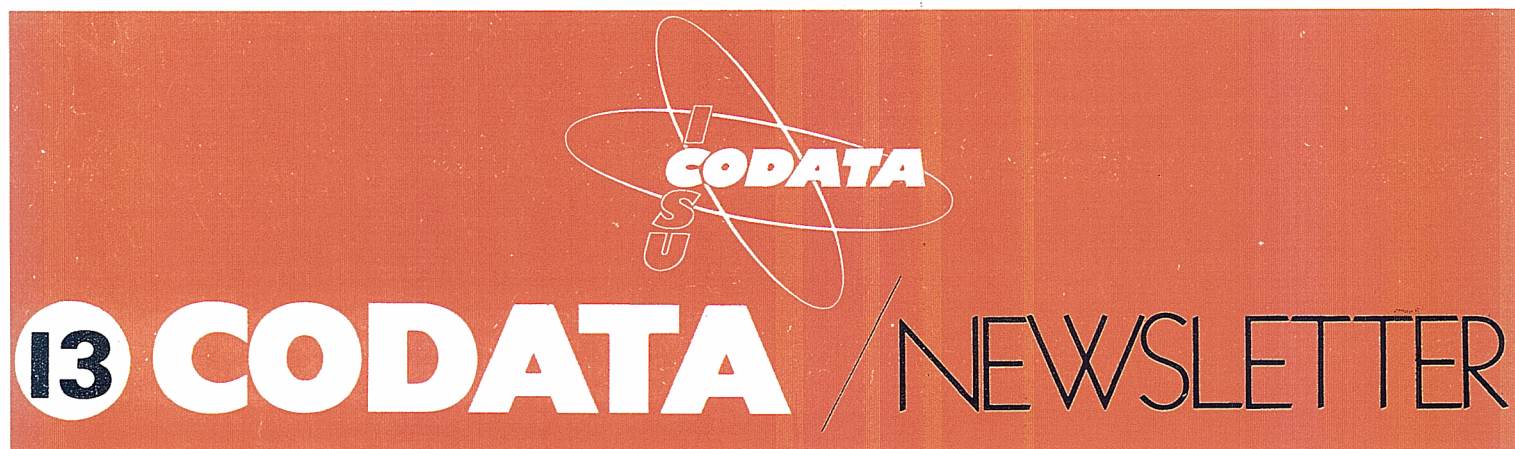


INTERNATIONAL COUNCIL OF SCIENTIFIC UNIONS  
COMMITTEE ON DATA FOR SCIENCE AND TECHNOLOGY



SEPTEMBER 1974

TABLE OF CONTENTS  
*TABLE DES MATIERES*

CODATA Elections  
*Elections à CODATA*

Fourth International CODATA Conference  
*IV<sup>e</sup> Conférence internationale CODATA*

Chemical Thermodynamics of the Actinides  
*Thermodynamique chimique des actinides*

1974 IAPS Conference  
*Conférence 1974 de l'IAPS*

Indian National Committee for CODATA  
*Comité national indien pour CODATA*

Programme - 4th International CODATA Conference  
*Programme de la IV<sup>e</sup> Conférence internationale CODATA*

The Importance of Accelerating Thermodynamic  
Compilation Endeavors  
*Importance actuelle d'une intensification des efforts  
de compilation des grandeurs thermodynamiques*

The Fundamental Constants, 1974 vs 1973  
*Evolution des constantes fondamentales de 1973 à 1974*

New publications  
*Publications récentes*

CODATA Members 1974  
*Composition de CODATA en 1974*

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

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

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## CODATA ELECTIONS

During the 9th CODATA General Assembly held in Yerevan, U.S.S.R. in June 1974, new CODATA officers and members of the Executive Committee were elected as follows:

### PRESIDENT:

Prof. P. MELCHIOR, Observatoire Royal de Belgique, 3, avenue Circulaire, 1180 Brussels, Belgium.

### PAST PRESIDENT:

Prof. B. VODAR, Laboratoire des Interactions Moléculaires et des Hautes Pressions, 1, place Aristide-Briand, 92190 Meudon, France.

### VICE-PRESIDENT:

Prof. T. PLEBANSKI, Division of Physico-Chemical Metrology, National Board for Quality Control and Measures, Elektoralna 2, Warsaw 1, Poland.

### TREASURER:

Prof. N. KURTI, The Clarendon Laboratory, Parks Road, Oxford OX1 3PU, U.K.

### SECRETARY GENERAL:

Prof. E. F. WESTRUM, Jr., University of Michigan, Dept. of Chemistry, Ann Arbor, Michigan 48104, U.S.A.

### MEMBERS:

Dr. P. L. ALTMAN, Office of Biological Handbooks, F.A.S.E.B., 9650 Rockville Pike, Bethesda, Maryland 20014, U.S.A.

