CODATA 8

NEWSLETTER

THIRD INTERNATIONAL CODATA CONFERENCE

on

Generation, Compilation, Evaluation, and Dissemination of Data for Science and Technology

Le Creusot, France, 26—29 June, 1972

Chairman: Prof. Boris Vodar, President of CODATA, Paris, France

Programme Chairman: Dr. Edward L. Brady, NBS, Washington, D.C., U.S.A.

CONFERENCE PROGRAMME

The programme of the Third CODATA Conference was designed with the following principles in mind. The programme should:

1. Provide an opportunity for scientists active in data compilation and evaluation to provide guidance to CODATA on appropriate activities for CODATA to undertake.

2. Rely heavily on input from the various Scientific Unions that are Members of CODATA.

3. Emphasize scientific areas included within the broadened scope of CODATA interests.

4. Concentrate as much as possible on activities of common interest to more than one discipline.

5. Identify activities needing international coordination that are within the resources of CODATA to undertake and, if possible, assess priorities.

There are to be eight sessions in all — morning sessions from 9:00 to 12:30 and late afternoon sessions from 16:00 or 16:30 to 18:30 or 19:00. The afternoon break is intended to make it possible for participants to hold informal discussions with others, several ad hoc groups will be organized and meeting rooms will be available. Discussion time is to be provided after each presentation and all attendees are encouraged to participate. The comments of Conference participants are desired by CODATA as an input to its programme planning.

MONDAY, June 26, 1972

Ceremonial Session: Chairman — *B. Vodar*, Paris, France
Words of Welcome from *M. Malaud*, Ministre de la Fonction Publique, and from other French Officials.

International Framework of CODATA

Session I: Chairman — *H. Viellard*, DRME, Paris, France

A. Introductory Remarks — Session Chairman

B. Rationale and Structure of the Conference
E. L. Brady, Chairman of the Conference Programme Committee, Washington, D.C., U.S.A.

C. Role of the Conference in Development of the CODATA Programme
L. M. Branscomb, U.S. Delegate to CODATA, Washington, D.C., U.S.A.

D. The UNISIST Programme
A. Wysocki, UNESCO, Paris, France

E. Role of CODATA
B. Vodar, President of CODATA, Paris, France

Session II: Chairman — *F. D. Rossini*, Past President of CODATA, Houston, Texas, U.S.A.

A. Introductory Remarks — Session Chairman

B. Activities of CODATA in Chemical Kinetics
S. Benson, Chairman CODATA Task Group on Chemical Kinetics, Menlo Park, Cal., U.S.A.

C. Activities of CODATA Relating to Computer Use
G. Black, Chairman CODATA Task Group on Computer Use, Manchester, U.K.

D. Proposed Values of the Fundamental Constants
E. R. Cohen, Chairman CODATA Task Group on Fundamental Constants, Thousand Oaks, Cal., U.S.A.

E. Key Values of Thermodynamic Properties
S. Sunner, Chairman CODATA Task Group on Key Values for Thermodynamics, Lund, Sweden

F. Presentation of Data in the Primary Literature
E. F. Westrum, Chairman CODATA Task Group on Presentation of Data in Primary Literature, Ann Arbor, Mich., U.S.A.

G. Proposed International Tables of Thermodynamic Properties

H. Discussion period — Activities and Accomplishments of CODATA

Sessions III, IV, V:

Consideration of Broadened Scope of CODATA

In each of the following areas, one or more survey papers are to be presented on the needs for data evaluation and compilation activities and on current projects in the area. Speakers are to be representatives of appropriate Scientific Unions. The aim is to stimulate a discussion that can bring out the common features of data evaluation and compilation projects, demonstrate whatever community of interests may exist, and suggest ways in which individual scientists, Scientific Unions, and CODATA can cooperate to achieve common goals. In some areas a specific activity will be described in some detail in order to illustrate specific solutions to general problems and, hopefully, to demonstrate the ways in which a single project serves the needs of several communities of users.

Earth and Atmospheric Sciences

Session III: Chairman — *M. Roubault*, CRPG, Nancy, France

A. Introductory Remarks — Session Chairman

B. COGEODATA and its Activities
P. Laffitte, Vice President of COGEODATA, Paris, France

C. Federation of Astronomical and Geophysical Services and its Activities
P. Melchior, IUGG Representative on CODATA, Brussels Belgium

D. ICSU Panel on World Data Centres
L. Perek, Prague, Czechoslovakia

E. Illustrative Example: Handling of Geo-Data in the French National Geological Service
F. C. Dumort, BRGM, Orléans, France

F. International Oceanographic Commission
G. Peluchon, Brest, France

Biological Sciences

Session IV: Chairman — *K. Egle*, University of Frankfurt/Main Germany, F. R.

A. Introductory Remarks — Session Chairman

B. Specialists' Needs for Data — Activities of Scientific Unions

(a) International Union of Biological Sciences (IUBS)
P. L. Altman, IUBS Representative on CODATA, Washington, D. C., U.S.A.

(b) International Union of Pure and Applied Biophysics
F. M. Richards, New Haven, Conn., U.S.A.

(c) International Union of Pure and Applied Chemistry (IUPAC)
S. Sunner, Lund, Sweden

C. Achievements of the International Biological Programme
H. A. W. Southon, London, U. K.

D. Activities of the Toxicology and Enzymology Data Centre
Mme. J. Zeraffa, Paris, France

WEDNESDAY, June 28, 1972

Astronomy and Astrophysics

Session V. 1: Chairman — *C. W. Allen*, London, U.K.

A. Introductory Remarks — Session Chairman

B. Numerical Data for Astronomers
G. A. Wilkins, IAU Working Group on Data for Astronomers, Greenwich, U. K.

C. Illustrative Example: Stellar Data Centre of Strasbourg, France
J. Jung, Strasbourg, France

Engineering Sciences

Session V. 2: Chairman — *T. Plebanski*, Warsaw, Poland

A. Introductory Remarks — Session Chairman

B. Data and other Information Needs of Engineers
F. K. Willenbrock, Washington, D. C., U.S.A.

C. Joint WFEO/CODATA Study on Engineering Data
(a) *C. Schäfer*, CODATA, Frankfurt/Main, Germany, F. R.
(b) *J. Larink*, Düsseldorf, Germany, F. R.

D. Illustrative Example: The International Steam Tables Project
K. R. Schmidt, Frankfurt/Main, Germany, F. R.

Computer Topics of Special Interest to Data Analysis Centres

Session VI: Chairman — *M. Kizawa*, University of Osaka, Japan

A. Introductory Remarks — Session Chairman

B. Computer Representation of Numerical and Graphic Data
P. Dubois, DRME, Paris, France,

C. Computerized Data Handling
J. Drobishev (speaker) and *Kaptug*, Novosibirsk, U.S.S.R.

D. Processing Natural Languages for Data Banks
M. P. Barnett (speaker) and Mrs. *B. H. Barnett*, New York, U.S.A.

E. Panel Discussion — Application of Computer Techniques to Data Analysis Centre Operations
Chairman: *Gordon Black*, Manchester, U. K.

F. A Demonstration of the Utility and Economics of on-line Access, Including Trans-Atlantic Access via Satellite, to Basic Reference Data Files,
J. Hilsenrath, Washington, D.C., U.S.A.

THURSDAY, June 29, 1972

Special Topics Important to Data Analysis Centre Operations

Session VII: Chairman — *P. Aigrain*, DGRST, Paris, France

A. Introductory Remarks — Session Chairman

B. The Role of Information Analysis Centres in Science and Technology,
C. Schäfer, CODATA, Frankfurt/Main, Germany, F. R.

C. The Thermophysical Property Data Centre of the Soviet Union as a Focus of a National Network,
E. Shpilrain, Moscow, U. S. S. R.

D. Problems and Solutions in the Development of Specialized Data Centres

(a) Operation of a Thermochemical Data Bank
E. Bonnier, Grenoble, France

(b) Information and Data Analysis Centres Relating to Heat
Mme. A. David, IFCE, Paris, France

(c) Mass Spectrometry Data Centre
W. M. Scott, Aldermaston, U. K.

E. General Discussion

Accessibility and Dissemination of Critical Reviews and Data Compilations

Session VIII: Chairman—*C.N.R. Rao*, Indian Institute of Technology, Kanpur, India

A. Introductory Remarks — Session Chairman

B. Statistical Distribution of Property Data in Published Literature
T. Golashvili, CODATA, Frankfurt/Main, Germany, F. R.

C. Accessibility of Experimental Data — Published and Unpublished
H. W. Koch, New York, N. Y., U.S.A.

D. The Role of Publishing Industry in Production and Dissemination of Critical Reviews and Data Compilations
P. N. Asser, Amsterdam, The Netherlands

E. Special Problems of Small and Developing Countries,
C. N. R. Rao, Kanpur, India

CLOSING REMARKS

A GUIDE TO PROCEDURES FOR THE
PUBLICATION OF THERMODYNAMIC DATA

This document represents the endeavours of an *ad hoc* Committee of Commission I.2 on Thermodynamics and Thermochemistry of IUPAC composed of:

V. P. Kolesov (USSR)

M. L. McGlashan (UK)

Jean Rouquerol (France)

Syûzô Seki (Japan)

C. E. Vanderzee (USA)

E. F. Westrum, Jr. (USA, *Chairman*)

At the 1971 Washington, D. C. Meeting of the IUPAC Commission on Thermodynamics and Thermochemistry it was resolved that the following guide should be given the widest publicity, in order to aid in the resolution of some current problems in scientific communication and in the hope that it might stimulate similar action by other organization concerned with specialized fields of science.

This guide was previously ratified by the All-Union Calorimetry Conference (USSR). The Calorimetry Conference (USA), the Experimental Thermodynamics Conference (UK), the Society of Calorimetry and Thermal Analysis (Japan), and the Société Française des Thermiciens (France).

