb, Cs) in both the condensed and vapour phases over wide ranges of temperature and pressure. The most reliable data have been selected and co-ordinated to produce a compilation of 310 tables.

For metals in the condensed state, the temperature dependence of density, viscosity, surface tension, thermal conductivity, electrical conductivity, and enthalpy is included. For the vapour phase, properties covered include thermophysical and transport properties, e. g., thermal conductivity, viscosity, thermodynamic properties of dry, saturated, and superheated vapours, and the dependence of the vapour pressure upon temperature.

Thermophysical Properties of Gaseous and Liquid Methane, by V. A. Zagurchenko and A. M. Zhuravlev, Publishing House for State Standards, Moscow, 1969, 236pp, 1r.

In this Soviet publication, the available experimental data on the thermophysical and thermodynamic properties of gaseous and liquid methane are compiled and critically analysed. The method of deriving the equations of state according to the experimental data for both the vapour and liquid phases is described, and the appropriate constants are given.

Tables of data on specific volume, enthalpy, entropy, specific heat, and velocity of sound in gaseous and liquid methane are given for temperatures and pressures up to 1000 K and 1000 bars respectively. For temperatures up to 500 K and pressures up to 500 bars, the experimental data on diffusion coefficients, thermal conductivity, viscosity, and Prandtl numbers are also correlated.

NBS Technical Note 385, *Thermal Conductance at the Interface of a Solid and Helium II (Kapitza Conductance)**, by N. S. Snyder, Cryogenics Division, Institute for Basic Standards, National Bureau of Standards, Boulder, Colorado 80302, U.S.A., 1969, 90pp, U.S. \$ 1.00, SD Catalog No. C 13.46:385.

Thermal Radiation Phenomena, edited by R. K. M. Landshoff, Lockheed Palo Alto Research Laboratory, Palo Alto, California, U.S.A., and J. L. Magee, Department of Chemistry, University of Notre Dame, Notre Dame, Indiana, U.S.A., Plenum Publishing Corporation, 227 West 17th Street, New York, N.Y. 10011, U.S.A., Volume 1: *Radiative Properties of Air*, 1969, 648pp, U.S. \$ 28.00.

Tracer Diffusion Data for Metals, Alloys and Simple Oxides, by J. Askill, Physics Department, Millikin University, Decatur, Illinois, U.S.A., Plenum Publishing Corporation, 227 West 17th Street, New York, N.Y. 10011, U.S.A., 1970, ca. 175pp, U.S. \$ 12.50.

NBS Technical Note 383, *Bibliography of Thermophysical Properties of Air from 0 to 300 K**, by L. A. Hall, Cryogenic

Data Center, National Bureau of Standards, Boulder, Colorado 80302, U.S.A., 1969, U.S. \$ 1.25, SD Catalog No. C 13.42:383.

SOLUTION PROPERTIES

Dissociation Constants of Inorganic Acids and Bases in Aqueous Solution (1970, 236pp, £ 2.4.), by D. D. Perrin, Department of Medical Chemistry, Institute of Advanced Studies, Australian National University, Canberra, Australia, is the third and most recent compilation produced under a programme of the Commission on Electroanalytical Chemistry, Analytical Chemistry Division, International Union of Pure and Applied Chemistry (IUPAC), and published by the Butterworth Group, 88 Kingsway, London, W.C. 2, U.K. (distributed in the U.S.A. by the Plenum Publishing Corporation). The tables include the compound name, chemical formula, thermodynamic dissociation constant with assessment of reliability, temperature, range of concentration, method of measurement, and literature reference. A similar format is followed in the two previous publications, *Dissociation Constants of Organic Acids in Aqueous Solution*, by G. Kortüm, W. Vogel, and K. Andrussov, Institute of Physical Chemistry, University of Tübingen, Germany-BRD, 1961, 340pp, £ 2.10., and *Dissociation Constants of Organic Bases in Aqueous Solution*, by D. D. Perrin, 1965, 515pp, £ 7.