Dr. W. W. HUTCHISON, Canadian Centre for Geoscience Data, 601 Booth Street, Ottawa, Ontario, Canada.

Prof. H. JANCKE, Amt für Standardisierung Messwesen und Warenprüfung der D.D.R., Wallstrasse 16, 102 Berlin, D.D.R.

Dr. R. N. JONES, Division of Pure Chemistry, National Research Council of Canada, 100 Sussex Drive, Ottawa 2, Ontario, Canada.

Prof. T. SHIMANOUCHI, Director of Computer Centre, University of Tokyo, 2-11-16, Yayoi, Bunkyo-ku, Tokyo, Japan.

Prof. V. V. SYTCHEV, Institute of High Temperatures, Korovinskoye Road, 127412 Moscow I-412, U.S.S.R.

A complete list of CODATA Members and Task Groups - 1974, can be found on pages 18 and 19 of this *Newsletter*.

## FOURTH INTERNATIONAL CODATA CONFERENCE

Amid the refreshing mountain air and the recreational facilities afforded by the Soviet high-altitude olympic village of Tsakhcadzor in the Armenian S.S.R., some 130 scientists from 19 countries met between June 24 and 27, 1974 in order to discuss means of improving the quality of data, enhancing its accessibility and dissemination, and implementing new procedures to ensure its critical evaluation. Participating in the scientific conference sections dealing with a) present needs for more and better data in geophysics, astronomy and biology; b) progress made in handling thermodynamical and spectroscopic data; c) the role of Data Centers in science, technology and industry proved to be a rewarding experience. The wealth and variety of the subjects covered can be gauged not only by the number of papers actually delivered (45), but also by the exceptionally wide range of items discussed, extending from the nomenclature of microorganisms to the standardization of celestial radio-sources and from the production of computer-generated movies to the numerical inclusion of spatial data in data bank memories. More traditional subjects, such as thermodynamic properties of substances, molecular spectra and methods of automatic retrieval of data were also discussed and a good deal of attention was devoted to the modus operandi of data centers and, more generally, to the computerized manipulation and handling of data and adjacent concerns. In addition, opportunities for broad participation in the work of CODATA Task Groups were provided by series of mutually beneficial parallel sessions in which exchange of ideas and suggestions took place between Task Group members and Conference participants. For example, means for providing appropriate training in the handling and evaluation of data, extension of the *Guide for the Presentation of Numerical Data* to bio- and geodata, as well as to observational data, and the tagging and flagging of data were typical of the concerns which provided general interest.

Excursions to nearby Lake Sevan and to the city of Yerevan supplemented the recreational and touristic opportunities offered by Tsakhcadzor and its environs. Appetites engendered by the high altitude were slaked by the camp canteen and a banquet at Lake Sevan. The meeting of the General Assembly following the Conference accepted the American invitation to hold the next International CODATA Conference in another mountain area, at Boulder, Colorado in June 1976.

The Conference Proceedings are scheduled to appear as a 100-odd page issue (No. 15) of the CODATA *Bulletin* early in 1975. Its Table of Contents, embodying the actual Conference can be found on p.4 of the present *Newsletter*. A detailed report on the parallel sessions will appear in the next issue.

## CHEMICAL THERMODYNAMICS OF THE ACTINIDES

Scientists from ten countries have combined their talents in the production of a critical evaluation of the thermophysics and the thermochemistry of the actinide elements and their compounds. This endeavor under the auspices of the International Atomic Energy Agency will appear initially as special issues of the *Atomic Energy Review*. The first of these are expected early in 1975. About 25 authors are involved under the editorship of an Advisory

Board composed of Dr. Vadim Medvedev (U.S.S.R.), Dr. Frank Oetting (I.A.E.A.), Dr. Malcolm Rand (U.K.) and Professor Edgar F. Westrum, Jr. (U.S.A.). The initial scope will include the elements, the binary and ternary compounds, alloys, but will exclude the complex ions in aqueous solution and the distribution between aqueous and non-aqueous solutions. It is possible that the excluded aspects may later be incorporated in the series.



## 1974 IAPS CONFERENCE - HYERES-GIENS

The International Association for the Properties of Steam (IAPS), the first Associate Organization to become affiliated with CODATA held its 8th International Conference on the Properties of Water and Steam at Hyères-Giens, France, September 23 through 27 under the joint sponsorship of the Société Française des Thermiciens and the Institut Français des Combustibles et de l'Energie.

Relatively isolated within the "Family-Vacation-Village" facilities, more than 120 participants from 14 countries examined recent progress in the experimental determinations of transport and equilibrium properties of water substance as well as their formulation into terse critically evaluated tables and equations. Invited and submitted papers together with panel discussions provided many opportunities for comment by participants.