... ... (US) Calorimetry Conference adopted a resolu-

publication, and so led the Calorimetry Conference to revise extend, and publish its recommendations in 1960. (1) A second revision was authorized in 1970, and it was intended that this new version should be submitted to various calorimetry and related conferences, (2) and to the International Union of Pure and Applied Chemistry for suggestions and ratification.

This has been done with the approval of Commission I.2 of IUPAC and the agreed text is hereby presented in accordance with the terms of the resolution cited at the head of this document. The Commission itself has also prescribed recommendations on the publication of thermochemical studies as early as 1934, (3) as has the scientific council on chemical thermodynamics of IONKh of the USSR Academy of Sciences.(4)

INTRODUCTION

This guide is addressed not only to specialists in calorimetry or in the various aspects of thermodynamics but also to all those who measure and publish thermodynamic quantities as adjuvant aspects of their research endeavors. We would urge all who ever publish thermodynamic values for whatever purpose determined to follow these suggestions so that maximum benefit from their studies will be realized. Journal editors and referees should note that this document embodies a set of consistent, carefully considered criteria for judging the completeness and acceptability of papers reporting thermodynamic quantities. The ultimate needs of the compiler and correlator of such data have been considered also.

Essential Information

The highly interdependent nature of thermodynamic data impos special obligations upon the author of papers reporting the resu of thermodynamic investigation. He must give enough informatic about his experiment to allow readers to appraise the precisic and accuracy of his results so they may be properly consolidat within the existing body of data in the literature. Further, as acce ted values of physical constants change or as new thermodyn mic data for related systems become available, subsequent inves gators often can recalculate results if it is clear that they are bas on good experiments for which adequate information is presel ed, however old they may be. For these reasaons, an autho prime responsibility is to report his results in a form related

terize the results adequately and to allow critical assessment of t accuracy claimed. For the convenience of the reader, the auth may interpret and correlate the primary results as appropriate a present derived results in a form easy to utilize. However, su derived (or secondary) results *never* should be published at t cost of omitting the primary results on which they are base Reference may be made to accessible earlier publications for sor details.

In addition to the presentation of the data themselves, estima of the precision indices and probable accuracy of the data shot be given by the authors. The various sources of uncertainty shot be rigorously described with clear separation of measureme imprecisions, numerical analysis deviations and possible sys matic biases. The methods and assumptions for the statisti analyses should be indicated. Possible sources and magnitudes systematic errors should be identified and enumerated.

Because temperature scales are of such great significance for thermodynamic measurements the considerations and conv sions cited by Rossini (5) and others should be observed. I accurately measured temperatures depending on an Internat nal Practical Temperature Scale, the scale used in calibration the temperature-measuring instrument(s) (e.g., "IPTS-48 as am ded in 1960") and the scale to which the specified temperatu values refer (sometimes these two scales are different, e.g. latter might by IPTS-68) should be stated.

In instances where requisite primary results are too extensive or for other reasons do not merit journal publication in full, the use of auxiliary publication services may be appropriate. (6) A footnote in the publication indicates how the reader may obtain the adjuvant data.

Apparatus and Procedures. A description of the apparatus including details of the reaction container or calorimeter vessel, the controlled environment, and measuring systems such as those for time, temperature, and pressure; the design of calibration heaters and heater lead placement; precautions as to shielding or isolation of calibration circuits; the method of calibration and the sensitivity of the instruments used in these measuring systems such as thermometers, bridges, and potentiometers, flowmeters, weighing devices should be given. The history of a particular apparatus which is used in an on-going series of researches should be maintained and documented as to modifications, improvements, etc., to the end that should corrections be made necessary by subsequent recalibrations or by revelation of systematic errors or bias, such corrections can by applied to all affected data either by the author or by compilers or reviewers. Information establishing the heat capacity of the calorimeter or the energy equivalent (preferably with traceability to a calibrating or standardizing laboratory), together with details of the observational procedures, the methods of evaluating the corrected temperature increment, methods of analysis of results, and the precision of the measurements should be given. The reliability of the results should be established by the use of recognized reference substances such as the samples likely to be recommended by the IUPAC Sub-commission on Standard Calibration Materials (7), those provided by the National Bureau of Standards (U.S.) (8) or by VNIIM (U.S.S.R.) (9), those authorized by the Calorimetry Conference for thermophysical or thermochemical measurements (10), or those systems generally recognized as standard for mixtures, e.g. the solubility of oxygen in water at 1 atm and 298.15 K for gas solubility (11), hexane + cyclohexane for enthalpy increments on mixing (12), and benzene + cyclohexane for volume increments on mixing (13). Determination of the same quantity by two or more independent methods is often an advisable alternative method for detection of systematic error.

Materials. The source of and/or method of preparation for all materials used, including calibration, reference, and auxiliary substances; experimental values for analyses and pertinent physical properties of materials, the criteria of characterization and purity, as well as the method, temperature, time interval, etc. of storing samples and preparing them for measurements should be stated whenever this is important. The density used in reduction of weighing to mass, and special procedures such as for dealing with partially filled ampoules, should be specified. For studies made on solutions, the source, preparation and quality of the *solvent* should always be included, as should information as to dissolved gases (CO_2, air, etc.) whenever these impurities may be of influence on the results. For all thermochemical studies, the methods and results of all analytical investigations on the initial and/or final system should be presented, including tests for incomplete reaction, side reactions, evaporation losses of components from mixtures, corrosion of appatus, etc. These considerations as well as possible dialysis of compounds prior to actual reaction, buffers employed, etc. may be especially important in biothermodynamic studies.

Symbols, Terminology, Units. Authors are encouraged to follow as closely as possible the recommendations of the International System (SI) of units (14) and the symbols and nomenclature approved by IUPAC (15). In particular, authors are urged (a) to use the recommended name for each physical quantity and the preferred symbol, (b) to use the internationally accepted symbols for units, (c) to use SI units, and (d) to adhere, particularly in the labels of columns or rows in tables and in the labels of the axes of graphs, to the implications of the convention: physical quantity = number × unit; for example by the use of $S/(\text{J K}^{-1}\text{mol}^{-1})$ as a label for a series of numbers rather than "S" (with or without a statement somewhere as to what the units are), "$S, \{\text{J}/(\text{K mol})\}$", $S\,\text{J}/(\text{K mol})$, and (e) to functional expressions such as S° (H_2O, g, 298 K) rather than expressions like $S^{\text{o,g}}_{298,\;H_2O}$. (Those authors who elect to use non-SI units should define them in terms of SI units. This might be done, for example, by means of such a footnote as: "Throughout this paper cal_{th} = 4.184 J, Torr = (101.325/760) kPa and Å = 0.1 nm.")

Mode of Presentation of Results. Although a table giving the appropriate independent and dependent variables is often the best form of presentation in that it permits recovery of the primary results, circumstances arise where especially for a great many determinations the same end may be achieved, for example, by the presentation of an equation representing the temperature dependence of the measured quantity and a *deviation* plot showing the individual points. This procedure saves space, promotes clarity and in many instances can be sensitive enough to permit full recovery of individual results without a table.

Occasionally, as in combustion calorimetry, each set of replicate measurements can be acceptably recorded as only the mean value, the magnitude and definition of its precision index, and the number of individual measurements made. For the precision indices on thermochemical data, the conventions suggested by Rossini (16) are recommended.

Occasionally, tabulation of high-temperature thermodynamic functions are given by empirical equations which, instead of being in predetermined form and number of disposable parameters, are derived to fit the enthalpy, vapor-pressure, or other data within their precision at every temperature of measurement. This not only provides ready analytic interpolation, differentiation, or integration (as by a computer), but can save the journal space of longer-than-abbreviated tables when this is an issue. It is obviously not expedient, of course, when the given property function shows major lack of monotonic behavior. Graphical and analytical representation of the primary results or secondary results are occasionally worthwhile for the convenience of the reader, but are not generally a satisfactory substitute for tabular presentation of accurate experimental results. Extensive tabulations of secondary values (e.g., smoothed values at rounded temperatures) should be so designed with values reported at temperatures (or pressures, etc.) so spaced that no serious loss of accuracy will result by using an interpolation formula equivalent to five-place Lagrangian interpolation (17). In particular, a sufficient number of digits should be retained to make such interpolation feasible.

It is not practicable to give detailed recommendations for presenting the results of all types of thermodynamic investigations. However, the following paragraphs do provide recommendations for some important kinds of thermochemical, thermophysical, and equilibrium studies and will serve as guides for related areas.

PRESENTATION OF THERMOCHEMICAL CALORIMETRIC DATA

Reaction Calorimetry. The following experimental quantities should be included if applicable: energy equivalent of the calorimetric system, mass of sample and/or mass of product used in

determining the amount of reaction, masses of auxiliary substances, corrected temperature increment (or if appropriate initial and final temperatures plus heat exchange adjustment), total observed energy change, ignition energy, chemical and physical specification of the initial and final states of the reaction, conversion to "standard" concentrations, correction for side reactions, reduction to standard states (e.g., the "Washburn corrections"), temperature of experiments, final experimental energy (or enthalpy) of reaction and uncertainty interval (with the chemical reaction to which the result applies precisely specified). Derived values such as standard enthalpy and standard Gibbs energy of formation may be provided for the convenience of the reader. Detailed discussion of procedures is available (18, 19).

Solution Calorimetry. Although most of the considerations and literature of the previous paragraph apply, additional material to be included would involve the specification of the temperature of the measurements, appropriately specified concentrations of all reactants, solvent, supporting electrolyte, ionic strength, the precise reaction occurring, etc. Thermochemical studies on solutions should present primary and derived results in sufficient detail that the actual calorimetric process is clearly discernible.

Dilution corrections to standard states should describe any approximations for unmixing (e.g., Young's rule (20) or approximations as to the relative apparent enthalpy of uncharged solutes such as NH_3, CO_2, etc. in the solution. Investigators of thermochemical properties of solutions are urged to ascertain densities of their solutions to facilitate theoretical comparison.

