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

CODATA 9 NEWSLETTER

DECEMBER 1972

CODATA BUREAU

At the 7th CODATA General Assembly, 30 June, 1972, Le Creusot, France, the proposals of a Nominating Committee were approved, and the following appointments were made to the Bureau of CODATA: Prof. K. Egle (Germany, Fed. Rep.) as Secretary-Treasurer, Prof. N. Kurti (U.K.) and Prof. T. Shimanouchi (Japan) as Members, and Dr. A. Hubaux as Observer. The Officers and Members of the CODATA Bureau, with their terms of office, are therefore now as follows:

President: (1970—1974)	Prof. B. VODAR Laboratoire des Hautes Pressions, 1, place Aristide-Briand, 92-Bellevue, France
Vice-Presidents: (1970—1974)	Academician M. A. STYRIKOVICH Academy of Sciences of the U.S.S.R., Leninskiy Prospekt 14, Moscow B-71, U.S.S.R.
(1972—1976)	Dr. R. Norman JONES National Research Council of Canada, Sussex Drive, Ottawa 7, Ontario, Canada
Secretary-Treasurer: (1972—1976)	Prof. K. EGLE Botanisches Institut, J. W. Goethe Universität, Frankfurt/Main, Germany, Fed. Rep.
Members: (1970—1974)	Dr. Lewis M. BRANSCOMB IBM Corporation, Armonk, New York 10405, U.S.A.
(1972—1976)	Prof. N. KURTI, F.R.S. The Clarendon Laboratory, Oxford OX1 3PU, England
(1972—1976)	Prof. T. SHIMANOUCHI, Department of Chemistry, University of Tokyo, Hongo, Tokyo, Japan
Observer:	Dr. A. HUBAUX EURATOM/CETIS, 21020 Ispra (Varese), Italy
Executive Director: (Ex Officio)	Dr. Christoph SCHÄFER, CODATA Central Office, Frankfurt/Main, Germany, Fed. Rep.

CODATA MEETINGS AND CONFERENCES 1972—1976

The **15th** (24—25 June) and **16th Bureau Meetings** (1 June), and the **7th General Assembly** (30 June) of CODATA were held before and after the **3rd International CODATA Conference,** 26—29 June, 1972, at Le Creusot, France.

The **17th Meeting of the CODATA Bureau** will take place 19—20 January, 1973, at Frankfurt/Main, Germany, Fed. Rep.

On the invitation of the Swedish Academy of Sciences, the **18th Bureau Meeting** and the **8th General Assembly** will be held 9—11 September, 1973, at Stockholm, Sweden.

The CODATA Task Group on Computer Use will hold a **Symposium on 'Man-Machine Communication for Scientific Data Handling',** at the University of Freiburg, Breisgau, Germany, Fed. Rep., 22—27 July, 1973.

The **4th International CODATA Conference** on the Generation, Compilation, Evaluation and Dissemination of Data for Science and Technology will be held in the last week of June 1974 on the invitation of the Soviet National Data Committee, who have offered the Olympic village, near Erevan, as a site for the Conference.

On the invitation of the U.S. National Data Committee, the **5th International CODATA Conference** is scheduled for mid-1976, near Washington, D.C., U.S.A.

CODATA NATIONAL MEMBERS

During 1972, new Representatives of three National Members of CODATA have been appointed, as follows:

Federal Republic of Germany

Prof. K. EGLE
Botanisches Institut,
J. W. Goethe Universität,
6 Frankfurt/Main

Prof. Egle has also succeeded Prof. W. Klemm as Secretary-Treasurer of CODATA.

Japan

Prof. T. SHIMANOUCHI
Department of Chemistry
University of Tokyo,
Hongo, Tokyo

United Kingdom

Prof. N. KURTI, F. R. S.
The Clarendon Laboratory,
Oxford OX1 3PU

Prof. Kurti is also the new Representative on CODATA of the International Union of Pure and Applied Physics (IUPAP).

AUSTRALIA

The membership of Australia on CODATA has now been accepted, bringing the number of CODATA National Members to 14.

CANADA

The Canadian National Committee for CODATA has been reorganized under more specific terms of reference. The following Members have been appointed for the period 1972—1976:

Chairman: R. N. JONES
Division of Chemistry,
National Research Council of Canada,
Ottawa

Secretary: W. B. PEARSON
Department of Physics,
University of Waterloo,
Waterloo, Ontario

Members: J. E. BROWN
National Science Library of Canada,
Ottawa

W. L. HANEY
Division of Radio and Electrical Engineering,
National Research Council of Canada,
Ottawa

H. PRESTON-THOMAS
Division of Physics,
National Research Council of Canada,
Ottawa

S. C. ROBINSON
Geological Survey,
Department of Energy, Mines and Resources
Ottawa

G. WADDINGTON
Victoria,
British Columbia

Ex officio: R. MARTINEAU
International Relations Office,
National Research Council of Canada,
Ottawa

The newly-constituted Committee met at the National Research Council Laboratories on 28 April, 1972. It reviewed the present status of data compilation and evaluation projects in Canada, and discussed what action should be taken to co-ordinate its activities with other Canadian organizations concerned with the more general problems of information storage and retrieval. Prominent among these are the National Science Library of Canada and the National Research Council Advisory Board on Scientific and Technological Information. The Committee is also taking steps to identify gaps in presently available data compilations that are of particular importance to Canada and to acquire a more complete overview of existing data compilation projects in Canada.
The assessment of computer-based methods to search the published literature for data collections is being continued in co-operation with the CAN/S.D.I. project of the National Science Library of Canada.

POLAND

A new Committee, entitled the **Scientific Committee on Metrology and Data for Science and Technology,** has been created by the Polish Academy of Sciences for the period 1972—74. This Committee, which combines the activities of the former Polish National Data Committee and the Committee on Metrology, has a two-fold scope (data and metrology), and the double function of organizing relevant research work throughout the country, and of representing Poland on CODATA. The new Committee is attached to Division IV (Engineering Sciences) of the Polish Academy of Sciences, and is supervised by the Scientific Secretary of this Division, Prof. Maciej Nalecz, former Chairman of both Committees (on Metrology and Data). The past Vice-Chairman of the Committee on Metrology and Member of the Polish National Data Committee, Prof. Wojciech Zielenkiewicz, has been named Chairman of the new Committee. The structure and membership of the Polish Scientific Committee on Metrology and Data for Science and Technology, Division IV, Polish Academy of Sciences, Palac Kulturyi Nauki 23p, Warsaw, is as follows:

Presidium

Chairman: Prof. Wojciech ZIELENKIEWICZ
Institute for Physical Chemistry,
Polish Academy of Sciences,
ul. Kasprzaka 44/52, Warsaw

Vice-Chairman: Prof. Edmund ROMER

Scientific Secretary and National Representative on CODATA: Prof. Tomasz PLEBANSKI
Division of Physico-Chemical Metrology,
Polish Committee for Standardization and Measures,
ul. Elektoralna 2, Warsaw

Members: Prof. Wladyslaw JAROMINEK
Prof. Maciej NALECZ
Mr. Zygmunt OSTROWSKI
Mr. Tadeusz PODGORSKI

Chairmen of Sections for Data Research and Co-operation with CODATA Task Groups

Solid State Physics Prof. Julian AULEYTNER
Institute of Physics,
Polish Academy of Sciences,
ul. Hoza 69, Warsaw

Chemical Kinetics Prof. Adam BIELAŃSKI
Department of Chemistry,
Jagellonian University,
ul. Krupnicza 41, Kraków

Physico-chemical Properties of Mixtures Section (formerly 'Data for Industry'): Prof. Andrzej BYLICKI
Institute of Physical Chemistry,
Polish Academy of Sciences,
ul. Kasprzaka 44/52, Warsaw

Computer Use Dr. Zbigniew KIERZKOWSKI
Polytechnic Institute of Poznań,
Regional Computer Centre,
M. Curie-Skleodowska Place 5, Poznań

Members
Dr. Zbigniew DUNAJSKI
Dr. Stanislaw DWOJAK
Prof. Leszek FILIPCZYŃSKI
Dr. Szymon FIRKOWICZ
Mr. Jerzy HUK
Prof. Andrzej JELLONEK
Dr. Wojciech KLIMECKI
Dr. Jozef KOSZEWSKI
Prof. Marian LAPIŃSKI
Prof. Artur METAL
Mr. Wojciech PIROG
Prof. Zbigniew PUZEWICZ
Prof. Stanislaw RYZKO
Prof. Andrzej SADOWSKI
Dr. Tomasz SLUSZKIEWICZ
Prof. Szczepan SZCZENIOWSKI
Dr. Wieslaw WARDZYŃSKI
Prof. Eugeniusz WOLNIEWICZ

The Chairmen of the various Sections for Data Research and Co-operation with CODATA Task Groups are at present completing the membership of their groups, with a view to developing activities within their field of interest, including closer contacts with the respective CODATA Task Groups.
The Committee as a whole has made efforts to introduce numerical reference data problems into the scientific programme of the 'Second Congress of Polish Science', the largest event in the Polish scientific calendar, which will take place in June 1973 at Warsaw. Prof. A. Bylicki has been named Chairman of a group preparing a report on the 'State-of-the-art and perspectives of data research', which will be presented at the Congress. The Board for Quality Control and Measures, recently reorganized as the Polish Committee for Standardization and Measures, is considering a programme on 'Numerical reference data for metrology', under the direction of Prof. T. Plebanski.