Transport properties such as viscosity and thermal conductivity at kilobar pressures as well as at more ordinary conditions and also for deuterium-rich materials equally competed with correlations and critical equations for the conferee's attention. Novel experimental techniques were compared with old. Equilibrium measurements (e.g., vapor pressure, liquid density, PVT properties, isobaric and isochoric heat capacities, Joule-Thomson coefficients, dielectric constants, structural, and spectrographic aspects, consideration of the critical region and of metastable states - especially that of undercooled water - as have been developed in the six-year interval since the last conference) were presented and reviewed. Scaling laws, universality conditions, and development of analytic equation-of-state equations, especially in the critical region, provided opportunities for theoretical virtuosity introduced at the very outset of the Conference by a lucid presentation on theories of dense fluids by G.S. Rushbrooke.

A special session on dilute solutions of "technically pure" water included interesting trends of parameters with pressure as well as chemical and crystallographic considerations involved in power plant operations. Although the subject was beyond the usual IAPS concerns, it did invoke unusual interest under the chairmanship of Dr. K. R. Schmidt. Yet despite the fact that participation in this section was greater than in most other technical sections, further endeavor by IAPS appeared unlikely, in the immediate future at least. In one sense, the Conference emphasis has shifted from the simple technological problem of providing uniform steam tables to a scientific concern with more adequate representation of the equation of state in critical regions and in the refinement of fits and the more critical evaluation of new data.

Among the papers most likely to be of special interest to *Newsletter* readers are those on critical evaluation and correlation by K. Watanabe and his coworkers, on correlation of equilibrium and transport properties by R.D. McCarty, on thermodynamic consistency of property tables by J. Kestin and on interrelationships between independently measured thermodynamic and transport properties by C.A. Meyer. These will, of course, be of special interest to thermodynamicists, but some are of even broader applicability in critical evaluation. The papers and discussion are expected to be published as proceedings in several volumes early in 1975.

An ovation to the retiring President of IAPS, Professor Boris Vodar of Paris, included praise

for the arrangements for the Conference. Vice-President, Professor Joseph Kestin of Providence, Rhode Island was honored with the Presidency and Dr. H.W. Bradly of the United Kingdom will serve as the new Vice-President. Professor S.R. Beitler of Columbus, Ohio, who has served for many years as the Executive Secretary, will be replaced by Dr. Howard White of Washington, D.C. in January 1975, and the Secretariat will at that time become resident in the Bureau of Standards. An invitation to hold the next meeting in West Germany in 1979 - possibly at Munich - was accepted.

## INDIAN NATIONAL COMMITTEE FOR CODATA

Following its decision to adhere to CODATA, the Indian Academy of Science has invited the following to serve on its National Committee:

**PROFESSOR C.N.R. RAO**, Chairman  
Department of Chemistry  
Indian Institute of Technology  
Kanpur 208016

**DR. A.S. DIVETIA**  
Bhabha Atomic Research Centre  
Variable Energy, Cyclotron Project  
Calcutta 64

**DR. V.K. GAUR**  
Professor of Geophysics  
Department of Geology and Geophysics  
University of Roorkee  
Roorkee 67

**SHRI S. PARTHASARATHY**  
Scientist-in-Charge  
I.N.S.D.O.C.  
Hillside Road, New Delhi 12

**DR. A.P. KUDCHADKER**  
Department of Chemical Engineering  
Indian Institute of Technology  
Kanpur 208016

**DR. R. ANANTHAKRISHNAN**  
Indian Institute of Tropical Meteorology  
University Road  
Poona 5

**MR. C.R.V. RAMAN**  
Deputy Director-General of Observatories (Climatology)  
Poona 5

**DR. S. RAMASESHAN**  
Deputy Director and Head  
Materials Science Division  
National Aeronautical Laboratory  
Post Bag No. 1779  
Bangalore 560017

**DR. J.G. NEGI**  
National Geophysical Research Institute  
Hyderabad

**DR. A.R. VERMA**, Member-Secretary  
Director  
National Physical Laboratory  
Hillside Road  
New Delhi 12

The Administrative Office of the Committee is at the following address:

Executive Secretary  
Indian National Science Academy  
Bahadur Shah Zafar Marg  
New Delhi 11001

PROGRAMME  
FOURTH INTERNATIONAL CODATA CONFERENCE

Tsakhadzor Olympic Village, near Yerevan  
Armenian S. S. R., U. S. S. R.