PRESENTATION OF THERMOPHYSICAL CALORIMETRIC DATA

The following information is important for delineating the temperature dependence of the thermodynamic (thermophysical) properties of nonreacting systems and ascertaining the influence of thermal history on measured properties and evaluating the reliability of the results: A table of experimental values of heat capacity or enthalpy increment values including the actual temperature increments used in the measurements (if important as e.g., in transition, pre-melting, or anomalous regions) the chronological sequence of data where the thermal history may be significant (either implicitly by chronological presentation or by a general statement), values of the energy (or enthalpy) increments and temperatures of essentially isothermal phase changes, and the reliability of the data indicated by an estimated uncertainty. These primary experimental results may be supplemented, but never supplanted, by a tabulation of smoothed values of thermodynamic properties at selected temperatures for the convenience of the reader. Where applicable, such tabulations should include values of the appropriate heat capacity, the standard entropy (S^o), the standard enthalpy increment $\{H^o(T) - H^o(0)\}$, the standard Gibbs energy functions $[\{G^o(T) - H^o(0)\}/T]$ (21). Frequently these have been tabulated at 5 K intervals from 0 to 50 K, at 10 K intervals from 50 to 300 K or slightly higher temperatures, at 100 K intervals at higher temperatures, and at the temperatures of phase transitions. Such details need not be given for all substances but are desiderata for important compounds. Use of auxiliary publication services as mentioned above may be more appropriate as repositories for such tabulations. Certainly values at the two important reference temperatures, 273.15 and 298.15 K, should be included in the tabulations. Definitive information on procedures is available (22).

PRESENTATION OF CALCULATED THERMOPHYSICAL FUNCTIONS

Because the usefulness of calorimetric data is extended if calculated thermodynamic function based upon them are provided recommendations for the presentation of such calculated values are incorporated here. The following information with appropriate sources is needed to characterize the results of statistical thermodynamic calculations: Details of the molecular model used, including bond distances and angles, specification of the exact conformation, moments of inertia or rotational constants, symmetry number, complete vibrational assignments, parameters used for calculating contributions of internal rotation, rotational isomerism, anharmonicity, centrifugal distortion, etc., the citation (usually by reference) of formulas and special tabulations used, comparison with experimental thermodynamic data. The functions tabulated should include those indicated in previous sections except that the heat capacity should be C_v^o or C_p^o and in addition, value of the standard enthalpy of formation $\Delta_f H^o$, standard Gibbs energy of formation, $\Delta_f G^o$, and the common logarithm of the equilibrium constant of formation, $\log_{10} K_f$ may be published if warranted. The criterion suggested above for the spacing of values if recommended; this corresponds, for example, to 50 K intervals to 300 K, 100 K intervals to 2000 K, 200 K intervals to 3000 K and 500 K intervals at higher temperatures. Again the values should be given also at the reference temperatures, 273.15 and 298.15 K.

For purposes of smoothness, interpolation and internal consistency, one (but seldom more than one) more digit may be retained than is justified by the absolute accuracy. For calculations on small, rigid molecules, involving anharmonicity, centrifugal stretching, rotation vibration interaction, Fermi resonance, isotopic composition, and any other significant effect, functions may be reported to three decimal digits, e.g.:

12.345 cal K^{-1} mol^{-1} or 51.651 J K^{-1} mol^{-1}.

For more approximate calculations, but with agreement with calorimetric values of C_p^o and S^o obtained by empirical anharmonicity corrections or other semi-empirical procedure, two decimal digits are appropriate. For calculations to the rigid rotator, harmonic-oscillator, independent-internal-rotator approximation, only a single decimal digit should be retained. For still more approximate calculations (based on non-definitive calorimetric data, rough incremental calculations, etc.) the single decimal digit should be subscripted, e.g.:

12.$_3$ cal K^{-1} mol^{-1} or 51.$_7$ J K^{-1} mol^{-1}.

PRESENTATION OF p, V, T DATA

Full disclosure of the use and calibration of the pressure gauge including buoyancy, local gravitational acceleration, fluid heads, pressure reference standards, and pressure point in the sample. Volumetric measurements should be referred to a calibration standard as, for example, the density of mercury or water, and the effects from combined pressure and temperature should be described. Also, volumetric data presented in mass or molar units should include the values assumed for atomic weights as well as a statement of the corrections applied for impurity in the sample.

Here also, the importance of the presentation of primary results should be observed. Primary results are not the instrument readings but the values of physical properties derived from these instrument readings after the application of all calibration corrections, and evaluating equations, etc. These experimental values should be reported in full, together with a brief discussion of the application of various corrections and adjustments. The steps necessary to transform experimental values into final results should be made clear. Particularly, methods of smoothing results and of numerical differentiation or integration should be given as well as the sequence in which they are used. The final results should be accompanied by a statement regarding the magnitude of the differences between the smooth and the unsmooth results. Care should be taken to indicate clearly any results of other workers which are included in the preparation of a composite table. The base for tabulating entropy or Gibbs energy of a compressed fluid should be defined in one of the following ways:

$$\{S(p,T,\text{real}) - S(p,T,\text{ideal})\} \text{ or } \{S(V,T,\text{real}) - S(V,T,\text{ideal})\}.$$

When results are presented in tabular form, the spacing of data should be sufficiently close to permit accurate mapping of the p, V, T surface. Consistency tests for anomalous trends should be applied whenever possible. A related guideline (23) for the specialized communication of results may be of interest.

The results of thermophysical measurements leading to Joule-Thomson coefficients or $(\partial H/\partial p)_T$ should include adequate descriptions of apparatus, procedures, calibrations, and comparison measurements, as well as procedures for data reduction.

Since more accurate characterization of the pressure scale to increasingly high values is now possible, (24) authors should be scrupulous in indicating the pressure scale involved.

PRESENTATION OF OTHER EQUILIBRIUM MEASUREMENTS

Included in this category are such diverse measurements as vapor pressures, either by equilibrium or effusion techniques; studies of solubility, distribution, dissociation, adsorption, or other chemical equilibria, by whatever techniques are applicable; electrochemical measurements, etc. Such measurements provide information leading to the standard Gibbs energy increment for a reaction ($\Delta_r G^0$), but care is needed before associating this value with a *particular* reaction. Here again, details of apparatus, calibration, and experimental procedures should be clearly presented, together with preparations of materials, analytical procedures, and any special procedures applicable to the problem. Evidence as to attainment of equilibrium should be given. Primary results, as defined in connection with p, V, T data, should be reported in full, together with results and methods for reduction of results to standard state conditions, including any auxiliary information or equations, such as those from the Debye-Hückel theory of electrolytes. The chosen standard state should be clearly defined, and the final results, such as $\Delta_r G^0$, $\log_{10} K$ or $\log_{10} p$, should be accompanied by an explicit description or statement of the related reaction, process, or change in state. The presentation should include a discussion of errors, estimates of other factors, including instrumental and analytical limitations, effects of non-attainment of equilibrium, side reactions, non-ideality corrections, etc., to the end that the precision indices for $\Delta_r G^0$ of reaction include such contributions.

Definitive studies on activity or osmotic coefficients should likewise present clear descriptions of apparatus, materials, experimental, and computational procedures, together with sufficient primary results to permit verification of derived results. A forthcoming book will discuss procedures in the areas of equilibrium measurement (25). In reporting adsorption studies, the mass of adsorbent used as well as the duration of the experiment are important.

NON-DEFINITIVE DATA

Although this resolution is concerned primarily with precise and accurate data taken by definitive techniques on well-characterized samples it is recognized that survey measurements are often made for technical and/or analytical purposes and these results are submitted for publication. Such values may be of doubtful significance as a basis for theoretical deductions or for incorporation in critical tables of scientific data. Therefore, the foregoing recommendations do not fully apply and presentation of a brief note summarizing the most important values and heralding a more detailed documentary presentation may be appropriate. However, in differential scanning calorimetric measurements, for example, the characterization of the solid phases before and after the experiment, the composition and pressure of the gas phase, the heating rate, the arrangement of the sample in the cell, the extent of base line drift during the thermal effect and the way it is taken into account should be noted. Additional recommendations for presentation of thermal analysis data have been cited (26).

References

1. *Science* **132**, 1658, (1960). *Physics Today* **14**, No. 2, 47, (1961).

2. The All-Union Calorimetry Conference (USSR), The Calorimetry Conference (USA), The Experimental Thermodynamics Conference (UK), The Society of Calorimetry and Thermal Analysis (Japan), La Section de Calorimétrie de la Société Française des Thermiciens, The International Conference on Calorimetry & Thermodynamics (meeting in Maine), and the Colloque International de Thermochimie (meeting in Marseille).

3. W. Swietoslawski and L. Keffler, "First Report from the Standing Commission for Thermochemistry", IUPAC General Secretariat, Paris, 1934.

4. Institute of General and Inorganic Chemistry (IONKh) *cf.* Zhur. Fiz. Khim. **39**, 1298, (1965).

5. F. D. Rossini, *J. Chem. Thermodynamics* **2**, 447, (1970).

6. For example, National Auxiliary Publications Service of the American Society for Information Science, c/o CCM Information Corp., 909 3rd Ave., New York, New York 10022.

7. IUPAC Subcommission on Standard Calibration Materials; personal communications.

8. U.S. National Bureau of Standards, Office of Standard Reference Materials, Washington, D.C., 20234. *E.g.*, NBS Standard Reference Material 720 (Sapphire heat capacity standard), benzoic acid combustion standard 39i, ‡ 736 tris-hydroxymethylaminomethane (THAM) for aqueous solution calorimetry.

9. Vsesoyuzny Nauchno-Issledovatel'skiĭ Institutt Metrologiĭ (All Union Scientific Research Institute for Metrology).

10. Calorimetry Conference standards such as *n*-heptane, benzoic acid, synthetic sapphire (aluminum oxide), and copper for heat capacity and/or enthalphy measurements.

11. *cf.*, R. Battino and H. L. Clever, *Chem. Rev.* **66,** 395, (1966).

12. *cf.*, M. L. McGlashan and H. F. Stoeckli, *J. Chem. Thermodynamics* **1,** 589, (1969).

13. *cf.*, R. Battino, *Chem. Rev.* **71,** 5, (1971).