UNITED KINGDOM

Several data centres and projects in the U.K. are sponsored by the **Office for Scientific and Technical Information (OSTI)**, Elizabeth House, York Road, London S.E.1, a part of the Department of Education and Science. Status reports on the progress of some of these centres are given below.

Crystallographic Data Centre, University Chemical Laboratory, Cambridge CB2 1EW (enquiries to Dr. Olga Kennard or Dr. D. G. Watson). This Centre maintains computer-based bibliographic and numerical data files on crystal structures of organic and organo-metallic compounds analysed by X-ray or neutron diffraction methods. The total number of entries in the bibliographic file as of May 1972 was ca. 7000, and during 1972 the following data elements were added to the 15 already stored: reliability factor (R), bond lengths corrected for thermal vibration, and flag for mode of intensity measurement. The numerical data are subjected to critical evaluation before incorporation into the data base, and are released from the file only after computer processing and evaluation for internal consistency.

From 1972, a repository system for protein crystallographic data will be operated jointly by the Crystallographic Data Centre and the Brookhaven National Laboratory, U.S.A. Atomic coordinates are stored, and provision will be made for the storage of structure factors and electron density maps. The two Centres maintain identical files, and distribution is on magnetic tape wherever possible. At present there is no charge for the service apart from handling costs. The total holdings will be announced annually in the bibliographic volumes of *Molecular Structures and Dimensions*, published by the Centre in co-operation with the IUCr. Requests for protein crystallographic data should be made to the Crystallographic Data Centre, or Dr. W. C. Hamilton, Brookhaven National Laboratory, Upton, N.Y. 11973, U.S.A., or Dr. E. F. Meyer, Department of Biochemistry and Biophysics, Texas A&M University, College Station, Texas 77843, U.S.A.

In order to complement the work of the Cambridge Centre and to fill a gap in the provision of evaluated reference data, OSTI is supporting the establishment of a computerized data base covering inorganic crystal structures, under the direction of Prof. D. Rogers, Department of Chemistry, Imperial College of Science and Technology, London. The project will utilize the bibliographic searches carried out by the Crystallographic Data Centre, and will benefit from the techniques, software and other expertise acquired by this Centre.

Data and Information Systems for Atomic and Molecular Physics, Director, Dr. F. J. Smith, Department of Applied Mathematics and Theoretical Physics, Queen's University, Belfast, Northern Ireland. In addition to the interatomic potentials already stored, it is planned to incorporate into the data system formulae for generating potentials from other related data. The data base will be broadened to include transport properties, collision cross-sections and similar properties; a second data base on wave functions will also be developed. Users of this computer-based data bank will not only have direct access to the data, but will be able to manipulate the data for their own requirements.

Computer Analysis of Thermochemical Data (CATCH) Tables, Dr. J. B. Pedley, School of Molecular Sciences, University of Sussex, Brighton. This project uses a set of computer programs for generating tables of self-consistent enthalpies of formation of chemical compounds from standard enthalpies of

reaction at 25°C. When revised experimental data on key compounds become available, or if changes are made in the weighting system used to assess data from various sources, the programs provide for rapid up-dating of the data. A co-operative project has been established under which thermochemists, principally in the U. K. and in Sweden, will supply critically evaluated input data for a continuing series of tables covering the following compound classes: halogen compounds, boron compounds, phosphorus compounds, compounds of germanium, tin and lead, compounds of transition metals (especially complex ions solution), silicon compounds, nitrogen compounds, compounds of molybdenum, chromium, tungsten and vanadium, organic free radicals, gaseous ions from lattice energy calculations, sulphur compounds, and dissociation energies of small molecules. To date, a set of three tables and a bibliography on 466 nitrogen compounds has been produced using experimental data compiled by Dr. G. Pilcher, University of Manchester. The tables, produced by computer type-setting, include chemical formula for each compound, molecular weights and enthalpies of formation together with the related reactions, enthalpies of the reactions, and bibliographic references. Data on inorganic halogen compounds and inorganic phosphorus compounds have also been processed, and are to be published in the near future.

Mass Spectrometry Data Centre, Director, Dr. R. G. Ridley, AWRE, Aldermaston, Reading RG7 4PR. As a further aid to retrieval, a chemical classification has been added to the data files, and over 30000 compounds have now been classified. The possibility of retrospective retrieval from the *Mass Spectrometry Bulletin* tapes is also being considered. This Centre is jointly supported by OSTI and the Department of Trade and Industry.

The following publications have been added during 1972 to the *OSTI Reports* series held by the U.K. National Lending Library for Science and Technology, Boston Spa, Wetherby, Yorkshire LS23 7BQ:

Cambridge Research on Data Processing in Geology, Reps 1—6 (one vol.), J. L. Cutbill, Department of Geology, University of Cambridge (June 1971);
Annual Report to OSTI, January 1971 — January 1972, and structural Data File Specifications, Program Documentation and Unimol Program Manuals, Report 1/72 (four vols), Crystallography Group, University Chemical Laboratory, Cambridge;
Final Report on Survey of Kinetic Data on Atomic and Free-Radical Addition Reactions, J. A. Kerr and M. J. Parsonage, University of Birmingham (1972);
Computer Analysis of Thermochemical Data. Final Report for the Period October 1969 — December 1971, J. B. Pedley, University of Sussex (May 1972);
Queens University On-Line Data Bank on Atomic and Molecular Physics. Annual Activity Report for Period ending 31 December 1971, Computer Laboratory and Department of Computer Science, Queen's University, Belfast (January 1972).

The **Department of Trade and Industry** is the second U.K. agency responsible for information and data services. An additional facility introduced during 1972 is the availability of the NBS-NSRDS series and other data items through the Department's Technology Reports Centre, St. Mary Cray, where the U.K. high-speed VDU link in the ESRO data network is also located Plans are well advanced for extending this latter facility through out the U.K. Other developments in 1972 have included a feasibility study on a cryogenic data centre by the National Physical Laboratory in association with the British Cryogenics Council. There has been recurrent interest in the provision of computerized data for chemical engineers, in the mechanical properties of polymer materials, and in high-temperature materials data. Computerized data services are being made available publicly to an increasing extent, and the Mass Spectrometry Data Centre, for example, now offers a computer mass spectra data matching service to its customers. Similar features form the core of services with which the Department has been associated in the planning stages, and which are shortly to be launched.

Biological Data Centres are the subjects of two recent reports in the *Biological Journal of the Linnean Society*, London:

The Biodeterioration Information Centre: Specialized Information Centre, by H. O. W. Eggins, University of Aston, Birmingham *Biol. J. Linnean Soc.* **3** 3 (1971) 245. The purpose and function of the specialized information centre are outlined, together with the importance of the relation of such a centre to current research users' needs. Methods of information storage and retrieval are discussed, and the publications and services of the Biodeterioration Information Centre are listed.

The Biological Records Centre — A Data Centre, by F. Perring Nature Conservancy, Abbots Ripton, *Biol. J. Linnean Soc.* **3** 3 (1971) 237. The Biological Records Centre collects data on the occurrence of species at a particular time in a particular place, which are used for the preparation of distribution maps, lists of species from localities and lists of localities for species. The Centre is encouraging the collection of data on a national and European basis; the establishment of both biological records centres and a complete biological recording network are important.