June 24 - June 27, 1974

**Monday, June 24, 1974**

**OPENING CEREMONIAL SESSION**

Co-chairmen: *Prof. V.V. Sytchev (USSR), Prof. E.F. Westrum, Jr. (USA)*

*Prof. V.A. Ambartsumian (USSR), Past President ICSU*

*Prof. V.V. Sytchev (USSR), Vice-Chairman U.S.S.R. Organizing Committee*

*Prof. B. Vodar (France), President CODATA*

**DATA CENTRES IN VARIOUS FIELDS**

Co-chairmen: *Dr. R. N. Jones (Canada)*

*Dr. A. Wysocki (UNESCO)*

The NSRDS Experience - *Dr. David R. Lide, Jr., National Standard Reference Data Service, Washington, D.C.*

State Service of Standard Reference Data - *Dr. L.M. Zaks, Director, All-Union Research Institute of Metrological Service, Moscow, U.S.S.R.*

Experience and International Cooperation of Nuclear Data Centre at Obninsk - *Prof. L.N. Usatchev, Nuclear Data Centre, Obninsk, U.S.S.R.*

Network of Data Centres for Dissemination of Data - *Prof. M. Kotani, Science University of Tokyo, Japan*

**Short communications:**

Problems of a Specialized Data Evaluation Centre - *Dr. O. Kennard, Crystallographic Data Centre, Cambridge, U.K.*

Presentation of Gaphyor: A Data Bank System for the Physics of Gases - *Prof. Y.L. Delcroix & Mr. G. Matthieussent, Université Paris-Sud, Orsay, France*

U.S.S.R. Research on Quantitative Kinetics - *Academician V.N. Kondratiev, Institute of Chemical Physics, Leningrad, U.S.S.R.*

**COMPUTER USAGE IN DATA SYSTEM ORGANIZATION**

Co-chairmen: *Prof. G. Black (UK)*

*Prof. Yu. Drobyshev (USSR)*

Computer Task Group Report on the Freiburg Man/Machine Symposium - *Dr. O. Kennard*

Role of the Regional Computer Centre in Reference Data Problems - *Prof. T. Shimanouchi, University of Tokyo, Japan*

Long-distance Handling of the Chemical Data Bank in Novosibirsk - *Prof. Yu. Drobyshev, Computer Center, Siberian Branch of the USSR Academy of Sciences, Novosibirsk, U.S.S.R.*

On the Rules of Numerical Data Publication in the Primary Literature - *Prof. D.O. Avetisyan & Prof. L.F. Sarukhyan, Institute of Scientific and Technical Information, Yerevan, U.S.S.R.*

Introduction to and Presentation of Motion Pictures on Data Banks - *Dr. R. L. Wigington, Chemical Abstracts Service, Columbus, Ohio, U.S.A.*

**Short communication:**

Polish Work on Information Systems - *Dr. J. Maluszynski, Regional Centre of Informatics, Technical University, Poznan, Poland.*

**Tuesday, June 25, 1974**

**DATA CENTERS FOR INDUSTRIAL NEEDS**

Co-chairmen: *Prof. H. Jancke (GDR)*

*Prof. Y.S. Touloukian (USA)*

Establishment of a Data Centre for the National Laboratories for Industry at the New Science City - *Tsukuba - Dr. Y. Mashiko, National Chemical Laboratory for Industry, Tokyo, Japan*

Thermodynamic Data for Engineering - *Dr. A. Bylicki & Dr. S. Malanowski, Institute of Physical Chemistry, Warsaw, Poland*

The Information System for Materials and Economic Use of Materials in the GDR - *Dr. K. Göttlich (presented by Dr. W. Künzel) - Amt für Standardisierung Messwesen und Warenprüfung der GDR, Berlin, G.D.R.*

User Aggregation for Data Center Development - *Dr. J. Murdock, Battelle Memorial Institute, Columbus, Ohio, U.S.A.*

Management of Technical Data Within Industry - *Mr. R. W. McIntyre, Rolls Royce (1971) Ltd., Bristol, U.K.*

Data Center for Thermodynamic Properties of Hydrocarbons and Oils - *Dr. S.D. Labinov, Thermodynamic Data Center, Kiev, U.S.S.R.*

**FORMULATION OF CODATA'S ROLE IN MEETING THE NEEDS OF THE BIOLOGICAL SCIENCES**

Co-chairmen: *Dr. K.P. Ivanov (USSR)*

*Dr. C. Schäfer (GFR)*

Characteristics of Data Collected by the Conservation Section of IBP, How They Will Meet Needs of Life Scientists, and How CODATA Can Assist in Fulfilling Needs - *Dr. G.L. Radford, International Union for the Conservation of Nature & Natural Resources, Huntington, U.K.*

Perspectives of a National (German) Biological Information and Data Center - *Dr. C. Schäfer, Biologie-Dokumentation, Forschungsinstitut Senckenberg, Frankfurt, G.F.R.*

Activities of the World Federation for Culture Collections as Related to Needs of the Working Scientist for Non-Numerical Data - *Dr. V.B.D. Skerman, University of Queensland, St. Lucia, Australia*