14. Le Systeme International d'Unites (SI), International Bureau of Weights and Measures, Sevres, France (1970). Authorized English translations are available: (a) H.M.S.O., London, 1970 and (b) C.H. Page and P. Vigoreux, eds. *N.B.S. Special Publication 330*, U.S. Government Printing Office, Washington, D.C., 1970.

15. A convenient source for this is: *Manual of Symbols and Terminology for Physiochemical Quantities and Units*, M. L. McGlashan, ed. *Pure and Applied Chemistry* **21,** 3, (1970).

16. F. D. Rossini, Chapter 14, in *Experimental Thermochemistry*, Vol 1, F. D. Rossini, ed., Interscience, New York, 1956.

17. *Tables of Lagrangian Interpolation Coefficients*, Prepared by the Mathematical Tables Project, Works Projects Administration of the Federal Works Agency, Columbia University Press, New York, 1944.

18. *Experimental Thermochemistry*, Vol 1, F. D. Rossini, ed., Interscience, New York, 1956.

19. *Experimental Thermochemistry*, Vol 2, H. A. Skinner, ed., Interscience, New York, 1962.

20. T. F. Young, Y. C. Yu, A. A. Krametz, *Discussions Faraday Society* **24,** 37, (1957).

21. The nomenclature "Gibbs energy function" (and "enthalpy function" for $(\{H^o(T) — H^o(0)\}/T)$ have been widely used They are presently being reconsidered by IUPAC and other international scientific unions.

22. *Experimental Thermodynamics*, Vol 1, J. P. McCullough and D. W. Scott, eds. Butterworths, London, 1969.

23. "A. S. M. E. Resolution on Communication of Experimental Data" *Mechanical Engineering* **80,** 147, Nov. 1958.

24. *Accurate Characterization of the High Pressure Environment* N.B.S. Special Publication 326. U.S. Government Printing Office, Washington, D.C. (1971). *cf.*, especially pp. 1—3 313—340.

25. *Experimental Thermodynamics*, *Vol II*, B. Vodar and B LeNeindre, eds. Butterworths, (to be published).

26. H. G. McAdie. *Anal. Chem.* **39,** 543, (1967).

GEOLOGICAL DATA FILES; A FIRST WORLD-WIDE SURVEY

by

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A geological data file may conveniently be defined as a collection of measurements and observations made on a series of geological objects of the same kind. Data files form the basis of practically all geological works. Possibilities offered by computers have, in these last years, given a new interest to these files, because it is now feasible to process great amounts of data and to exchange these data on a wide scale. Benefits to the geological community, when data will be widely circulated on computer processable means, will be enormous. A number of problems remain, however, before this ultimate goal is obtained. The most difficult pertain to the methodology of building consistent data files. Experience has shown that the building of great geological data files encounters difficulties, which could hardly have been foreseen at the start. These difficulties, however, will not appear before the file has already reached an important volume and represented a conspicuous investment in man/years. Coping with these difficulties by modifying the recording system represents a costly task. Hence, the experience acquired by others when attempting to build a storage system is valuable. It is therefore of interest to know (1) who has collected a given type of geological data and (2) who has experience with the methodology to be used.

Among the tasks of Cogeodata figures the creation and updating of an international index to geological data. As a first step, a questionnaire has been sent in 1970, (a) to the recipient of "Computer Contributions" of the Kansas Geological Survey thanks to Professor Daniel F. Merriam, (b) to the geologist mentioned in the G.O.S.S.I.P. list of T.V. Loudon (I.G.S. London), and (c) individually to a series of geologists likely to possess a data file. The questionnaire has also been published in *Geo-Sciences Documentation* (Graham Lea, ed., London), and has been announced in *Atlas* (Elsevier) and in the I.U.G.S. Geological *Newsletters*. For France, use has also been made of an inquiry on current activity in "informatique géologique" carried out in 1969 by B. de Jekhowsky, secretary of the French "Comité d'informatique géologique". In 1967 and 1969, Dr. G. H. Scott (New Zealand Geological Survey) disseminated questionnaires to geological organizations in Australasia on behalf of Cogeodata The answers he received have been incorporated in the list. The collaboration offered by these editors and specialists has made

possible the present inquiry and is gratefully acknowledged. To present in a consistent way the 159 answers, it has been necessary to introduce several types of classification; they are explained in Section 2. The files are listed in Section 3, grouped by countries in alphabetical order. Some files kept on manual supports (plain cards, folders, . . .) have been included because a number of these files is likely to be computerized in the near future. For about one third of the data files, thought to be representative of the various kinds of existing files, a description is given in Section 4. These descriptions have been checked by the persons in charge of the file.

Files thus described are asterisked in the main list. Section 5 contains indexes by themes (paleontology, oil, petrography . . .); by purposes of files (inventory, pilot file, catalogue . . .); by degrees of availability of contents and by types of physical supports. A list of files to which original and available computer programmes are directly related, is also included.

As it stands, the list is probably a fair representative sample of the diversity of geological data files which are created and processed to-day. The degree of coverage obtained by the inquiry is difficult to estimate and varies considerably from country to country. The difficulties to assemble information from various continents with limited means should not be forgotten. The task was further complicated here by the fact that the list is, in all likelyhood, the first of its kind to be established on an international level.

It is therefore to be considered as a first effort towards the creation of a permanent index.

After the present draft has been duly corrected, it is intended to publish it in the CODATA *Bulletin*.

NEW PUBLICATIONS

NUCLEAR PROPERTIES

Periodic System of the Elements, Journal of the Academy of Science, "Chimia i jizh", Moscow, U.S.S.R., 1971.

The table suggested to the readers was compiled by I. Selinov according to data as of June 1971. It has several features that distinguish it from former tables.

First, refined atomic masses, computed by A. Mekhtiyeva and I. Selinov on the basis of the new table of atomic masses of isotopes by A. Wapstra and M. Gova and according to more reliable relative distributions of isotopes in nature, are included in it for many elements. The international table of atomic masses has remained practically unchanged since 1964, when the former table of atomic masses of isotopes was published. In the new table the atomic masses of monoisotopic elements are determined 1,000 times more accurately on the average; the reduced atomic masses of other elements are also much more accurate. In those cases when the atomic masses, after rounding off (according to the usual rules), give the same number in the fifth position as the international table of atomic masses, the old accepted values are given; in those cases when the differences are greater, new refined values are presented.

Second, the table includes hypothetical data on not yet synthesized but predicted elements, up to 118, since ambitious programs are already under way to synthesize the far trans-uranic elements (they are preliminary reports of the discovery of isotopes of elements 107 and 112), and also to determine the nature of the 114th element. The symbols of these elements are made up of the symbols of their lighter analogs preceded by the letter E, denoting the prefix "eka", introduced by D. I. Mendeleyev to signify predicted, but not yet discovered elements. The names and symbols of elements No. 102, 103, and 104 are placed in parentheses, since they have not yet become generally accepted: the now synthesized element No. 105 is given without any name at all and is denoted by the symbol "E-Ta" ("eka-tantalum"), since the

question of its name and symbol had not yet been considered by anybody at the time the table was compiled. A. Giorso suggests that element No. 104 be called "rutherfordium" (Rf) and element No. 105 — "hahnium" (Ha). G. Flerov calls element No. 105 "Nielsbohrium" (Ns).

Third, all s- and p-elements are placed in this table in a-subgroups, and d-elements, in b-subgroups; the double position of hydrogen, helium and thorium is denoted by the fact that the numbers of both groups to which these elements may be related are indicated in the corresponding boxes.

Finally, the relationship is shown between the periodic chart of the elements and the periodic system of the atomic nuclei, in which the relationship between the atomic masses of the elements is shown, and also the relationship between the mass numbers of the central isotopes and the ordinal numbers of the elements, (see I. P. Selinov, **Izotopy** (Isotopes), Vol. 3, "Nauka" Publishing House, 1970).

Tables of Rotational Wavefunction d_{MK}^{I}, $I \leq 13$ **AND** $I \leq 25/2$ — Compilations of Experimental and Theoretical Results in Nuclear — Structure Physics, by A. N. Behkami, J. Nuclear Data Tables, ed. Katharine Way, Volume 10, Number 1, September 1971.

Harmonic – Oscillation – Relative – Coordinate Transformation Coefficients. Compilations of Experimental and Theoretical Results in Nuclear – Structure Physics, by A. Barber and B. S. Cooper, J Nuclear Data Tables, ed. Katharine Way, Volume 10, Number 1, September 1971.

Table of Electromagnetic M1 Reduced Transition – Probability Matrix Elements between Nilsson States in Odd-A Nuclei. Compilations of Experimental and Theoretical Results in Nuclear Structure Physics, by E. Browne and F. R. Femenia, J. Nuclear Data Tables, ed. Katharine Way, Volume 10, Number 1, September 1971.

Tables of Energies of Gamma Rays Occurring during Decomposition of Radioactive Nuclei, by B. S. Dzhelepov, S. F. Koshkareva, "Nauka" Publishing House, Moscow, U.S.S.R., 1970.

Selective compilation of $\pi^-p \to \pi\pi N$ Events from Hydrogen Bubble Chambers, CERN/HERA fat 71-1 by L. D. Jacobs, M. Roos and S. Santiago, Sixteen hydrogen bubble-chamber experiments on the reaction $\pi^-p \to \pi\pi N$ at beam momenta 1.7 — 3.2 GeV/c are compiled in the form of fitted events (four-vectors) on a Data Summary Tape. Consistent data are added to give a numerical Chew-low table, graphs and tables of spherical moments as functions of beam momentum and dipion mass, and numerical tables of $\cos \theta_{\pi\pi}$ versus azimuth as a function of dipion mass.

Nuclear Data for Reactors, Proceedings of the Second International Conference on the Subject Convened by the IAEA, Helsinki, 15, 19 June 1970. Volume 1, 1970, 742 pp, $ 21.00; Volume 2, 1970, 960 pp, $ 24.00.