Two publications of relevance to the work of CODATA have recently been issued by ASLIB, 3 Belgrave Square, London SW1X 8PL: **Quantitative Data in Science and Technology,** by Brenda Mountstephens, Averil Osborn, and Margaret Slater, Aslib Occasional Publication No. 7 (1971, 24 pp, £ 1.24 for non-members, £ 0.90 for members); **Data and the Chemist,** by Margaret Slater, Averil Osborn, and Alexandra Presanis, Aslib Occasional Publication No. 10 (1972, 82 pp, £ 3.50 for non-members, £ 2.90 for members).

These reports result from a continuing project of the Aslib Research and Development Department, started in late 1969, to explore the need in science and technology for factual and quantitative data. The earlier publication (No. 7) provides a review of present knowledge on the provision and use of scientific and technical data under three headings: the data problem as seen in recent literature, data search in technical libraries, and a sampling of data centres. *Data and the Chemist* reports on the second phase of the project, a detailed field survey of 500 chemists with respect to their opinions and practices in the provision and use of data. In view of the particular interest of this survey, the findings will be reviewed in detail by one of the authors in Newsletter No 11.

U.S.A.

The **U.S. National Standard Reference Data System (NSRDS)** was established in 1963 as a means of co-ordinating on a national scale the production and dissemination of critically evaluated reference data in the physical sciences. Under the Standard Reference Data Act, the National Bureau of Standards (NBS) of the Department of Commerce has the primary responsibility in the Federal Government for providing reliable scientific and technical reference data. The **Office of Standard Reference Data (OSRD)** of the NBS co-ordinates a complex of data evaluation centres, located in university, industrial and other Government laboratories, as well as within the NBS, which are engaged in the compilation and critical evaluation of numerical data on physical and chemical properties retrieved from the world scientific literature. The participants in this NBS-sponsored programme, together with similar groups under private or other U.S. Government support and which are pursuing the same aims, comprise the National Standard Reference Data System.

A revised status report on the NSRDS has recently been published as **NBS Technical Note 747**, *Critical Evaluation of Data in the Physical Sciences — A Status Report on the National Standard Reference Data System, June 1972* (Nov. 1972, 79 pp, $1.25, SD Catalog No. C13.46:747, available from the Superintendent of Documents, U.S. Government Printing Office, Washington, D. C. 20402, U.S.A.), Stephen A. Rossmassler, Ed. This report describes the activities and progress of the NSRDS since the publication of the last status report (NBS Tech. Note 553) in June 1970, with respect to general background and new developments, progress of the data evaluation programmes in the seven property areas covered, data systems design activities, and information services. Appendices include a directory of continuing U.S. data centres and a listing of NSRDS publications.

New projects sponsored or co-ordinated under the NSRDS during the past year include the following:

1) A planning effort to develop a programme for mechanical properties of materials.

2) In the area of chemical kinetics, new emphasis on data relevant to air pollution problems. Representatives of the OSRD and the U.S. Chemical Kinetics Information Center participated in activities of the CODATA Task Group on Data for Chemical Kinetics under which new co-operative initiatives were undertaken.

3) In the area of solid state data, formation of an ad hoc Panel on Electrical Properties, and beginning of a compilation of elastic constant data for metals and alloys. A co-operative arrangement between the NBS Single Crystal Data Centre and the Crystallographic Data Centre, U.K., has been concluded for handling future compilation and evaluation of single crystal data.

4) In the atomic and molecular properties area, a meeting of the ad hoc Panel on Interatomic Distances, and planning for relevant data compilation activities. A new Data Center on Spectral Line Shapes and Shifts has been established within the Optical Physics Division of the NBS, with the objectives of collection and cataloguing of all literature relevant to the broadening and shift of atomic spectral lines, and preparation and publication of bibliographies and critical reviews of various topics in atomic line broadening. The Center has already published a first bibliography on atomic line shapes and shifts (see page 10), which will be up-dated by the periodic issue of supplements as the volume of new literature warrants. A critical review on the present status of the hydrogen Stark-broadening problem is in the planning stage. Future plans include other critical reviews of well-defined topics in atomic line broadening, and the compilation and critical evaluation of line-broadening data.

5) In the area of thermodynamics and transport properties, projects on thermodynamic properties of propane, and on phase equilibrium data for cryogenic fluid mixtures.

6) Concerning nuclear data, expansion of interrelationships between the OSRD and the U.S. Atomic Energy Commission to provide ex officio OSRD membership on the U.S. Nuclear Data Committee.

A particularly noteworthy event was the publication in March 1972 of the first issue of the **Journal of Physical and Chemical Reference Data,** a co-operative undertaking of the NBS, the American Chemical Society (ACS), and the American Institute of Physics (AIP). The Journal will provide a primary outlet for NSRDS products and will also include, as appropriate, high quality data compilations and critical reviews from other sources. The purpose of the Journal is to provide improved accessibility for compilations of evaluated data through a publication channel more compatible with the information-acquiring patterns of individual users and organizations. The Journal will appear quarterly, with an anticipated annual volume of approximately 1200 pages. It is expected that international users of NSRDS products will benefit particularly from the improved access to this material through the new medium. The contents of Nos 1—4, Vol 1 (1972) of *J. Phys. Chem. Ref. Data* are detailed in the CODATA Newsletter No.11.

The presentation of numerical data in the primary literature is a topic of great importance which is gaining increasing and deserved attention. Two relevant articles have recently been issued, as follows:

Presentation of Concepts and Numerical Data in Physics (Oct. 1971 AIP ID 71—3) by H. William Koch, AIP, presented at the U.S./Japan Symposium on Data Evaluation and Compilation, 15—17 Nov. 1971, Tokyo. Available from: AIP Physics Information Division, American Institute of Physics, 335 East 45 St., New York, N.Y. 10017, U.S.A.

Guidelines for the Reporting of Numerical Data and Experimental Procedures

(*J. Res. Nat. Bur. Stand., A. Phys. Chem.* **76A** 2 (1972) 67) by David Garvin, Institute for Materials Research, NBS, gives general recommendations on the reporting of data and experimental procedures, in order that the measurements may be evaluated, re-interpreted or repeated. The recommendations are intended as instructions to authors of papers in which quantitative physical or chemical data are reported. A bibliography of standards documents and more detailed guidelines is included.

Recent U.S. conferences in the field of numerical data have included the following:

Forum on the Management of Information Analysis Centers, sponsored by the COSATI Panel on Information Analysis Centres and organized by the NBS, 17—19 May 1971, Gaithersburg, Maryland. The Proceedings of this Forum, entitled *The Management of Information Analysis Centers. Proceedings of a Forum sponsored by the COSATI Panel on Information Analysis Centers* (1972, 192 pp, $3.25 paper, $0.95 microfiche, COSATI Rep. No. 72—1), are now available from the National Technical Information Service, Springfield, Va. 22151, U.S.A. Topics include: automatic data processing systems, establishment of computerized files, semi-automated scientifically-orientated data centres, interactive retrieval systems, and computer usage in a large data centre. Sessions also covered abstracting and indexing services (case studies and information service profiles included),

and marketing information analysis centres (including service charge policies). A reprint of a paper presented in the latter session, entitled *Marketing the Products and Services of Information Analysis Centres*, by H. William Koch, AIP, and W. Grattidge, General Electric Co., is available from the AIP Physics Information Division (AIP ID 71—2, May 1971).

Gordon Research Conference on Numerical Data of Science and Technology, 21—25 August 1972, Tilton, New Hampshire. Session topics and chairmen, and invited speakers of this most recent Gordon Conference on Numerical Data were as follows: Data of Biological Systems (Irving Fatt, University of California (Chairman); Edward C. DeLand, Santa Monica, Calif.; Philip L. Altman, Office of Biological Handbooks, FASEB; Paul Webb, Webb Assoc.); Value Judgement (David R. Stull, The Dow Chemical Co. (Chairman); Donald D. Wagman, NBS; Harold Hoge, U.S. Army Natick Labs); Factors involved in Critical Evaluation (Howard White, NBS (Chairman); Richard Stewart, University of Idaho; Max Klein, NBS); Utilization of Computerized Abstracts in Critical Evaluation (Joseph Hilsenrath, NBS (Chairman); N. B. Gove, ORNL; R. C. Thompson, NBS; V. E. Hampel, LRL); An Evaluator's View of Non-Stoichiometric Compounds, or Can Too Much Freedom Be Understood? (Edmund Storms, Los Alamos Scientific Lab. (Chairman); Louis Toth, University of Minnesota; Wendall Williams, Materials Research Lab.; John Jennings, Food and Drug Administration); The Art and Science of Critiques of Experimental Numerical Data (Y.S. Touloukian, TPRC (Chairman); C. Y. Ho, TPRC; S. J. Schneider, NBS).