CHEMICAL KINETICS

Handbook of Rate Constants of Gas Phase Reactions, by V. N. Kondratiev, Institute for Chemical Physics, Academy of Sciences of the U.S.S.R., Moscow, U.S.S.R., Nauka Publishing House, Moscow, 1970, 351pp, 2r.38k.

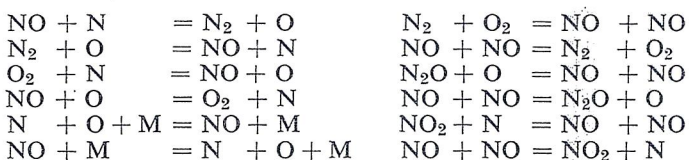
This extensive compilation comprises tables of rate data for more than 2000 elementary reactions in the gas phase. Reactions covered include exchange reactions of atoms and radicals, combination reactions, and disintegration reactions of radicals and of electronically excited particles.

The Handbook is based mainly upon data published in the primary scientific literature, but the content of other relevant compilations and reviews has been taken into consideration. Many of the data have been critically evaluated to derive recommended values of the rate constants.

High Temperature Reaction Rate Data, No. 4, December, 1969

The fourth report in the series entitled *Critical Evaluation of Rate Data for Homogeneous, Gas Phase Reactions of Interest in High-Temperature Systems*, by D. L. Baulch, D. D. Drysdale, D. G. Horne, and A. C. Lloyd, is now available free of charge from Dr. D. L. Baulch, School of Chemistry, The University, Leeds LS2 9 JT, U.K.

The following homogeneous, gas phase reactions leading to the production of NO in high-temperature systems are considered:



For each reaction, the available experimental rate data are tabulated, together with the experimental method and evaluators' comments, and a recommended value of the rate constant is derived. An Arrhenius plot of these data is given. A discussion and bibliography for each reaction are also provided.

The first report in the series (May 1968) included similar information for eight reactions of CO and CO₂, while the second (November 1968) and third reports (April 1969) covered respectively eight and twelve hydrogen/oxygen reactions.

* Available from: Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402, U.S.A. Order by SD Catalog No. if given.

Bibliography of Chemical Kinetics and Collision Processes, by A. R. Hochstim, Science and Technology Division, Institute for Defense Analysis, Arlington, Virginia, U.S.A., Plenum Publishing Corporation, 227 West 17th Street, New York, N.Y. 10011, U.S.A., 1969, 953pp, U.S. \$ 35.00.

Bibliography of Ion-Molecule Reaction Rate Data (JILA Information Center Report No. 9), by G. A. Sinnott, Joint Institute for Laboratory Astrophysics (JILA) Information Center, University of Colorado, Boulder, Colorado, U.S.A., 1969, 80pp, free of charge.

EARTH SCIENCES

Handbook of Geochemistry, Executive Editor, K. H. Wedepohl, Professor of Geochemistry, University of Göttingen, Germany-BRD, Editorial Board, C. W. Correns, D. M. Shaw, K. K. Turekian, and J. Zemann, Springer-Verlag, Heidelberger Platz 3, 1 Berlin 33, Germany-BRD, or 175 Fifth Avenue, New York, N.Y. 10010, U.S.A., Volume 1, 1969, 444pp, Volume 2, Part 1, 1969, loose-leaf binder, DM 224,—.

Feldspars, by T. F. W. Barth, Mineralogisk-Geologisk Museum, Oslo, Norway, John Wiley and Sons, Ltd., Baffins Lane, Chichester, Sussex, England, 1969, 274pp, £ 6.16.

Handbook of World Salt Resources, by S. J. Lefond, United States Borax and Chemical Corporation, U.S.A., Plenum Publishing Corporation, 227 West 17th Street, New York, N.Y. 10011, U.S.A., 1969, 384pp, U.S. \$ 30.00.