The book deals mainly with the nuclear data aspects most important for nuclear technology. A great part of it is devoted to the measurement and analysis of neutron cross-sections due to the importance of the development and systematic exploitation of high-intensity neutron sources, such as modern linear accelerators, modern cyclotrons and underground nuclear explosions, improvements in instrumentation and in sample-preparation techniques, etc. It also discusses the systematic evaluation of fission, capture and inelastic-scattering cross-sections of the most important fissile and fertile nuclei and of capture cross-sections of the main structural materials. It contains: Cross-sections and techniques for high-precision neutron nuclear data measurements. Nuclear data in the thermal and resonance-energy region: A>220 and A<220. Nuclear data above the resonance energy: A>220 and A<220. Relationships of microscopic and integral data. Evaluation problems.

Bulletin of the Center on Nuclear Data. State Committee on the Utilization of Atomic Energy, U.S.S.R., No. 6, Atomizdat, 1969, 447 pp; No. 7, Atomizdat, 1971, 87 pp; Scientific editor, V. A. Kuznetsov. Contains nuclear-physics constants, reactor constants, shielding characteristics and constants. The results are presented in the form of tables and graphs.

Defense Nuclear Agency Cross Section Library. The Defense Nuclear Agency (DNA) has established a comprehensive program to provide cross section data adequate to allow its contractors to make transport calculations to the degree of accuracy required on their projects. This means the evaluations will contain both neutron interaction and secondary gamma-ray production data. Two key features of the library are that it is in ENDF format and it is a working library – that is, a library that will change as rapidly as is necessitated by the availability of new information. The main factor in the DNA program is the concept of a single evaluator responsible for a given material. He is funded and has complete responsibility for updating and seeing that the best information is inserted into the evaluated cross-section data.

RSIC's role is as a clearinghouse. We receive the data from evaluators, check for format conformity, process through syntax and physics checking codes, plot the data, coordinate reviews, correct errors, and package the data for distribution. We communicate with the evaluator about possible changes but update only when directed by the evaluator.

The present contents of the library are listed in the table. The library is not restricted for use by DNA contractors but is generally available to the scientific community.

MATERIAL	EVALUATORS	DATE
Iron	Penny, Kinney, Wright, Perey – ORNL	Sept. 71
Nitrogen	Young, Foster – LASL	July 71
Oxygen	Young, Foster – LASL	August 71
Aluminium	Young, Foster – LASL	July 71
Lead	Fu, Perey – ORNL	Sept. 71
Hydrogen	Stewart, LaBauve, Young – LASL	March 71
Silicon	Kinsey, Drake – BNL	Sept. 71
Calcium	Perey, Fu, Kinney – ORNL	Sept. 71

(from Radiation Shielding Information Center, *Newsletter,* No. 87 February 1972).

Nuclear Physics Investigations in the U.S.S.R., A Collection of Annotations, Chief Scientific Editor, V. A. Kuznetsov; Chief Editor, D. A. Kardashchev, Information Center on Nuclear Data, Obninsk; Number 8, 1969, 20 pp; Number 9, 1969, 31 pp; Number 10, 1970, 53 pp; Atomizdat, Publishing House of the State Committee on the Utilization of Atomic Energy, U.S.S.R. Contains works (tables and graphs) on nuclear data from the Institute of Physics and Energetics, Obninsk; Theoretical and Experimental Physics, Moscow; Khlopin Radium Institute, Leningrad; Joint Institute of Nuclear Investigations, Dubna; Institute of Physics Academy of Sciences UkrS.S.R.; I. V. Kurchatov, Institutes of Atomic Energy, Moscow.

ATOMIC AND MOLECULAR PROPERTIES

Physics of Atomic Collisions, Second Edition, by J. B. Hasted Butterworth, London, 1972, 784 pp, £ 20.00, contains information on collisions, populations, energy distributions, the elastic scattering of electrons by atoms and molecules, excitation of atoms and molecules by electrons, ionization by electrons, positive ion recombination, electron attachment and detachment photon emission and absorption, elastic collisions between atomic particles, ionization and excitation by atomic particles, charge transfer processes, collisions of excited species, chemical interchange collisions.

Low Temperature Spectroscopy; Optical Properties of Molecules in Matrices, Mixed Crystals, and Frozen Solutions, by B. Meyer American Elsevier, New York, 1971, 653 pp, $ 33.50. The text is on low temperature spectroscopy of matrix isolated atoms, diatomics and polyatomics, trapped free radicals, mixed organic crystals, and aromatic hydrocarbons. Only electronic spectra of samples below 100 K are considered. Complementary infrared data are included to support identification of species. Numerous tables, some figures, 101-page bibliography.

OSTI Report Series. The following reports have been added to the OSTI (Office for Scientific and Technical Information, London) Report Series held by the National Lending Library for Science and Technology, 5086, 5087 – Information storage and retrieval on atomic and molecular physics, (from OSTI *Newsletter,* No. 2, June 1971).

Atomic and Molecular Data Series – American Society for Testing and Materials (ASTM) Publications, 1916 Race Street, Philadelphia, Pennsylvania 1903, U.S.A.
Data publications providing mass, infrared, and ultraviolet spectral information and chromatographic information.

Title	Designation	Former Designation	Pages
– Mass Spectral Data-Chemical Structure Cards	AMD 10a	DS 27–1a	12
– Mass Spectral Data-Name Cards	AMD 10b	DS 27–1c	12
– Mass Spectral Name-Formula Cards	AMD 10c	DS 27–1b	12
– Mass Spectral-First Supplement to AMD 10a	AMD 10a–S1		12
– First Supplement to AMD 10b	AMD 10b–S1		12
– First Supplement to AMD 10c	AMD 10c–S1		12
– Index of Mass Spectral Data	AMD 11	DS 27	12
– Gas Chromatographic Data Compilation	AMD 25 A	DS 25 A	7
– Supplement	AMD 25 A–S1		
– Gas Chromatographic Data on Magnetic Tape	AMD 26		8
– Gas Chromatographic Data on Microfilm	AMD 27		8
– Molecular Formula List of Compounds, Names, and References to Published Infrared Spectra; Through the 13th Supplement	AMD 31	DS 24	11
– Fourteenth Supplement	AMD 31–S14		
– Serial Number List of Compound Names and References to Published Infrared Spectra; through the 13th Supplemeet	AMD 32	DS 29	11
– Supplement	AMD 32–S14		
– Infrared Spectral Index, magnetic tape	AMD 33 A		11
– Thirteenth Supplement to the Infrared Spectral Index, magnetic tape	AMD 33–S13		11
– Fourteenth Supplement, magnetic tape	AMD 33–S14		11
– Alphabetical List of Compound Names, Formulae, and References to Published Infrared Data	AMD 34		11
– Superseded by AMD 35 A	AMD 35		N.A.
– Computerized Search System	AMD 35 A		12
– Infrared Spectral Index on Disk	SIRCH		12
– Infrared Spectral on Tape	SIRCH 360		11
– Infrared Name-Formula Index on Magnetic Tape	AMD 36		11
– Fourteenth Supplement, Magnetic Tape	AMD 36–S14		11

SPECTRA

The Solar Spectrum from λ 7498 to λ 12016, A Table of Measures and Identifications, Volume Hors Série, no. 5, by J. W. Swensson, W. S. Benedict, L. Delbouille and G. Roland, Société Royale des Sciences de Liège, Belgium, 1970. 449 pp, $ 16.00. This book is intended as a description of the solar spectrum between λ 7498 and λ 12016 as derived from measures of the 10,840 solar and telluric absorption lines appearing on a series of photometric records obtained by L. Delbouille and G. Roland with a high resolution prismgrating spectrometer installed at the Jungfraujoch International Scientific Station, Switzerland (altitude: 3,580 meters).

Photometric Atlas of the Solar Spectrum from λ 3000 to λ 10,000, by L. Delbouille, G. Roland, Institut d' Astrophysique, Université de Liège, Belgium, and L. Neven, Observatoire Royal de Belgique, Uccle, Belgium, Information from: Dr. G. Roland, Institut d' Astrophysique, B-4200 Cointe-Ougree, Belgium, First Delivery, Summer 1972, 106 pp, $ between 20.00 and 30.00. It will cover the region λ 4300 to λ 6200, in a loose leaf binder which will hold the complete set of records. Final issue expected 1974.

Selected Tables of Atomic Spectra. The latest critical compilation in the NSRDS series is Section 4 of NSRDS-NBS 3, Selected Tables of Atomic Spectra, Atomic Energy Levels and Multiplet Tables N IV, N V, N VI, N VII by Charlotte E. Moore (55 cents, SD Catalog No. C13.48:3/Sec. 4). This publication is part of a series being prepared in response to the increasing demand for a current revision of two sets of tables containing data on atomic spectra as derived from analyses of optical spectra. Meanwhile, work is underway to update and revise the first set, Atomic Energy Levels, NBS Circular 467, which will be reprinted and published at a later date as NSRDS-NBS 35, Volumes I, II, and III. (from NSRDS News, November 1971).

Infrared Spectra of Inorganic Compounds, by R. A. Nyquist, R. O. Kagel, Academic Press, New York, 1971, 495 pp, $ 24.95. It gives information on Experimental, Arrangement of spectra, Spectra-structure correlations, References, Numerical index of spectra, Alphabetical index of spectra, Spectra. A reference work for scientists specializing in analytical chemistry, presents a collection of spectra of nearly 900 compounds. The spectra are in two parts, from 2.6 to 25 μm and from 17 to 220 μm.

The Hydrogen Molecule Wavelength Tables of Gerhard Heinrich Dieke, Editor, H. M. Crosswhite, John Wiley & Sons Ltd., U. K., gives information on Energy Levels of H_2, The Spectrum of H_2. 1972, approx. 656 pp, approx. £ 9.35.