The **U.S. Association of Scientific Information Dissemination Centers** (**ASIDIC**) has recently published *A Survey of Information Center Services*, compiled by Martha E. Williams and Alan K. Stewart, Information Sciences, ITT Research Institute. This survey is presented as the report of the ASIDIC Co-operative Data Management Committee (CDMC), which was formed to study ways, means and feasibility of sharing experiences, resources, processing activities, etc., between ASIDIC information centres (and possibly others), in order to standardize, simplify and economize information centre activities and to establish an informal network. As a first step towards such co-operative arrangements, the CDMC undertook this survey of the information centre data bases and services. Copies are available for $ 7.50 either from the authors, ITT Research Institute, 10 West 35th St., Chicago, Ill. 60616, or from the ASIDIC Secretary, Mr. R. Bruce Briggs, Center for Information Services, Campus Computing Network, University of California, Los Angeles, Calif. 90024, U.S.A.

The **Panel on Nuclear Data Compilation** of the U.S. National Research Council's Committee on Nuclear Science has been directing an intensive programme, now entering its second year, to bring nuclear data compilations up to date by the end of 1974. Supported by the National Science Foundation, 23 Nuclear Information Research Associates are working under the supervision of senior physicists at the same number of universities and laboratories in order to reduce the backlog. In co-operation with the Nuclear Data Group at Oak Ridge National Laboratory, the new compilations are being published by Academic Press as part of the *Nuclear Data Sheets* series. Compilations, known as 'A-chains', have already been published for mass numbers 71 and 92. 'A-chains' for an additional ten mass numbers are nearing publication, leaving approximately 60 to be completed by the end of the project.

A **Rock Properties Information Center** has been established within the Thermophysical Properties Research Center (TPRC), West Lafayette, Ind. 47906, U.S.A., with the aims of providing quick response to technical and bibliographic inquiries, generating recommended reference data, and performing relevant experimental research. A programme specializing in the properties of geological substances was initiated at TPRC in June 1972 with the support of the National Science Foundation. The programme is based at TPRC, but constitutes an interdisciplinary effort involving investigators from three Purdue University Departments: Civil Engineering (W. R. Judd), Geosciences (T. R. West), and Mechanical Engineering (D. P. DeWitt).

As presently constituted, the programme has four major areas of activity:

1) generation of data tables for the mechanical, physical and thermal properties of minerals and rocks; 2) identification and organization of the unclassified literature on nuclear blast, explosion phenomena for parametric studies; 3) organization of the literature on rapid excavation and tunnelling, in order to provide information on techniques, rock formations, geographic locations, cost, and other pertinent variables in support of research and development in this field; and 4) an experimental programme with the objectives of developing and refining theories of heat conduction in rocks, and of correlating thermal and mechanical properties of rocks which have been petrographically characterized. The capabilities and experience of TPRC in scientific documentation and data tables generation will provide a productive environment for support of the new Rock Properties Information Center.

U.S.S.R.

A **Scientific Information Centre on Thermophysical Properties of Pure Substances** is planned for establishment as a part of the Institute of High Temperatures by the Academy of Sciences of the U.S.S.R. The function of this Centre is to compile, systematize, correlate and distribute thermophysical property data of substances of scientific and technological interest, under the guidance of the Soviet National Data Committee.

CODATA UNION MEMBERS

During 1972, new Representatives of four Union Members of CODATA have been appointed, as follows:

International Union of Crystallography (IUCr)
Dr. D. G. WATSON
University Chemical Laboratory,
Cambridge CB2 1EW, U.K.

International Union of Pure and Applied Physics (IUPAP)
Prof. N. KURTI, F.R.S.
The Clarendon Laboratory,
Oxford OX1 3PU, U.K.

International Geographical Union (IGU)
Prof. G. VERGER
Laboratoire de Geomorphologie,
Ecole Pratique des Hautes Etudes,
75-Paris 5e, France

International Union of Geodesy and Geophysics (IUGG)
Prof. P. MELCHIOR
Observatoire Royal de Belgique,
1180 Brussels, Belgium

INTERNATIONAL UNION OF BIOLOGICAL SCIENCES (IUBS)

With the support of CODATA, a survey of the Section Chairmen of the various IUBS Divisions was undertaken during the latter part of 1971 to determine the existence of data-collecting activities in the biological sciences. Survey sheets requesting information on organization, coverage, analysis, and publications were sent to the members of the IUBS Executive Committee, National Committees, International Organizations, as well as the Chairmen of Divisions, Sections, Commissions and Working Groups.

Of the 156 survey sheets mailed out, only 16 were returned. Eleven individuals provided information on their data-collecting activities, and the other five indicated that such work was not being done by their groups.

In response to a letter in the 7 January 1972 issue of *Nature*, nine positive replies were received. Through personal solicitation, five other organizations with data-collecting projects submitted completed survey sheets. The data being collected by various organizations are listed below:

Responses from IUBS Affiliates

1. General agricultural data (Commonwealth Agricultural Bureaux, Farnham House, Farnham Royal, Slough, England)
2. Taxonomy and identification of algae (Freshwater Biological Association, Windermere Laboratory, The Ferry House, Ambleside, Westmorland, England)
3. Major ecosystems relative to conservation (International Biological Programme, Section CT, The Nature Conservancy, Monks Wood Experimental Station, Abbots Ripton, Huntington, England)
4. Strain characteristics of micro-organisms and cell lines (World Federation of Culture Collections Information Center, Department of Microbiology, University of Queensland, St. Lucia, Brisbane, Queensland, Australia)
5. Morphology and taxonomy of oribatid mites (Dr. Eduard Piffl, Department of Zoology, University of Vienna, Austria)
6. Fish data (Laboratory of Limnology, University of Wisconsin, Madison, Wisconsin, U.S.A.)
7. Plant data (Institute of Botany, Academia Sinica, Nankang, Taipei, Republic of China)
8. Food additives (Food Chemicals Codex, National Academy of Sciences — National Research Council, 2101 Constitution Avenue, Washington, D.C., U.S.A.)
9. Plant physiology data (Institute of Plant Biology and Physiology, University of Lausanne, Palais de Rumine, Place de la Riponne, Lausanne, Switzerland)
10. Plant pathology data (International Society for Plant Pathology, Department of Botany, Imperial College, London, England)
11. Primate data (Regional Primate Research Center, University of Washington, Seattle, Washington, U.S.A.)

Responses to 7 January 1972 Letter in NATURE

1. Animal pest species (Centre for Overseas Pest Research, College House, Wrights Lane, London, England)
2. Limnology data (Fishery Research Unit, Malawi Ministry of Agriculture, P. O. Box 27, Monkey Bay, Malawi, Africa)
3. Physiological clearance curves (Dr. M. E. Wise, Physiology Laboratory, Leiden University, Wassenaarseweg 62, Leiden, Netherlands)
4. Agro-ecological atlas of cereal growing in Europe (Centre for Agricultural Publishing and Documentation, 6a Duivendaal, P.O. Box 4, Wageningen, Netherlands)
5. Experimental tumour data (Research Data Unit, Imperial Cancer Research Fund, Burtonhole Lane, Mill Hill, London, England)
6. Blood data (Blood Information Service, 508 Getzville Road, Buffalo, New York, U.S.A.)
7. Numbers of plastids in cells (Dr. Theodor Butterfass, Max-Planck-Institut für Pflanzengenetik, 6802 Ladenburg, Rosenhof, Germany, Fed. Rep.)
8. Taxonomy of grass genera (Dr. Leslie Watson, Research School of Biological Sciences, The Australian National University, P. O. Box 475, Canberra City, Australia)
9. Tree data (Commonwealth Forestry Institute, University of Oxford, South Parks Road, Oxford, England)

Responses to Personal Solicitations

1. General biological data (Office of Biological Handbooks, Federation of American Societies for Experimental Biology, Bethesda, Maryland, U.S.A.)
2. Catalogue of North American Coleoptera (Entomology Research Division, Plant Industry Station, U.S. Department of Agriculture, Beltsville, Maryland, U.S.A.)
3. Mammalian taxonomy codes (Seamak-Zoogad System, Veterans Administration Hospital, 54th St. and 48th Ave. South, Minneapolis, Minnesota, U.S.A.)
4. Marine data (National Oceanographic Data Center, Environmental Data Service, NOAA, Rockville, Maryland, U.S.A.)
5. Protein and nucleic acid sequences (National Biomedical Research Foundation, Georgetown University, 3900 Reservoir Road, N.W., Washington, D.C., U.S.A.)