Evaluation of Numerical Data in Biology and Biological Data Centers - *Dr. K.P. Ivanov, Pavlov Institute of Physiology, Leningrad, U.S.S.R.*



Wednesday, June 26, 1974

FORMULATION OF CODATA'S ROLE IN MEETING THE NEEDS OF THE GEOLOGICAL, GEOPHYSICAL, GEOGRAPHICAL, AND ASTRONOMICAL SCIENCES

Co-chairmen: Prof. I.G. Magakian (USSR)  
Prof. P. Melchior (Belgium)

Characteristics of Data Required by Geophysicists - Prof. P. Melchior, Observatoire Royal de Belgique, Brussels, Belgium

World Data Center A - Dr. A.H. Shapley, Environmental Data Service, National Oceanic & Atmospheric Administration, Boulder, Colorado, U.S.A.

Characteristics of Data Required by Geologists; How Needs Are Being Met - Dr. G.Y. Craig, Grant Institute of Geology, University of Edinburgh, Edinburgh, Scotland

Cooperation in the Provision of Astronomical Data - Dr. G.A. Wilkins, Royal Greenwich Observatory, Sussex, U.K.

Spatial Data Characteristics and Handling Techniques - Dr. R.F. Tomlinson, International Geographical Union, Ottawa, Ontario, Canada

Short communications:

The Role of Data Banks in Astronomy: Experience with the Stellar Data Center in Strasbourg - Prof. J. Jung, Observatoire de Strasbourg, Strasbourg, France

Appreciation of Reliability of Astronomical Data Processing by Computer - Dr. R.A. Sargsian & Dr. V.S. Khitrova, Computer Center, Academy of Sciences of the Armenian S.S.R., Yerevan, U.S.S.R.

Standardization of Sky Radiosources for Guarantee of Unity of Radiotechnical Measurements - Dr. P.M. Geruny, Academy of Sciences of the Armenian S.S.R., Yerevan, U.S.S.R.

On Numerical Data of Earth's Physical Parameters - Prof. A.G. Aslanyan, Academy of Sciences of the Armenian S.S.R., Yerevan, U.S.S.R.

PROGRESS IN HANDLING SPECTROSCOPIC DATA

Co-chairmen: Dr. D. R. Lide, Jr. (USA)  
Prof. C.N.R. Rao (India)

Molecular Spectral Data Center of Novosibirsk - Dr. V.A. Koptug, Institute of Organic Chemistry, Siberian Branch of the USSR Academy of Sciences, Novosibirsk, U.S.S.R.

Recent Developments in the Display, Evaluation, and Storage of Molecular Spectral Data - Dr. R. N. Jones, National Research Council of Canada, Ottawa, Canada

Spectra and Spectroscopic Properties of Diatomic Molecules - Dr. R. F. Barrow, Physical Chemistry Laboratory, Oxford, U.K.

Some Recent and Ongoing Compilations of Atomic Spectral Data - Dr. W.C. Martin, National Bureau of Standards, Washington, D.C., U.S.A.

Short communications:

Standardization and Accumulation of Data Used in Interpretation of Molecular Spectra - Dr. M.A. El'yashevich, Minsk University, Minsk, U.S.S.R. & Dr. L.A. Gribov, Vernadsky Institute of Geochemistry and Analytical Chemistry, USSR Academy of Sciences, Moscow, U.S.S.R.

Measurement Methods of Transition Probabilities in Faculté des Sciences of Brest - Prof. A. Johannin-Gilles, Faculté des Sciences, Brest, France

Thursday, June 27, 1974

PROGRESS IN HANDLING THERMODYNAMIC DATA

Co-chairmen: I. Ansara (France)  
L.V. Gurvich (USSR)

Academy of Science Series of Reference Books on Thermodynamic Properties of Substances - Dr. V.P. Glushko, Academy of Sciences of the U.S.S.R., Moscow, U.S.S.R.

Key Values for Thermodynamics: A Project Servicing Science and Industry - Prof. S. Sunner, Thermochemistry Laboratory, Chemical Center, Lund University, Lund, Sweden

The IUPAC Thermodynamic Tables Project - Dr. S. Angus, IUPAC Thermodynamic Tables Project Centre, Imperial College of Science and Technology, London, U.K.

Thermophysical Data Project - Prof. Y. S. Touloukian, Thermophysical Properties Research Center, Purdue University, West Lafayette, Indiana, U.S.A.

Short communications:

Automatic Search System in IHT Thermophysical Center - Prof. E.E. Shpilrain & Prof. K.A. Jakimovich, Institute of High Temperatures, Moscow, U.S.S.R.

Computer Analysis of Thermochemical Data - Dr. J.B. Pedley, University of Sussex, Brighton, Sussex, U.K.