Carbon-13 NMR Spectra: A Collection of Assigned, Coded and Indexed Spectra, by Le Roy F. Johnson, W. C. Jankowski, John Wiley & Sons Ltd., U. K., 1972, approx. 680 pp, approx. £ 9.35. This book consists of a collection of 500 proton noise decoupled Carbon-13 NMR spectra of a variety of organic molecules. All chemical shifts are listed and approximately 3000 chemical shift assignments with structural coding are collected in functional group and chemical shift indices. A wide selection of organic substances were carefully chosen to produce a collection of Carbon-13 spectra which would be useful as reference material in the elucidation of the structure of unknown chemical substances.

DMS Working Atlas of Infrared Spectroscopy, by N. A. J. Luff, Butterworth, London, 1972, 318 pp illustrated, £ 7.00. A selection of spectral tracings compiled from the 20.000 card collection of the Documentation of Molecular Spectroscopy Index, which has just completed its 14th year. The 825 spectra have been specially selected to illustrate important chemical aspects such as ring size. It contains: Spectra, Formula Index, English Alphabetical Index, German Alphabetical Index.

A Review of the Structure and Physical Properties of Liquid Crystals, by Glenn H. Brown, J. W. Doane and Vernon D. Neff. Butterworth, London, U.K., 1971, 94 pp, £ 5.00.
Covers recent basic work on the structure and physical properties of the thermotropic and Iyotropic liquid crystals. Infrared and Raman Spectra of Liquid Crystals. Light Scattering and Spin-Iattice Relaxation. Magnetic Resonance. Other Physical Properties.

SOLID STATE PROPERTIES

CRYSTALLOGRAPHIC PROPERTIES

Molecular Structures and Dimensions. Volume 3 of the new reference series published by the Crystallographic Data Centre and the International Union of Crystallography has appeared in February 1972. The new volume contains classified bibliographic information on organic and organometallic structures published during 1969–1971. The arrangement is identical with the first two volumes in the series with entries arranged in chemical classes and extensive cross-references. There are three indexes: author, formula and transition metal. All are cumulative for the years 1935-1971 and give references to entries in Volumes 1–3.

The books are available from any bookseller, directly from A. Oosthoek, Domstraat 5–13, Utrecht, Netherlands, and from the Polycrystal Book Service, P.O. Box 11567, Pittsburgh, Pennsylvania, U.S.A.

Prices for the three volumes are:

	Personal	Library
Vol. 1 (1935–1969)	£ 3.90 ($ 10.00)	£ 5.40 ($ 14.00)
Vol. 2 (1935–1969)	£ 3.30 ($ 8.50)	£ 4.30 ($ 11.00)
Vol. 3 (1969–1971)	£ 4.70 ($ 12.50)	£ 6.50 ($ 17.00)

Landolt-Börnstein New Series, Group III: Crystal and Solid State Physics, Volume 5, parts a and b: Structure Data of Organic Crystals, by E. Schudt and G. Weitz, Editors: K. H. Hellwege and A. M. Hellwege, XXII, VIII, 1971, 1626 pp, $ 277,20. Volume 6, Structure Data of Elements and Intermetallic Phases, by P. Eckerlin and H. Kandler, with the assistance of A. Stegherr. Editors: K. H. Hellwege and A. M. Hellwege, XXVIII, 1971, 1019 pp, $ 179,10, Springer-Verlag, Berlin, Heidelberg, New York. Volume 6 continues the compilation of structural data on crystals, started with volume 5. It contains the data on elements and intermetallic phases. Compiled are the space groups, the lattice constants with their dependance on temperature and pressure, as well as other information. A complete presentation of all atomic parameters was not possible within the limits of this volume, but references are given when the cited original paper contains a complete structure analysis. The substances are arranged alphabetically within each chapter. A list of mineral and common names is given at the end of the volume. Distribution of substances within volumes 5 and 6. Volume 5: Organic compounds, Elemento-organic compounds, Salts with at least one organic substituent, Coordination compounds with at least one organic substituent. Volume 6: Elements and all inorganic phases which do not contain, O, N, F, Cl, Br, I, At and do not belong to volume 5.

Crystal Data. Determinative Tables, third edition. Recognizing the need for updated crystallographic information, the Office of Standard Reference Data has sponsored the issuance of the third edition of *Crystal Data*, Determinative Tables. The publication should be of particular interest not only to crystallographers but also to chemists, mineralogists, physicists and individuals in related fields of study. The current edition, which comprises two volumes, Organic and Inorganic, is a thoroughly revised and updated work, containing over 30,000 entries. The entries 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. In addition, the following information is given: axial ratio(s) and interaxial angles not fixed by symmetry, cell dimensions, space group or diffraction aspect, number of formula units per unit cell, crystal structure (whether determined), measured density and x-ray calculated density. Also listed is the name of the compound and synonym(s), chemical formula, literature reference and transformation matrix. When available, the crystal structure type, crystal habit, cleavages, twinning, color, optical properties, indices of refraction, optical orientation, melting point and transition point are also listed.

The first edition of *Crystal Data* was published as Memoir 60 of the Geological Society of America in 1954. The second edition was issued in 1967 as Monographs 5 and 6 of the American Crystallographic Association. Both editions proved extremely valuable to crystallographers throughout the world. The present edition culminates years of effort by J. D. H. Donnay, John Hopkins University; Helen M. Ondik, National Bureau of Standards; Sten Samson, California Institute of Technology; Quintin Johnson, Lawrence Radiation Laboratory; Melvin H. Mueller, Argonne National Laboratory; Gerard M. Wolten, Aerospace Corporation; Mary E Mrose, U.S. Geological Survey; Olga Kennard and David G. Watson, Cambridge University, England and Murray Vernon King, Massachusetts General Hospital.

The third edition of *Crystal Data* will be available in the very near future. For further information and price schedules, please write directly to:

Joint Committee on Powder Diffraction Standards
1601 Park Lane, Swarthmore, Pennsylvania 19081

(from NSRDS News, November 1971).

Alloys of Silicon with Transition Metals of the Fourth Period, P. V. Gel'd, and F. A. Sidorenko, Metallurgiya, Moscow U.S.S.R., 1971, 3 r. 30 k. The most important physical and physicochemical characteristics of solid and liquid alloys of transition metals of the fourth period with silicon are described systematically. Data are given for the temperature and concentration regions where silicides are stable and for their basic thermodynamic characteristics. Data are correlated concerning the crystal structure of the silicides, the complexity of their lattices, and the solutions they form. Information is given concerning their electrical conductivity, magnetic susceptibility, and other electrophysical and magnetic properties. The varied properties of liquid silicides and possible models for their short-range order are examined.

Phase Diagrams of Silicate Systems, No. 3. Ternary Systems, Part I, Silicate Systems. Handbook, Nauka, Leningrad, U.S.S.R., 1971, (I. V. Grebenshchikov Institute for Silicate Chemistry), 2. r. The handbook contains the primary information about silicate systems. In addition to the large quantity of graphic material and tables, methods of synthesis and phase transformations are described, and some constants are cited.

THERMODYNAMIC, THERMOPHYSICAL AND

TRANSPORT PROPERTIES

International Thermodynamic Tables of the Fluid State – Argon 1970 IUPAC, (in preparation), Butterworth, London, 1972, will be a compilation of internationally agreed values of the equilibrium thermodynamic properties of liquids and gases of interest to scientists and technologists. The range covered for each fluid is that for which exists reliable experimental data. It will contain, introduction, symbols and units, conversion factors: 1. the constituent tables. 2. the IUPAC tables, acknowledgements, references, saturation properties, single-phase properties, tolerance diagrams.

Thermodynamic Tables in SI (metric) Units, by R. W. Haywood, Cambridge University Press, 1972, 42 pp, £ 0,80, contains thermodynamic tables for students in SI units, all units are carefully defined and conversion factors listed. It includes general data, thermochemical tables, steam tables, refrigerant tables, air at low temperatures, transport properties of various fluids, appendices, pull-out charts (also available separately) of the enthalpy-entropy diagram for steam and pressure-enthalpy diagram for Refrigerant-12.

Thermophysical Properties of Nonmetallic Materials, by R. Ye. Krzhizhanovskiy, Z. Yu. Shtern, Energiya, Leningrad, U.S.S.R., 1970, 432 pp, 1 r. 63 k. Data on the physical properties of oxides and carbides over a wide temperature range and other parameters are cited in the handbook. For these materials chief attention is given to thermophysical and thermodynamic properties such as thermal conductivity, heat capacity, linear expansion, and others. On the basis of the experimental data available the effect on these properties of such factors as temperature, heat treatment, amount of impurities, material density, and medium is considered. In addition to thermophysical properties, as a rule, data characterizing structure, degree of interaction with other materials, and some other general information are given for each material.

Thermodynamic Constants of Compounds, No. IV, Part 2, by V. A. Medvedev, V. S. Yungman, G. A. Bergman, V. P. Kolesov, L. V. Gurvich, A. F. Vorob'yev, V. P. Vasil'yev, V. N. Kostryukov, L. A. Reznitskiy, N. T. Ioffe, V. F. Baybuz, V. I. Alekseyev, G. L. Gal'chenko, G. G. Malenkov, N. L. Smirnova, et al (under the scientific supervision of V. P. Glushko), VINITI, Academy of Sciences, Moscow, U.S.S.R., 1971, 431 pp, 2 r. 32 k.

Thermodynamic Constants of Compounds, No. V, by V. A. Medvedev, G. A. Bergman, L. V. Gurvich, V. P. Vasil'yev, V. S. Yungman, V. P. Kolesov, V. N. Kostryukov, L. A. Reznitskiy, G. L. Gal'chenko, V. I. Alekseyev, N. L. Smirnova, A. F. Vorob'yev, V. F. Baybuz, et al (under the scientific supervision of V. P. Glushko), VINITI, Academy of Sciences, Moscow, U.S.S.R., 1971, 530 pp, 2 r. 55 k.

Thermodynamic and Thermophysical Properties of Combustion Products, 5 Volumes. Volume 1, Calculation Methods, by V. Ye. Alemasov, A. F. Dregalin, A. P. Tishin, V. A. Khudyakov, (under the scientific supervision of V. P. Glushko), VINITI, Academy of Sciences, Moscow, U.S.S.R., 1971, 266 pp, 1 r. 73 k.