INTERNATIONAL ASTRONOMICAL UNION (IAU)

An **International Information Bureau on Astronomical Ephemerides** was established by the IAU in 1970, and has now commenced operation at the Bureau des Longitudes in Paris, under the direction of Dr. B. Morando. The task of the Bureau is to gather from relevant observatories, computing centres, laboratories, ephemerides offices, etc., information on the material or data that they are prepared to communicate to any user; and to distribute this information to the scientific community through information cards. It should be emphasised that the Information Bureau is not a data centre as such, and neither collects nor distributes the material itself. The fields covered include: ephemerides of bodies in the solar system (excluding artificial satellites and space probes, comets and minor planets other than Ceres, Pallas, Juno and Vesta), lists of reduced observations of such bodies, and catalogues of star positions. A first series of 29 cards have already been distributed to a number of recipients. Institutions interested in receiving and/or contributing information should contact Dr. B. Morando, Bureau International d'Informations sur les Ephémérides Astronomiques, 3 rue Mazarine, 75-Paris 6e, France.

Several **IAU publications** of interest have recently been issued, as follows:

IAU Colloquium No. 8, 'Techniques for the Measurement of Fundamental Spectroscopic Data' (report by B. W. Shore), *Quart. J. Roy. Astron. Soc.* **11** (1971) 48.

IAU Colloquium No. 9. 'The IAU System of Astronomical Constants', T. Lederle and B. Emerson, Eds, *Celest. Mech.* 4 2 (1971).

IAU Symposium No. 50, 'Spectral Classification and Multicolour Photometry', *Proceedings of the International Astronomical Union Symposium held in Villa Carlos Paz, Argentina, October 18—24, 1971*, J. Landi Dessy, R. F. Sistero and M. C. Sistero, Eds, D. Reidel Publishing Co., P. O. Box 17, Dordrecht, Holland. Four introductory papers discuss classification of slit-spectra, classification of objective-prism spectra, photometric classification, and catalogues and documentation. In

the three sessions on classification, particular interest was shown in criteria for identification and classification of supergiant stars, peculiar stars, cool stars, and Population II stars, as well as in the astrophysical interpretation of the data. The possibilities of automatic classification of objective-prism spectra were discussed extensively. In the last session, the main topic was the problem of making existing and forthcoming spectroscopic and photometric data easily available as catalogues and/or via data centres. In all, 50 papers were presented at this Symposium, which was attended by 46 participants from 14 countries.

Catalogue of Cometary Orbits, 1972, a special publication of the IAU Central Bureau for Astronomical Telegrams, prepared by B. G. Marsden. Orbital information, including osculation epochs and non-gravitational parameters, is included for 924 cometory apparitions (referring to 600 individual comets) observed between the year 1886 and February 1972. Supplementary tables give statistical listings of the 97 short- and 503 long-period comets. Available for $2.50 (plus $1.50 for air-mail delivery) from: Smithsonian Astrophysical Observatory, Fiscal Section COO., 60 Garden St., Cambridge, Mass. 02138, U.S.A.

INTERNATIONAL UNION OF CRYSTALLOGRAPHY (IUCr)

At the 9th International Congress of Crystallography in Kyoto, the following persons were elected to the **Commission on Crystallographic Data** for the period 1972—75:

R. ALLMANN (Germany, Fed. Rep.)
I. D. BROWN (Canada)
F. L. HIRSHFELD (Israel)
G. G. JOHNSON (U.S.A.)
M. NARDELLI (Italy)
H. M. ONDIK (U.S.A.)
D. ROGERS (U.K.)
N. L. SMIRNOVA (U.S.S.R.)
D. G. WATSON (U.K., Chairman)

The Commission has undertaken to prepare an up-dated list of crystallographic information services, which will be made available to CODATA to assist in the production of the revised edition of the *International Compendium of Numerical Data Projects*. As a result of recent publication trends, in particular the custom of depositing numerical data rather than publishing them, the Commission has decided to produce a check-list for non-IUCr journals. It is intended that the check-list should provide reasonable recommendations to assist journal editors in the handling of crystallographic publications.
At a meeting of the IUCr General Assembly in Kyoto, it was proposed that the Executive Committee should set up a working party on information services. The working party has been appointed under the chairmanship of S. E. Rasmussen, General Secretary of the IUCr. The terms of reference proposed by the Executive Committee are: 1) to evaluate the present situation in relation to needs in IUCr information services (e. g. publication, collection, storage, retrieval, critical appraisal and dissemination of data and other information pertinent to crystallography); 2) to project these needs into the future and to determine how the IUCr, primarily through its Commissions, could best meet them; 3) to make specific proposals for needed innovations to and extensions of services in this field (in these proposals, feasibility on economic, manpower and cost bases are to be specifically considered); and 4) to report to the Executive Committee at its meetings in 1973 and 1974, and to prepare a full report for circulation before and submission at the 10th General Assembly of IUCr in 1975.

INTERNATIONAL UNION OF GEOLOGICAL SCIENCES (IUGS)

Cogeodata, the IUGS Committee on Storage, Automatic Processing and Retrieval of Geological Data, was established by the Executive Committee of IUGS in January 1967. Its members were appointed from nominees proposed by member countries, the Committee membership being selected to represent the world geographically and to represent the various geosciences.
The four principal tasks of Cogeodata (see *Geological Newsletter* 1 (1967) 22) are in essence to appraise existing systems; to establish factors common to all records of geological data; to work out formats for machine-processible files in a limited number of specific fields; and to establish an index of geological data. In addition, the Committee has served as a focus for international activities in its field, such as the working group on data processing of the International Geological Correlation Program, and the interests of geology in CODATA, UNISIST, oceanography (IOC), and the World Data Centres.
The main results of the Committee's efforts since its formation are seen in a series of documents which a·e o will shortly be available through the Cogeodata Secretary, Dr. C F. Burk, Jr., Canadian Centre for Geoscience Data, 601 Booth Street, Ottawa K1A CE8, Ontario, Canada. These documents include:

Two series of recommendations on the building of geological data files (*Geological Newsletter* 3 (1971) 175, 2 1972,) which after up-dating and editing, will be reissued in the form of a separate booklet. Chapters will include reference numbering, geographic location, stratigraphic data, palaeontological data, geochemical data, rock description, and mineral deposits. These recommendations should not be considered as standards, but rather as guidelines which will hopefully be tested in a wide variety of environments.

A series of documents, prepared by the Working Group on Geochemical Data, concerning the normalization of field and laboratory data for geochemical samples, notably rock samples. They may be obtained by writing to Prof. H. de la Roche, CRPG-CNRS, Case Officielle No. 1, 54-Vandoeuvre-les-Nancy, France. An inquiry on present usage in rock names and descriptions, undertaken by submitting equivalent samples of 23 rocks (eruptive, metamorphic and sedimentary) to petrographers of 18 geological surveys and institutes from various regions of the world. Preliminary results, showing an important scatter of names even after thin-section inspection, were presented at the XXIV International Geological Congress, Montreal, August 1972, and an analysis of the significant conclusions stemming from the answers will be published in 1973.

A bibliography, entitled *Computer-Based Storage and Retrieval of Geoscience Information: Bibliography* 1946—69 (1971, 52*pp*) by J. Hruska and C. F. Burk, Jr., published by the Geological Survey of Canada as GSC Paper 71—40. This bibliography lists in alphabetical order by author 336 papers dealing with 1) use of computers and/or computer-readable records for the storage and retrieval of geoscience information (data, bibliographies, abstracts, indexes, text, and graphical representations), and 2) techniques, codes, thesauri, studies, or other aids of direct assistance to the above. Entry to the bibliography is provided through six indexes by geoscience discipline and/or topic, information aspect, system name and acronym, nation, organization, and author. A supplement in the same series for the years 1970—71 is in press.

A survey of existing geological data files world-wide, compiled and prepared by A. Hubaux, Cogeodata Chairman, has been published as *CODATA Bulletin* 8 (November 1972), 'Geological Data Files: Survey of International Activity'.

NEW PUBLICATIONS

NUCLEAR PROPERTIES

Compilation of Cross Sections, I - π^- and π^+ Induced Reactions CERN/HERA 72-1 (May 1972, 183 pp) is the latest computer-based compilation of particle properties from the High-Energy Reactions Analysis (HERA) Group of the European Organization for Nuclear Research (CERN). This compilation of cross-sections of reactions produced by negative and positive pions on targets of protons, neutrons and deuterons is an updated version of *CERN/HERA* 70-5 (Sept. 1970) and *70-7* (Oct. 1970), and contains 40% more data values than the earlier publications. Graphs of the variation of cross-section with incident laboratory momentum are plotted, and values of the rate of decrease of cross-section with incident momentum are given.