The Compilation and Critical Analysis of Thermodynamic Data for Ternary Alloy Systems - Dr. I. Ansara, Laboratoire de Thermodynamique et Physico-Chimie Métallurgiques, St. Martin d'Hères, France

Data for Solid State Physics Obtained by Neutron Scattering - Dr. I. Sosnowska, Institute of Experimental Physics, University of Warsaw, Warsaw, Poland

Soviet Commission on Thermodynamic Data - Prof. V.V. Sytchev, CODATA Delegate, USSR Academy of Sciences, Moscow, U.S.S.R.

Data Tables for Metallic Mixtures - Prof. M. Laffitte, Institut de Microcalorimétrie du C.N.R.S., Marseille, France

CLOSING REMARKS

Prof. L.V. Gurvich (USSR) - Programme Chairman



# THE IMPORTANCE OF ACCELERATING THERMODYNAMIC COMPILATION ENDEAVORS\*\*

BY LEO BREWER

[An excerpt from a Talk entitled "The Relevance of Thermodynamics to National Energy Problems" presented by Professor Leo Brewer of the Inorganic Materials Research Division of Lawrence Berkeley Laboratory and Department of Chemistry, University of California, Berkeley, California 94720, at a Conference on Thermodynamics and National Energy Problems at Airlie House, Warrenton, Virginia, June 10-11, 1974]

I will devote most of my time to the question of accelerating compilation efforts to enhance the usefulness of thermodynamics.

In the 1920's, a very ambitious effort was initiated which was aimed at bringing together and critically evaluating all of the available thermodynamic data. It was hoped at the time that this compilation would be a continuing effort that would keep up to date with the new experimental data. This effort was the International Critical Tables<sup>1</sup> and a most remarkable job was done. Unfortunately, it was not possible to maintain the effort of keeping up to date. Bichowsky and Rossini's tabulation<sup>2</sup> of thermochemistry followed by the Bureau of Standards' Circular 500 tabulation<sup>3</sup> were efforts in a more limited area to carry on the function of the International Critical Tables. The Standard Reference Data program of the Bureau of Standards has continued the effort of compilation and of coordinating thermodynamic compilations around the country. However, as the years have gone by, these compilation efforts have fallen more and more behind the accelerating accumulation of experimental data. The present level of effort is quite inadequate for the demands of the expanding energy development program. Of even more concern is the fact that support of these compilation programs has been decreasing in recent years. How to expand these programs to meet the new needs posed by the energy programs is a very serious question. The typical developmental scientist or engineer does not have the time nor the background to go through the multitudes of journal publications that might have data of interest to him and evaluate the different determinations to arrive at a most reliable value. I have continually encountered situations in industrial laboratories where data that were very important for their operations were not being used by them because they were not aware of their existence. It is of greatest importance that every effort be made to increase the rate of critical evaluation and compilation of values judged to be the most reliable. Such an effort will help avoid dead-end developmental programs which could waste not only large amounts of money, but large numbers of valuable personnel who would be used on more fruitful endeavors.

The problem of expanding compilation efforts is not an easy one to solve. It will require not only an increase in the level of operation of funding existing compilation centers, but it will also require an active recruiting program to bring individual compilers into the program to

supplement the activities of large groups such as the Bureau of Standards. The requirements for a person to engage in compilation activities are rather unique. It is important that the person have had some experience in the laboratory with a variety of thermodynamic techniques; so that he has the background for evaluating the reliability of experimental measurements. It is important that he have some understanding of the possible sources of error that have to be taken into account and, in particular, he must be able to judge the order of magnitude of systematic errors that have to be considered in judging the discrepancies between different determinations. It has been difficult to find enough people who have the qualifications and who are willing to devote the time required for a compilation program. I do not think that it will be possible to recruit sufficient numbers of qualified people as full-time compilers. There are a number of specialists who are quite familiar with the work that has been done in a relatively narrow field and who might be willing to devote a portion of their time to the compilation effort as a side-line of their regular research program. It would be necessary to obtain funds to back up such a person with assistants who can do the literature work and some of the trivial calculations so that he can concentrate on the job of critical evaluation and the application of judgment in deciding the weighting to be given to the various data. There are hazards in such a program in that not all individuals may be qualified to carry out compilations and a system of critical review of compilation quality would have to be devised to insure that all of the input from the small groups would be of comparable quality. Because all areas would not be equally covered, the large compilation centers like the Bureau of Standards would have to take specific responsibility for areas that might not be of great current interests to individual research workers.

I would like to devote my remaining time to a technical aspect of compilations which is rarely discussed. That is the question about the role of models as an aid in evaluating experimental thermodynamic data. One can describe compilations in terms of two different points of view. One is the compilation in which the data are critically evaluated in terms of the experimental methods used and possible systematic errors and evaluation of other results from the same laboratory compared to laboratories with established reliability. Such compilations can be carried out independently of any models to establish what appear to be the best experimental thermodynamic results. Another type of compilation is carried out in the context of some model where the data are examined with respect to the expectations of the model. An example where this is now routinely done is in the treatment of aqueous electrolyte data in terms of the Debye-Hückel theory. In this instance, the model is of very great importance because its greatest validity is in the extremely dilute range where it is particularly difficult to obtain reliable experimental data.