Refractory Compounds, Thermodynamic Characteristics, by R. F. Voytovich, Naukova dumka Publishing House, Ukr.S.S.R., 1971, 1 r. The manual discusses problems characterizing the high-temperature stability of refractory compounds in various media. Data are presented on thermodynamic stability of borides, yttrides and silicides in a vacuum. Tables of the thermodynamic functions of certain borides, carbides and yttrides are given in the appendix.

Dissociating Gases, by A. K. Krasin, V. B. Nesterenko, Nauka Publishing House, Minsk, U.S.S.R., 1970, 311 pp, 1 r. 72 k. Presented in the book are the thermodynamic and transport properties, heat exchange and gas dynamics of dissociating gases.

Heat Exchange in Chemically Reacting Gaseous Heat Carriers, by A. K. Krasin, V. B. Nesterenko, A. I. Devoyno, Nauka Publishing House, Minsk, U.S.S.R., 1971, 168 pp, 0.74 k. Presented are theoretical and experimental data for the gas N_2O_4.

NBS Technical Note 270-6, Selected Values of Chemical Thermodynamic Properties, Tables for the Alkaline Earth Elements (Elements 92 through 97 in the Standard Order of Arrangement), by V. B. Parker, D. D. Wagman, W. H. Evans, $ 1.25, SD Catalog No. C13.46:270-6, is the 6th in a series of Notes containing tables of numerical values prepared as a revision of NBS Circular 500, Selected Values of Chemical Thermodynamic Properties. This Note contains tables of values for the standard heats and Gibbs free energies of formation, entropies and enthalpies at 298.15 K, and heats of formation at 0 K for compounds of beryllium, magnesium, calcium, strontium, barium, and radium.

NBS Technical Note 384, Thermophysical Properties of Oxygen from the Freezing Liquid Line to 600 R for Pressures to 5000 Psia by Robert D. McCarty and Lloyd A. Weber, $ 1.50, SD Catalog No. C13.46:384, was compiled on the properties of oxygen commonly used for engineering calculations. The values presented have been critically evaluated by the authors and represent the "best values" available at this time.
The tables include entropy, enthalpy, internal energy, density, volume, speed of sound, specific heat, thermal conductivity, viscosity, thermal diffusivity, Prandtl number and the dielectric constant for 79 isobars. Also included in the isobaric tables are quantities of special utility in heat transfer calculations (from N.S.R.D.S. News, December 1971).

Physical Properties of Sedimentary Rocks at High Pressures and Temperatures, by G. M. Avchyan, Nedra Publishing House, U.S.S.R., 1972, 1 r. 14 k. Results are presented on experimental investigations of the effect of up to 2,500 kg/cm² hydrostatic pressure, up to 1,000 kg/cm² stratal pressure and of temperatures up to 250°C on the velocity of an elastic longitudinal wave, specific resistivity, density, porosity, and compressibility of sedimentary rocks saturated with various fluids. The relations between the physical parameters of the rocks and various thermodynamic conditions are characterized, the setups for high pressure and temperature developed in the U.S.S.R. and abroad are described.

Manual of Thermodynamic Values (for Geologists), by G. B. Naumov, B. N. Ryzhenko, I. L. Khodakovskiy, Editor, A. I. Tugarinov, Atomizdat, Moscow, U.S.S.R., 1971, 239 pp, 1 r. 60 k.

Thermodynamic and Transport Properties of Chemically Reacting Gas Systems, by A. K. Krasin, V. B. Nesterenko, Nauka Publishing House, Minsk, U.S.S.R., 1971, 234 pp, 1 r. 8 k.

Specific Energies of Galvanic Reactions: and Related Thermodynamic Data, by J. Sudworth and J. G. Gibson, Chapman & Hall, 1971, 1088 pp, £ 7.50. Consideration of those reactions involving the compounds of oxygen, sulphur and the halogens has produced calculations for approximately 50.000 reactions which cover most of those which are likely to be considered for novel battery systems. The chapters in the book are divided into the following sections: Thermodynamic data; Elemental reactions; Displacement reactions-Transition elements, B-sub group elements.

CHEMISTRY   CHEMICAL KINETICS

NBS-OSRDB-71-2, A Bibliography of Kinetic Data on Gas Phase Reactions of N_2, O_2 and Nitrogen Oxides, by Francis Westley (COM-71-00841, Hard Copy $ 3, Microfiche 95 cents) is the latest publication in the NBS Office of Standard Reference Data Bibliography Series published by the National Technical Information Service.
This Bibliography lists papers and reports on the gas phase reaction kinetics in the nitrogen-oxygen system through 1970. Only reactions among N, N_2, O, O_2, O_3, and the nitrogen oxides are considered. The material is presented in two methods: by reaction, with a listing of each pertinent article; and in a general reference list, which has been arranged alphabetically by first author.

Evaluated Kinetic Data for High-Temperature Reactions, Volume 1: Homogeneous Gas Phase Reactions of the $H_2 - O_2$ Systems, by Baulch, Drysdale, Horne and Lloyd, Butterworth, London, 1972, approx. 448 pp, £ 10.00. The thermodynamic data for each reaction and its reverse are recorded, together with all available reaction rate measurements, which are displayed in tabular and graphical form. The data are critically evaluated and discussed and, whenever possible, a rate expression is derived. The error limits and conditions under which the recommended rate parameters are applicable are defined. The reactions considered have been selected by a panel consisting of representatives from industry, government research establishment and universities. The reactions covered in this volume are of importance in combustion and air pollution research, upper-atmosphere studies, re-entry problems and high-temperature systems generally. As such they will be of use to chemist, physicists and mechanical and chemical engineers. Two other volumes are scheduled for future publication: Homogeneous Gas Phase Reactions of the H_2-N_2-O_2 Systems and Homogeneous Gas Phase Reactions of the H_2-O_2-CO and H_2-O_2-S Systems.

Investigation of Vanadium Compounds of Elements of Groups I and II. Ural'sk Affiliate of U.S.S.R. Academy of Sciences Publishing House, 1971, 170 pp, 60 k. The collection pertains to analysis of the properties of vanadium compounds of groups I and II and the conditions of their formation. The results of experiments on the kinetics of the reaction of vanadium pentoxide with com-

pounds of the alkali and alkaline-earth metals are published; the optical, thermal and other properties of individual vanadates are analyzed; phase diagrams are constructed and corrected for the systems: oxides of S-elements — vanadium pentoxide, and also vanadate-vanadate. Data obtained lead to individual generalizations and in a number of cases permit critical review of certain fundamental concepts of the phase composition in the examined systems and the chemistry of the reaction of salts of the S-metals with vanadium pentoxide. Considerable attention is devoted to analysis of oxygen vanadium bronzes of the alkali and alkaline-earth elements. The results of the work are of practical importance and represent a considerable contribution to the physical chemistry of vanadium.

IUPAC. Selected Constants: Oxidation Reduction Potentials of Inorganic Substances in Aqueous Solution (IUPAC Supplement), by G. Charlot, Mme A. Collumeau, M. J. C. Marchon, Butterworth, London, 1972, 80 pp, £ 3.50. A presentation of tables intended to provide the chemist with a convenient working tool which will enable him to find rapidly the best or most probable values of the normal or formal oxidation-reduction potential of a given oxidation-reduction system.

Phase Diagrams of Silicate Systems, Handbook, No. 2, Metal-Oxygen Components of Silicate Systems, by N. A. Toropov, V. P. Barzakovskiy, I. A. Bondar', and Yu. M. Udalov, Nauka, Leningrad, U.S.S.R., 1970, 2 r.

Characterization of Chemical Purity: Organic Compounds, IUPAC, Editor, L.A.K. Staveley, 1971, £ 5.00.

The Chemistry of the Transuranium Elements, by Cornelius Celler, Kernchemie in Einzeldarstellungen, Volume 3, Verlag Chemie, Germany, Fed. Rep., 1971, XV, 675 pp., DM 188, with 190 tables and 299 figures. This book provides an up-to-date account of the chemistry of the transuranium elements. Particular attention is also given to physical and nuclear-physical data. None of the other elements show such close correlations between chemistry and physics as the transuranium elements.
The work is divided into two parts. The first part deals with transuranium elements within the larger group of the actinides and stresses analogous and different behaviors, e.g., as compared to the lanthanides. Ten chapters describe the preparation, stability, and application of the isotopes and elements, the electronic configuration (which has only recently been established unequivocally), valences and coordination chemistry, metallurgy, organometallic and analytical chemistry, as well as separation procedures and behavior in solution and in the solid state. This first part is rather an accurate description and a representation of common and contrasting features of the actinides than a compilation of details. It therefore contains an up-to-date review of all actinide elements including thorium, protactinium and uranium.
The second part describes the preparation and properties for the individual transuranium elements neptunium ($Z = 93$) to hahnium ($Z = 105$) and contains predictions about the chemistry of the superheavy elements. All these chapters follow a common scheme: discovery, preparation, and production of the isotopes, metallurgy, solid state chemistry, organometallic chemistry, chemistry in aqueous solutions, separation prodecures, and analytical chemistry. Numerical values of the literature have been critically selected. Numerous tables, figures and diagrams supplement the text.

MECHANICAL PROPERTIES AND ENGINEERING DATA

Engineering Materials and Methods, by E. G. Semler, The Institution of Mechanical Engineers, London, 1971, 184 pp, $ 2.50, includes information on mechanical properties of materials at high temperature, properties of cast iron, high-strength light alloys, rubber as an engineering material, self-lubricating composites for bearings, refractories and other ceramics, diamond as an engineering material, choosing a fuel.

The Study of Metal Structures and Their Mechanical Properties, by W. A. Wood, Pergamon, New York, 1971, 383 pp, $ 15.00, includes the crystalline state, lattice geometry and crystal symmetry, electrons in metals, alloys and dispersions, lattice faults, some properties of dislocations, experimental approach, elastic strain and internal stress, unidirectional plastic strain and static strength at normal temperature, cyclic strain and fatigue strength, combined unidirectional and cyclic strain, deformation at elevated temperatures and creep strength, search for strong solids, appendixes.