Review of Particle Properties, in *Physics Letters* 39*b* 1 (April 1972), by the Particle Data Group covers the properties of leptons, mesons, and baryons, and is an updating of "Review of Particle Properties" by the same Group (*Rev. Mod. Phys. 43*,2 Suppl. S1 (1971). The relevant data are evaluated, listed, averaged, and summarized in tables.

A Compilation of Data on Inclusive Reactions, NSRDS-LBL-80 (Aug. 1972, 757 pp) by the Particle Data Group, is a self-contained compilation of the most relevant data, graphs and references on multiparticle inclusive reactions. The majority of the compilation consists of the published data graphs, upon which grids have been superimposed to facilitate their use. Relevant references are given on the reverse side of each graph. The single particle spectra are presented in seven sections arranged according to the nature of the beam and target, as follows: pp, p-Nucleus, $K^{\pm}$ p, $\pi^{\pm}$ p, ep(μp), and γ p. Within each section, the plots are given in order of increasing beam momentum, and a bibliography follows each section. Sections on comparative plots and two-body correlations, and also a review article on the kinematics and phenomenology of inclusive spectra, are provided.

Publications of the CERN-HERA Group and reprints of reports from the Particle Data Group are distributed in North and South America, Australasia, and the Far East by Technical Information Divison, Lawrence Radiation Laboratory, Berkeley, California 94720, U.S.A., and in the rest of the world by Scientific Information Service, CERN, CH-1211 Geneva 23, Switzerland. For detailed descriptions of the membership, activities and previous publications of both Groups, see *CODATA Newsletter 5* (Dec. 1970) 22, and *6* (June 1971) 8.

Newsletter Bulletin 13 (CCDN-NW/13, February 1972, 336 pp) of the ENEA Neutron Data Compilation Centre, B.P. 9, 91-Gif-sur-Yvette, France, provides an up-dated listing through February 1972 of the content of the CCDN Experimental Neutron Data Library, superseding a previous index (CCDN-NW/11) published in October 1969. In the three intervening years, the data base has been greatly enlarged due to the collaboration of neutron data users in the ENEA area (Western Europe and Japan) and to the effective world-wide co-operation between the four existing neutron data centres (see below).

Newsletter Bulletin 14 (CCDN-NW/14, May 1972, 133 pp), entitled "A Compilation of Evaluations of Neutron and Photon Cross Sections Available May 1972", lists the existing compilations of evaluated data under the headings, nuclide (material), energy range, date of evaluation, laboratories, reference, data media (i. e. form in which data are available), data bank (i. e. data centre from which copies of evaluated file can be requested), reactions considered, data type, and comments. Listings of computer programs for format conversion from one evaluated data library to another, and for evaluated data handling, are also included. The present publication is a revised version of *Newsletter Bulletin 12* (CCDN-NW/12) issued in October 1970.
The ENEA Neutron Data Compilation Centre has announced that in future shorter updates in loose-leaf form will be published quarterly, containing only the new evaluations entered in its file since the preceding issue. As from September 1972, the Centre has assumed responsibility for the compilation and publication of the *Neutron Nuclear Data Evaluation Newsletter* (*NNDEN*), previously prepared by P. Ribon, CEN-Saclay, France.

CINDU-10, Catalogue of Numerical Neutron Data Available from the IAEA Nuclear Data Section (May 1972, 304 pp), H. D. Lemmel, Ed., is an up-dated index to the experimental and evaluated neutron data sets held by the IAEA Nuclear Data Section, and supersedes *CINDU-9*. The IAEA Nuclear Data Section Kärnterring 11, P. O. Box 590, A-1011 Vienna, Austria, which services countries in Eastern Europe, Asia (except Japan), Africa, Central and South America, and Australasia, shares responsibility for world-wide data collection, compilation and dissemination with the ENEA Neutron Data Compilation Centre (OECD member countries) and two other centres as follows: National Neutron Cross-Section Center, Brookhaven National Laboratory, Upton, N.Y. 11973, U.S.A. (U.S.A. and Canada); and Nuclear Data Information Centre, Obninsk, U.S.S.R. (U.S.S.R.). These four centres also co-operate in the preparation of a world-wide compilation of requests for neutron data measurements (RENDA) that are needed for fission-reactor development. *RENDA-72* is to be published by the IAEA towards the end of 1972.

Gammaenergien is a three-volume computer-based compilation of evaluated data produced by a group under the direction of Chr. Meixner at the Zentralinstitut für Reaktorexperimente, Kernforschungsanlage Jülich GmbH, Jülich, Germany, Fed. Rep. The first part (Jül-811-RX, Dec. 1971, 335 pp) comprises a listing of the approx. 600 nuclides covered with gamma-energies (keV) and other relevant data, schematic diagrams of the gamma spectra, and a chart of the nuclides. Part 2 (Jül-812-RX, Dec. 1971, 362 pp) is a table of neutron-produced nuclides ordered by energies (excluding fission products), and Part 3 (Jül-813-RX, Dec. 1971, 327 pp) includes tables of fission products ordered by energies, and of nuclides and gamma-energies ordered by half-lives. *Gammaenergien* is available free of charge on an exchange basis from Tauschstelle der Zentralbibliothek Kernforschungsanlage Jülich.

A publication of interest has recently been issued by the Institute for Nuclear Study, University of Tokyo, Tanashi, Tokyo, Japan. **Table of Bands in Even-Even Nuclei** by Mitsuo Sakai (INS-J-127, June 1971, 35 pp) lists for even-even nuclei the probable members of quasi-ground, quasi-beta and quasi-gamma bands of the spherical regions and the corresponding ground, beta and gamma bands of the deformed region. This compilation, covering the literature up to May 1971, is a revision of "Quasi-ground, quasi-beta, and quasi-gamma bands" (*Nuclear Data Tables A8* (1970)323).

Nuclear Physics Investigations in the U.S.S.R. — A Collection of Annotations, Issue No. 12 (1971, 112 pp), Information Centre on Nuclear Data, Obninsk; V.A. Kuznetsov and L. N. Usachov, Scientific Eds, D. A. Kardashev, Chief Ed., "Atomizdat", Publishing House of the State Committee on the Utilization of Atomic Energy, U.S.S.R. This report contains tables and graphs of nuclear data from the following Soviet Institutes: Institute of Physics and Energetics, Obninsk; Theoretical and Experimental Physics Institute, Moscow; Khlopin Radium

Institute, Leningrad; Joint Institute of Nuclear Investigations, Dubna; Institute of Physics, Academy of Sciences of the Ukr. S.S.R.; T.V. Kurchatov Institute of Atomic Energy, Moscow.

Nuclear Constants, Issue No. 7 (1971, 471 pp), Information Centre on Nuclear Data, Obninsk; V.A. Kuznetsov and L. N. Usachov, Scientific Eds, D. A. Kardashev, Chief Ed., "Atomizdat" Publishing House. Data tables and graphs are given for delayed neutrons, fission products, α for Pu, fission constants for ^{244}Cm, inelastic and elastic neutron cross-sections, reactor constants and parameters, and shielding constants. Supplement 2 (1971, 158 pp) to Issue No. 7 of "Nuclear Constants" includes tables and graphs for systematization of the average radiation width for neutron resonance.

Bulletin of the Information Centre on Nuclear Data, Obninsk, Issue No. 7, Supplement 1 (1971, 87 pp) by A. F. Saveliev, "Atomizdat" Publishing House. This Bulletin contains data, tables and graphs on prompt radiation with nuclear fission.

ATOMIC AND MOLECULAR PROPERTIES

Atomic Data is a compilation journal covering a broad range of experimental and theoretical results in atomic physics. Contents of 1972 issues are as follows: Vol. 4, No. 1 (March 1972):

Energy loss, range, and bremsstrahlung yield for 10-keV to 100-MeV electrons in various elements and chemical compounds, L. Pages, E. Bertel, H. Joffre and L. Sklavenitis (127 pp).

Vol. 4, No. 2 (April 1972):

Theoretical electron scattering amplitudes and spin polarizations.