BIOCHEMISTRY

Atlas of Protein Sequence and Structure, 1969, Volume 4, Editor, Margaret O. Dayhoff, National Biomedical Research Foundation, 11200 Lockwood Drive, Silver Spring, Maryland 20901, U.S.A., 1969, 361pp.

SPECIAL SUBSTANCE CATEGORIES

Semiconducting II—VI, IV—VI, and V—VI Compounds, by N. Kh. Abrikosov, V. F. Bankina, L. V. Poretskaya, L. E. Shelimova, and E. V. Skudnova, A. A. Baikov Institute of Metallurgy, Academy of Sciences of the U.S.S.R., Moscow, U.S.S.R., translated from Russian by A. Tybulewicz, Plenum Publishing Corporation, 227 West 17th Street, New York, N.Y. 10011, U.S.A., 1969, 252pp, U.S. \$ 19.50.

This publication describes the physico-chemical properties and crystal structures of semiconducting compounds formed from elements of groups II, IV, or V, and sulphur, selenium, or tellurium ($A^{II}B^{VI}$, $A^{IV}B^{VI}$, $A_2^{VI}B_3^{VI}$ compounds).

Phase diagrams, particularly of the pressure-temperature-composition type, are included, and the influence of stoichiometry on electrical properties is considered.

Properties of Liquid and Solid Hydrogen, by B. N. Yeselson, Yu. M. Blagoi, V. N. Grigoriev, V. G. Manzheliy, S. A. Michailenko, and N. P. Neklud, Publishing House for State Standards, Moscow, 1969, 135pp. 43k.

In this reference book, information on the physical properties of hydrogen in the liquid and solid states is compiled. Tables (58) and charts of critically evaluated data are included.

NOMENCLATURE, SYMBOLS, UNITS, STANDARDS

International Union of Pure and Applied Chemistry (IUPAC)

Final Recommendations (reprinted from *Pure and Applied Chemistry*), The Butterworth Group, 88 Kingsway, London, W.C. 2, U.K.

Manual of Symbols and Terminology for Physicochemical Quantities and Units, by M. L. McGlashan, 1970, £ 1.

Recommended Nomenclature for Titrimetric Analysis, by E. B. Sandell and T. S. West, 1969, 5 s.

Recommendations for Abbreviations of Terms Relating to Plastics and Elastomers, 1969, 5 s.

Recommended Symbols for Solution Equilibria, by Y. Marcus, 1969, 5 s.

Atomic Weights of Elements 1969, 1969, 5 s.

Sodium Carbonate and Sulphamic Acid as Acid-Base Primary Standards, 1969, 5 s.

Recommendations for the Presentation of the Results of Chemical Analysis, by R. W. Fennel and T. S. West, 1969, 5 s.

Appendices on Tentative Nomenclature, Symbols, Units, and Standards, IUPAC Secretariat, 2/3 Pound Way, Cowley Centre, Oxford OX4 3YF, U.K.

Information Bulletin Number 2, December 1969, *Catalog of Physicochemical Standard Substances*, Physical Chemistry Division, Commission on Physicochemical Measurements and Standards, Chairman, D. R. Stull, Building 1707, Dow Chemical Company, Midland, Michigan 48640, U.S.A.

Information Bulletin Number 3, January 1970, *Manual of Definitions, Terminology and Symbols in Colloid and Surface Chemistry*, Physical Chemistry Division, Commission on Colloid and Surface Chemistry, Chairman, D. H. Everett, Department of Physical Chemistry, University of Bristol, Bristol BS8 1TS, U.K.

Information Bulletin Number 4, January 1970, *Recommendations for the Presentation of NMR Data for Publication in Chemical Journals*, Physical Chemistry Division, Commission on Molecular Structure and Spectroscopy, Chairman, R. N. Jones, Division of Pure Chemistry, National Research Council of Canada, Sussex Drive, Ottawa, Canada, (Comments to: N. Sheppard, School of Chemical Sciences, University of East Anglia, University Plain, Norwich NOR 88C, U.K.).

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