Another example is the use of pair-interaction theory as a basis for use of a second virial-coefficient equation of state for extrapolation of gaseous thermodynamic data to the low pressure gaseous standard state. A similar pair-interaction theory is often used as the basis for a Gibbs energy of dilution equation for solutions corresponding to a linear deviation from the Henry's Law slope.

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In using models of these types in compilations, one must be cautious about the implications of some of the assumptions of the model. In evaluating uncertainty limits for the compiled results, one must include uncertainties introduced by the model. As example, one would not use an equation of state based on just a second virial coefficient for an ionized gas just as a linear deviation from Henry's Law is not applicable to an aqueous electrolyte. In the extrapolation of the thermodynamic data to the infinitely dilute or solute standard state, one must consider which systems might have long-range forces which would cause substantial deviations from Henry's Law even at the most dilute concentrations which can be studied experimentally. There is also the problem that the component being assumed may be dissociated at the low concentrations such as to make Henry's Law inoperable even in the limit of infinite dilution. It is important to use bonding models as a guide that warns when difficulties can be expected and provides for reformulation of the thermodynamic data in terms of a component which is actually the major species at the lowest concentrations. These are standard thermodynamic problems, but it is very important that the role of these essential models be clearly defined by the compiler.

Models are of value to the compiler aside from the problem of extrapolating to the infinitely dilute standard state or for carrying out the Gibbs-Duhem integration to infinite dilution. For example, it is sometimes convenient to express solution data in terms of the solubility parameter of the regular solution theory as a valuable means of tabulating the data more compactly. However, one must consider the implications of entropy assumptions that are implicit in the model. All of these models are useful in compilation efforts, but the possible influence of the model upon the resulting values must be clearly spelled out.

I would like to discuss specific examples to present my views on how to handle the role of the model in compilations. There are many instances where a straightforward thermodynamic treatment of the data is not possible and some extra-thermodynamic treatment is necessary. One of the most troublesome examples is that of determination of Third Law entropies of magnetic compounds of the transition metals, the lanthanides, or actinides. It is difficult to determine from the available data, in many instances, whether magnetic ordering has removed contributions to the entropy at low temperatures or whether additional amounts of entropy will be extracted at lower temperatures. Thus some of the tabulated entropies must be considered as lower limits until the magnetic contributions are fully elucidated. It is important to attempt to estimate the magnitude of this uncertainty and to clearly include the uncertainty prominently displayed with the tabulated entropy value.

A common example of use of an implicit model without warning to the user of the thermodynamic data is that of compilations of entropies and other thermodynamic data for high temperature gases. In many instances, one finds tabulated thermodynamic data based on just the spectroscopic levels tabulated by Herzberg<sup>4</sup> or in other spectroscopic compilations as if no other levels would be expected. For many molecules at high temperatures, and particularly for

compounds of the transition metals, the lanthanides, and the actinides, the available models clearly indicate that there should be many yet-unobserved low-lying levels that can have a very marked influence on the thermodynamic properties at high temperatures. For many of these molecules, the ground electronic state has not yet been established. In part, the problem is a matter of education to convince scientists who publish their thermodynamic calculations based on spectroscopic data that their values are merely limits and the fact that these are limits should be clearly pointed out and reflected in the uncertainty cited.

An example of two contrasting but equally appropriate treatments can be cited for the gaseous diatomic oxides. Gerd Rosenblatt and I have compiled<sup>5</sup> the thermodynamic data for all of the gaseous diatomic oxides of the elements using a model based on the spectroscopic data for the free gaseous ions to approximate the electronic contribution to the entropy of the diatomic oxides over a range of temperatures. The electronic contributions to the entropy were tabulated separately so that their magnitude is clearly evident. The uncertainty due to use of the model was reflected in the uncertainties cited for the derived thermodynamic data. It was shown that the model would generally be expected to give somewhat higher entropies than the actual value by comparison with examples for which rather complete spectroscopic data were available. However, the model was expected to give consistently more correct results for all molecules as a group compared to values based only on observed spectroscopic data. The JANAF Tables<sup>6</sup> have recently reviewed the data for some of these oxides. The choice was made to calculate the entropies using only the observed spectroscopic data, but it was clearly pointed out that the values were lower limits and a comparison was made with the values that Rosenblatt and I had tabulated to indicate the range of possible values and the tabulated probable errors reflected that range of uncertainty. There should be no ambiguity in the reader's mind about the magnitude of the uncertainty and the role of models in arriving at the values tabulated. In contrast to those two examples, one must admonish the Bureau of Standards for a complete lack of indication of uncertainties in the NBS Technical Note 270 series<sup>7</sup> aside from the lack of any discussion of the role of models or references to sources of data. This is due in part to lack of funds. The Bureau of Standards' Standard Reference Data Program is the keystone to the compilation effort and it is most important that adequate funds be obtained not only to bring the NBS Technical Note 270 series to a successful completion but to carry on a continuing program of updating these compilations and providing extensions to higher temperatures. The expansion of the number of compiling programs under the supervision of the Standard Reference Data Program is especially important for insuring sufficient manpower to maintain an adequate compiling rate.