Electron energies 100 to 1500eV. Part II. Be, N, O, Al, Cl, V, Co, Cu, As, Nb, Ag, Sn, Sb, I, and Ta targets, M. Fink and J. Ingram (79 pp).

Vol. 4, No. 3 (July 1972):

Tables of secondary-electron-production cross sections, C. B. Opal, E. C. Beaty, and W. K. Peterson, (47 pp);

Hartree-Fock values of energies, interaction constants, and atomic properties for excited states with p^N configurations of the negative ions, neutral atoms, and first positive ions from boron to bromine, S. Fraga and K. M. S. Saxena (15 pp);

Hartree-Fock values of energies, interactions constants, and atomic properties for excited states with $3d^N$ 4s0 and $3d^N$ $4s^2$ configurations of the negative ions, neutral atoms, and first four positive ions of the transition elements, S. Frage and K. M. S. Saxena (21 pp);

Polynominal approximations to the Stark perturbed rotational energy levels of the rigid symmetric top rotor, I. Roeggen (12 pp).

Correspondence on contributions to *Atomic Data* should be addressed to the editor, Dr. Katharine Way, Department of Physics, Duke University, Durham, N.C. 27706, U.S.A. Subscription information from Academic Press, Inc., 111 Fifth Avenue, N.Y. 10003, U.S.A.

Selected Tables of Atomic Spectra, *Atomic Energy Levels and Multiplet Tables, H_I, D, T,* NSRDS-NBS 3, Section 6 (Sept. 1972, 36 pp, $0.40, SD Catalog No. C13.48:3/Sec. 6) by Charlotte E. Moore is the sixth in a series comprising a current revision of two sets of tables containing data on atomic spectra derived from analyses of optical spectra (*NSRDS-NBS* 35, Vols I-III (see below); *NSRDS-NBS* 40 (see below) and *NBS Circular* 488, Sections 1-5 (1950-1962)). The present series includes both sets of data, energy levels and multiplet tables, as parts A and B respectively; additional sections are published at irregular intervals as revised analyses become available.

Atomic Energy Levels, NSRDS-NBS 35, Vols I, II and III (Vol. I: Dec. 1971, 359 pp, $5, SD Catalog No. C13.48:35/V.I.; Vol. II: 1971, 259 pp, $4.25, SD Catalog No. C13.48:35/V.II; Vol. III: Dec. 1971, 282 pp, $4.50, SD Catalog No. C13.48: 35/V.III) by Charlotte E. Moore is a reprint of *NBS Circular* 467 (Vols I-III, 1949—1958), issued in response to the continuing demand for the widely-used critical compilation of atomic energy levels prepared at NBS from analyses of optical spectra. The present volumes are now included in the NSRDS series, and in addition contain cross-references for certain atomic or ionic spectra to other NBS publications with more recent data. Volume I contains data on elements ^{1}H to ^{23}V; Volume II on ^{24}Cr to ^{41}Nb; and Volume III on ^{42}Mo to ^{57}La and ^{72}Hf to ^{89}Ac. Spectra of the lanthanides (Z = 58-71) and actinides (Z = 90—?) are to be covered in Volume IV, now in preparation.

A Multiplet Table of Astrophysical Interest. *Part I-Tables of Multiplets; Part II-Finding List of All Lines in the Table of Multiplets,* NSRDS-NBS 40 (1971, $2, SD Catalog No. C13.48:40) by Charlotte E. Moore is a reissue of *NBS Tech. Note* 36 (1959, out of print), which was in turn a reprint of the *Princeton University Observatory No.* 20, 1945 *Multiplet Table.* The leading lines in 196 atomic spectra of 85 elements are listed in related groups (multiplets). Part I includes the multiplets, with the spectra of each element in order of increasing ionization, and the elements in order of increasing atomic number; Part II is a "Finding List" comprising all spectral lines in Part I in order of increasing wavelength.

Bibliography on Atomic Energy Levels and Spectra, July 1968 through June 1971, NBS Special Publication 363 (June 1972, 103 pp, $1, SD Catalog No. C13.10:363) by Lucy Hagan and W.C. Martin is the first in a bibliographic series expected to be issued under the same title as a successor to *NBS Spec. Publ. 306,* Sections 1—4 (Sept. 1968—Aug. 1969). The present publication contains approximately 1100 references classified by subject for individual atoms and atomic ions, and covering the following data: energy levels, classified lines, wavelengths, Zeeman and Stark effects, hyperfine structure, isotope shift, ionization potentials, and also relevant theory.

Bibliography on Atomic Line Shapes and Shifts (1889 through March 1972), NBS Special Publication 366 (Sept. 1972, 165 pp, $1.75, SD Catalog No. C13.10:366) by J. R. Fuhr, W. L. Wiese and L.J. Roszman is the first output from a new Data Center on Atomic Spectral Line Shapes and Shifts, recently established in the Optical Physics Division of the NBS. The objectives of the Center are to collect and catalogue the relevant literature and to prepare and publish bibliographies and critical reviews on various topics in atomic line broadening (a first review on the present status of knowledge on hydrogen Stark broadening is in the planning stage). The present bibliography covers about 1400 references through March 1972, classified according to 1) general scope and content, 2) numerical data content, ordered by element, ionization stage, and broadening mechanism, 3) date of publication, and 4) authors names.

Theory of Charge Exchange (1972, $19.95, Wiley-Interscience, New York) by R.A. Mapleton is the second NSRDS volume in the Wiley-Interscience Series on Atomic and Molecular Collision Processes, produced under the sponsorship of the Atomic and Molecular Processes Information Center, Oak Ridge National Laboratory, Oak Ridge, Tenn. 37831, U.S.A. This critical review includes comparisons of theoretical and experimental cross-sections up to 10^5 keV, indicating where improvements in approximation methods are required.

Excitation in Heavy Particle Collisions (1972, ca. 464 pp. ca. £8.85, Wiley-Interscience, New York) by E. W. Thomas is another recent critical review in the same Wiley-Interscience Series. The formation of excited atoms induced in collisions between atomic and molecular systems is discussed, and the available experimental data are critically reviewed. The reliable measurements are compiled in tabular form.

Molecular Wave Functions and Properties: *Tabulated from SCF Calculations in a Gaussian Basis Set* (1972, 652 pp, ca £5.00, Wiley, Chichester) by L.C. Snyder and H. Basch gives SCF wave functions and derived properties computed in a uniform basis set of Gaussian functions for over 50 molecules. The theoretical context and the methods used in the computations are also discussed.

Tables of Molecular Vibrational Frequencies, Consolidated Volume I, NSRDS-NBS 39 (June 1972, 164 pp, $3, SD Catalog No. C13.48:39) by Takehiko Shimanouchi supersedes, revises and extends the data on fundamental vibrational frequencies of molecules previously published as *Tables of Molecular Vibrational Frequencies*, Part 1 (NSRDS-NBS 6, 1967), Part 2 (NSRDS-NBS 11, 1967), and Part 3 (NSRDS-NBS 17, 1968). The present consolidated volume covers 52 additional molecules, bringing the total to 223. Selected values of the fundamental vibrational frequencies are given for each molecule, together with observed infrared and Raman spectral data and citations to the original literature. Available from the Superintendent of Documents, U.S. Government Printing Office, Washington, D. C. 20402, U.S.A.

Landolt-Börnstein, Numerical Data and Functional Relationships in Science and Technology, New Series, K.-H. Hellwege and A. M. Hellwege, Eds; Group II, Atomic and Molecular Physics, Vol. 6, *Molecular Constants from Microwave-, Molecular beam-, and ESR-spectroscopy*, is a supplement and extension to *Molecular Constants from Microwave Spectroscopy* (Vol. 4, Group II, New Series, 1967), and is scheduled for publication in 1973.

Vibrational Spectra of Polyatomic Molecules (Nov. 1972, 560 Russian pp. $32, Keter Publishing House Ltd., distributors for Israel Program for Scientific Translations, P.O.B. 7145, Jerusalem, Israel), by L.M. Sverdlov, M.A. Kovner, and E. P. Krainov, "Nauka" Publishing House, Moscow (1970), translated 1972. Following a theoretical treatment of the vibrational spectra of polyatomic molecules, including a discussion of new methods for the determination of force constants and electro-optical parameters and the calculation of frequencies and intensities, this reference book is devoted to analysis and interpretation of vibrational spectra of various groups of compounds, including paraffins, naphthenes, unsaturated hydrocarbons, halogen-substituted parafins, halogen-substituted unsaturated hydrocarbons, halogen-substituted benzene, oxy-compounds, and nitrogenous, organosulphur, organosilicon, organoboron and organophosphorus compounds. Over 500 molecules are considered, and for each molecule and its isotopic substituents a table of fundamental frequencies in IR and Raman spectra is given. Much of the material is based on the original work of the authors.