Protective Coatings on Metals, Volume 3, by G. V. Samsonov, translated from the Russian, Consultants Bureau, New York, 1971, 202 pp, $ 27.50, includes information on production of coatings on metals in a glow discharge, influence of prior cold plastic deformation on carbon diffusion, some aspects of the alloying of metal surfaces with various elements, diffusion impregnation of carbon steels with titanium and boron, the boriding of sperical powders of refractory metals, structure and properties of aluminized Kovar alloy, nickel aluminide coatings from composite powders, evaluation of the effectiveness of coatings used for protection against gas pick-up, approximate calculation of the thickness of diffusion coatings, surface protection of heat-resistant alloys against oxidation.

Cryogenic Fundamentals, Editor, G. G. Haselden, Academic Press, New York, 1971, 757 pp, $ 33.00. Refrigeration and liquefaction cycles. Heat transfer. Insulation. Fluid dynamics. Materials of construction and techniques of fabrication. Adsorption. Expanders and pumps. Superconductivity. Instrumentation. Safety. Thermophysical data for cryogenic materials. A reference work on the field of cryogenics below the temperature of 150 K. Unites the fields of industrial gas liquefaction and separation and the lower temperatures necessary for the use of liquid hydrogen and helium for nuclear, propulsion and superconduction studies. On the graduate level, designed for the experimentalist and the plant designer.

Phase Diagrams of Silicate Systems, Handbook No. 2, Metal-Oxygen Components of Silicate Systems, by N. A. Toropov, V. P. Barzakovskiy, I. A. Bondar, Yu. M. Udalov, Nauka, Leningrad, U.S.S.R., 1970, 2 r. The book contains exhaustive handbook data on "metal-oxygen" system for those properties most important for modern technology. There are described the oxides of all the rare earths, titanium, zirconium, vanadium, niobium, tantalum, chromium, molybdenum, tungsten, uranium, manganese, iron, cobalt, nickel, and other metals, whose oxygen compounds are distinguished by high melting points. The lower oxides of Si, Al, Ge, Sn, and Pb as well as the polymorphism of the ordinary oxygen compounds of these elements are examined in detail. Besides the stability range characteristics of the corresponding oxide phases and their polymorphism (in T and P parameters) some physical (structural and optical) properties are listed.

Electronic Properties of Materials, A Guide to the Literature, Volume 3, parts 1 and 2, Editor, D. L. Grigsby, Plenum, New York, 1971, part 1, 1161 pp, part 2, 756 pp, $ 150.00. It updates previous volumes with material published since January 1967. This volume has a much deeper indexing system than the first two, as well as a section on laser materials.

Engineering Properties of Nickel and Nickel Alloys, by J. L. Everhart, Plenum, New York, 1971, 229 pp, $ 17.50, covers the mechanical and physical properties of nickel and a number of high nickel-containing alloys, including proprietary alloys protected by trademarks, but low-alloys and constructional nickel-containing alloys have been excluded. Illustrated with numerous tables and graphs which in many instances are a compilation of data from several sources.

Piezoelectric Ceramics, Non-Metallic Solids, Volume 3, by Jaffe, Bernard, et al, Academic Press, New York, 1971, 317 pp, $ 16.00, includes: Properties of $PbTiO_3$, $PbZrO_3$, $PbSnO_3$, and $PbHfO_3$ plain and modified, Solid solutions of $Pb(Ti, Zr, Sn, Hf)O_3$, Perovskite niobates and tantalates and other ferroelectric and antiferroelectric perovskites, Non-perovskite oxide piezoelectrics and ferroelectrics, Interpretation of some experimental results, Manufacture of piezoelectric ceramics, Applications of piezoelectric ceramics, Appendixes, Author index, Subject index. A detailed review of the properties of ceramic materials which are of actual or potential value for industrial purposes. Many tables, charts, diagrams and drawings, as well as references.

Mechanical Properties of Solids and Fluids, by R. C. Stanley, Butterworth, London, 1972, 250 pp, £ 3.90, includes: Elasticity, Applications of Elasticity, Plasticity, Viscosity, Viscosity of Gases and Non-Newtonian Fluids, Vacuum Physics, Further Reading, Appendix 1: SI Units and Conversion Factors. Appendix 2: Useful Physical Constants and Values.

Properties of Engineering Materials, by J. B. Moss, Butterworth, London, 1971, 338 pp, £ 4.50, contains information on atoms and molecules, atomic movements in crystalline solids, thermal equilibrium diagrams and their applications, metallic materials, polymeric materials, ceramic materials, composite materials, failure of engineering materials.

NBS-OSRDB-70-2 The NBS Alloy Data Center: Author Index, by G. C. Carter, D. J. Kahan, L. H. Bennett, J. R. Cuthill, and R. C. Dobbyn (COM-71-00722, Hard Copy $ 10, Microfiche 95 cents) was recently published for inclusion in the NBS Office of Standard Reference Data Bibliography Series by the National Technical Information Service.

This Index contains literature references to 12,000 research papers on physical properties of metals and alloys. It was created from the "Biblio-Master-File", a computer tape containing the master file of the NBS Alloy Data Center. The material has been arranged in accordance with three categories of properties. The first contains all NMR Knight Shift papers and many other papers dealing with NMR, NQR, FNR, and other nuclear resonances in metals. This section is complete for the period 1949–1969 and contains several 1970 papers. The second contains all soft x-ray emission papers since 1940 as well as some earlier papers and many soft x-ray absorption papers. The third section represents papers of

general interest to the Alloy Data Center, on related topics such as Mössbauer effect, susceptibilities, specific heats, hyperfine fields and band structures. This section does not represent a complete set of such papers. The referenced papers are annotated in depth and coded information (journal citation, physical properties, material studied, material composition, and temperature) was put onto the Biblio-Master-File. The Author Index was created from this tape, listing each paper under first author. The full annotation of each paper is given in the reference. For each metal or alloy system reported in a paper, a separate line appears in the Index.

The Biblio-Master-File can be manipulated in a number of ways with various available computer programs. A related publication developed from one such manipulation is NBS Special Publication 324, The NBS Alloy Data Center: Permuted Materials Index, by G. C. Carter et al. SD Catalog No. C13.10:324, $ 7.00.

Electronic Design Data Book, by R. F. Graf, Van Nostrand Reinhold, New York, 1971, 312 pp, $ 17.95, contains frequency data, communication, passive components and circuits, active components and circuits, mathematical data, formulas, symbols, physical data, index. This is a reference book containing tables, charts and formulas that are most frequently encountered in electronics design. Presents solved examples, thus facilitating the use of the monographs. The book is not limited to electronics, but also includes data in acoustics, mathematics and optics, as well as some engineering data.

GEO AND COSMIC SCIENCES

Computer Processing of Meteorological Data, by S. L. Belousov, et al, W. Heffers & Sons Ltd., U.K., translated from the Russian, 1971, 216 pp, approx. £ 7.50.

Tables for Microscopic Identification of Ore Minerals, second edition, by W. Uytenbogaardt, E. A. J. Burke, American Elsevier, New York, 1971, 430 pp, $ 18.50. Ore minerals listed in order of increasing minimum micro-identation hardness (VHN). Ore minerals listed in order of increasing minimum reflectance in air (R). Ore minerals listed in order of increasing polishing hardness (H). Selenides. Tellurides. Mineral descriptions. 1700 references.

Interpretation of Observation Data from Meteorological Satellites, by K. Ya. Kondratiev, et al, W. Heffers & Sons Ltd., U.K., translated from the Russian, 1970, 376 pp, £ 5.50.

Statistical Analysis of Geological Data, Volume II, by George S. Jr. Koch, Richard F. Link, Wiley, New York, 1971, 438 pp, $ 17.50. Analysis of multivariate data. Ratios and variables of constant sum. Delineation of ore deposits. Specialized geological sampling. Electronic computers and geology.

Algorithms of Interpretation of Seismic Data. Computer Seismology, No. 5, by Shmidt, Institute of Physics, Moscow, U.S.S.R., Nauka Publishing House, Moscow, U.S.S.R., 1970, 1 r. 50 k. The collection pertains to analysis of seismic observations on electronic computers. Described are a method and a program for determining the mechanism of earthquakes according to the signs of arrival of P and S waves. A new method is proposed for pattern recognition and examples of its use for distinguishing seismic phenomena are presented. Examples of the solution of inverse problems are given; determination of velocity cross sections of the earth's crust, upper mantle and earth's core according to seismic data. The first results of statistical analysis of earthquake catalogs are presented for the purpose of revealing the local properties of a seismic regime and for calculating the seismic danger.

MATHEMATICAL METHODS AND COMPUTER PROGRAMS FOR DATA

Data Banking for Science and Technology, by R. N. Jones, NRC, Ottawa, Canada, *Chemistry in Canada.* February 1972. The report is devoted to computer utility network including computer coding of organic structural formula, computer matching of infrared spectra.

Random Data: Analysis and Measurement Procedures, by J. S. Bendat, A. G. Piersol, Interscience, New York, 1971, 407 pp, $ 18.50, contains basic descriptions of physical data, review of physical system response properties, review of stationary random processes theory, review of statistical principles, input-output relationships for physical systems, statistical errors in random data analysis, general considerations in data acquisition and processing, analog data analysis procedures, digital data analysis procedures, nonstationary, transient, and multidimensional data.

NBS Technical Note 525 OMNITAB II, User's Reference Manual by D. Hoghen, S. T. Peavy, R. N. Varner, $ 2.00, SD Stock No. 0303–0918, has been designed to make computing easy, accurate, and effective, particularly for persons who are not programmers. OMNITAB II is a general purpose program, which can be learned quickly, for both simple and complex numerical, statistical, and data analysis. OMNITAB executes instructions written in the form of simple English sentences.

Numerical Error Propagation with Computer Assistance, by R. D. Nelson, M. R. Ellenberger. A paper submitted to the *Journal of Chemical Education*, January 15, 1972.