John Wiley and Sons Ltd., Baffins Lane, Chichester, Sussex, U.K., have announced that as from October 1972 they are distributing the entire IPST (Keter) Ltd. list (which includes numerous Soviet data compilations translated from Russian into English) throughout the U.K., Continental Europe, Africa, and the Middle East (excluding Israel).

Atlas of Spectral Data and Physical Constants for Organic Compounds (Jan. 1973, 1500 pp, approx, £50, Chemical Rubber Co., Cleveland, Blackwell Scientific Publications, Oxford), Jeanette G. Grasselli, Ed., is the first volume to combine in a single reference source the name, synonyms, formula, Wiswesser Line Notation, Chemical Abstracts Registry Number, literature references, and critically evaluated and reviewed data entries for molecular weight, specific rotation, melting and boiling points, density, refractive index, solubilities, and coded spectral data from infrared, ultraviolet, NMR, and mass spectral curves, as available. In addition, numerous computer-generated indexes of the physical and spectral data and of the compound names and synonyms, and also spectral reference curves, are provided.

The Hydrogen Molecule Wavelength Tables of Gerhard Heinrich Dieke (1972, 629 pp, $19.95, Wiley-Interscience, New York), H. M. Crosswhite, Ed., presents the most recent experimental data on the energy levels and spectrum of molecular hydrogen. The bulk of the book comprises spectral tables which include wavelength and associated wave numbers, corresponding estimated intensities, upper and lower electronic and vibrational states, and the branch type and rotational quantum number of the lower state. References are given to earlier work in the literature.

Digest of Literature on Dielectrics, Vol. 34, 1970 (1972, 515 pp, $35, National Academy of Sciences, Washington, D.C.) prepared by the Committee on Digest of Literature of the Conference on Electrical Insulation and Dielectric Phenomena, Division of Engineering, National Research Council, U.S.A. The *Digest*, issued annually since 1936, is a compilation of information published during the year on dielectric phenomena; tables of dielectric constants, dipole moments and dielectric relaxation times are included. Available from the Printing and Publishing Office, NAS, 2101 Constitution Ave N.W., Washington, D.C. 20418, U.S.A.

SOLID STATE PROPERTIES

CRYSTALLOGRAPHIC PROPERTIES

Crystal Structures, 2nd Edn, Vol. 6, Part 2 (1971, 615 pp, $37.50, £17.55, Wiley Interscience, New York) by R. W. G. Wyckoff, is the second part of a three-part volume on the structure of benzene derivatives in this continuing compilation of crystal structures. The present publication covers compounds containing two, three, four, and five or more benzene rings, derivatives of naphthalene and anthracene, and complex condensed-ring compounds. The bibliography is arranged by dates of references in the literature from 1921 through 1968. Part 1 of Volume 6 of the second edition of *Crystal Structures* (1969, 455 pp, $27.50, £ 13) covered compounds containing one benzene ring. For details of earlier publications in this series, see CODATA *International Compendium of Numerical Data Projects*, 3.3.2.

Crystal Data, Determinative Tables, 3rd Edn, Vol. 1, *Organic Compounds* (1972, sectional pagination, $30, National Bureau of Standards and Joint Committee on Powder Diffraction Standards, U.S.A.), J.D.H. Donnay and Helen M. Ondik, General Eds, Olga Kennard and D. G. Watson, Organic Section Eds, has now been published under the sponsorship of the NBS Office of Standard Reference Data. This volume covers approximately 7500 carbon-containing crystalline compounds, which are listed, within each crystal system, according to increasing values of a determinative number: a/b ratio in trimetric systems, c/a ratio in dimetric systems, and cubic cell edge a in the isometric system. For each crystalline species, the following information and properties are listed: axial ratio(s) and interaxial angles not fixed by symmetry, cell dimensions, space group or diffraction aspect, number of formula units per cell, crystal structure, measured and X-ray calculated densities, compound name and synonym(s), chemical formula, literature reference, and trans-

formation matrix (when relevant). Additional information includes some or all of the following: crystal structure type (if any), goniometric axial ratio(s), crystal habit, cleavages, twinning, colour, optical properties, indices of refraction, optical orientation (except in anorthic system), and melting and transition points. The data were computer-tested for self-consistency, and errors found in the original or abstracting literature are specifically mentioned: erroneous values are thus identified. Formula, and organic and mineral name indexes facilitate location of the data.
The second volume of *Crystal Data, Determinative Tables* (3rd Edn) covering inorganic compounds is scheduled for publication in the near future. *Crystal Data* is a collaborative international data project dating back to 1954: for further details, see *CODATA Newsletter* 8 (May 1972)12, and CODATA *International Compendium of Numerical Data Projects*, 3.3.1. Orders should be addressed to: Joint Committee on Powder Diffraction Standards, 1601 Park Lane, Swarthmore, Pa. 19081, U.S.A.

Landolt-Börnstein, Numerical Data and Functional Relationships in Science and Technology, New Series, K.-H. Hellwege and A. M. Hellwege, Eds; Group III, Crystal and Solid State Physics, Vol. 8, *Epitaxy Data of Inorganic and Organic Crystals* (1972, 193 pp, $37.50, DM118, Springer, Berlin, Heidelberg, New York) by M. Gebhardt and A. Neuhaus, is the most recent volume to be published in the New Series of "Landolt-Börnstein". Epitaxy data, i. e. planes, directions and misfits of orientation, are compiled for about 3700 inorganic and organic epitaxial systems. An alphabetical formula list, and organic compound name and mineral name indexes are included. The literature is covered from 1836 through 1970.

Absolute Configuration of Metal Complexes (1971, 362 pp, $19.50, Wiley-Interscience, New York) by C. J. Hawkins, is a recent monograph reviewing the topics of absolute configurations and conformational analysis, and which includes useful compilations of relevant data.

Crystal Structure Transformations in Binary Halides. NSRDS-NBS 41 (July 1972, 53 pp, $0.55, SD Catalog No. C13.48:41) by C.N.R. Rao and M. Natarajan, is a critical compilation of the data describing crystal structure transformations in binary halides. In addition to crystallographic data, thermodynamic, spectroscopic and electronic properties are given for each transformation. The most-relevant literature references are covered up to 1970. Similar compilations on transformations in binary oxides and other systems are planned for future publication.

Standard X-ray Diffraction Powder Patterns, NBS Monograph 25, Section 9 (1972, $1.25, SD Catalog No. C. 13.44:25/Sec. 9) by H. E. Swanson, et al., is the 19th and most recent in a series of publications on X-ray diffraction powder patterns. In this section, standard X-ray diffraction patterns are presented for 63 substances. The compilation, evaluation, and experimental work at NBS are part of a continuing programme to extend and up-date the *Powder Diffraction File* (see CODATA *International Compendium of Numerical Data Projects*, 3.3.3.).

ELECTRICAL AND MAGNETIC PROPERTIES

Electroconductivity of Ferroelectrics (1971, 368 pp, £ 11.50, IPST (Keter) Ltd., and Wiley, Chichester) by V. M. Gurevich, Publishing House of the Committee on Standards, Measures and Measuring Instruments, Moscow (1969), translated 1971. This recently-translated monograph presents data on the electrical conductivity and related properties of 60 compounds, 58 solid solutions, and 10 ferroceramics having ferro- and antiferroelectric properties.

Aluminum Wire Tables, NBS Handbook 109 (Feb. 1972, $0.65, SD Catalog No. C13.11:109), D. Peterson and J. L. Thomas, Eds, is a handbook prepared by the NBS and the U.S. Aluminum Association, presenting data on the conductivities and resistivities of both solid and stranded aluminium wires of various sizes and compositions, together with a variety of other data of interest to the designer of electrical equipment and installations. This publication is a companion volume to NBS Handbook 100, *Copper Wire Tables* (Feb. 1966, $0.50, SD Catalog No. C13.11: 100*).

Properties of Selected Superconductive Materials, NBS Technical Note 724 (1972, $1, SD Catalog No. C13.46:724*) by B.W. Roberts, is a non-critical compilation of data on superconductive materials, extending the data published earlier in *NBS Tech. Note* 482 (May 1969). Properties compiled are composition, critical temperature, critical magnetic field, crystallographic data, and lowest temperature tested for superconductivity.

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