The availability of up-to-date critically evaluated compilations of thermodynamic data together with the availability of models that can predict the missing data can have a very large impact upon the solution of our energy problems. With such data, it should be possible to select the most promising processes at any early stage before large investments of money and manpower have been made. Such compilations will be indispensable for surmounting the materials problems which are usually the main obstacles to development of economical, practical processes.

I do have some comments on the type of experimental work that I think should be encouraged.



In regard to the types of new measurements needed, one finds many complaints about the measurements being carried out. Some of the complaints are that measurements are on materials not likely to be of any practical importance; other complaints are directed to the duplication of measurements. These complaints are sometimes valid; I would like to examine them and to describe what I would consider to be the criteria for determining whether a measurement is worth doing.

Duplication of a measurement already reported in the literature may well be warranted in many circumstances. In some instances the duplication is carried out to test a new type of apparatus as a test of systematic errors. In other instances, duplication is important because of some uncertainty in the previous determinations either because of large contradictions between independent measurements or because of some theoretical basis for suspecting an error in the reported values. However, duplication of a measurement because of unfamiliarity with the literature is not warranted. If one considers the various combinations of the elements that might be studied, one finds the number of systems to be astronomical. It is important to limit the measurements to those systems which yield data of greatest significance. This requires more than a random selection of systems and, in general, it is of great importance to have some model to which the measurements could be related. It is not possible to hope to measure properties of all the systems that might be of interest or might possibly be considered for the variety of new energy developments. It is important to develop models that allow one to predict the properties of materials that have not been studied.

The question always comes up whether certain areas or certain groups of compounds should be emphasized. It may be harmful to limit measurements to certain groups of compounds inasmuch as quite unusual compounds are often of importance for testing of models. However, there are certain areas that appear to be of special importance, at least in the near future. In spite of the fairly large amount of work that has been done in the past on the hydrocarbons, the emphasis on new methods of shale utilization, liquefaction and gasification of coal, as well as the development of methods of separating impurities from the hydrocarbons makes it clear that additional information is needed on hydrocarbons in general and for large classes of organic compounds. Bonding models are well developed for organic compounds and work in this area should be related to improvement of these models. The push to high temperatures for the processing of materials and to higher temperatures to achieve better Carnot cycle efficiencies places emphasis on refractory compounds such as carbides, nitrides, borides, silicides as well as the oxides. Proposed geothermal processes would require thermodynamic data of multi-component aqueous saline solutions as well as thermodynamic data on high pressure systems. Semiconductor materials in general are of great importance today and will certainly become increasingly important in the future and thermodynamic data for these classes of compounds would be of great value, particularly in devising different and cheaper methods of preparation of single crystals. Of special importance for all types of processes would be the development of container materials of high-strength

steels for shells of nuclear reactors or for chemical reactors. Stronger materials will be needed for carrying high-pressure gas or for extremely cold environments where normal steels tend to become brittle. The availability of thermodynamic data for metallic systems can be of very great help in the development of methods of preparing these materials and fabricating them into suitable forms.

However, in spite of my cataloguing these various groups of compounds for which thermodynamic data would be very valuable, I would not recommend an exhaustive determination of thermodynamic properties of all the members of these groups of materials. It would be too large an effort to be practical, and, in general, the examples chosen in these classes should be ones which test the reliability of applicable models in an effort to improve those models or to clearly define the areas of applicability. In some instances compounds which could be relatively easily studied would be by-passed in favor of more difficult materials that might provide crucial tests of current models.

To develop really new processes, it is not possible to restrict ourselves to commonly used materials for which properties are readily available and one must, at the first stages of examination of the possibility of a process, consider all possible materials. In many cases the amount of material required might be small enough so that even rare and expensive materials could be considered. At the first stages of examination of such processes, it is not even necessary to have highly accurate models. Even models which yield order-of-magnitude values would be useful in establishing whether, in fact, any materials are capable of meeting the design criteria and if there are such possibilities, what general classes of materials should be considered. Once we have established the general classes of materials which might be useful for the particular project, then one would like to have more accurate models. When one is dealing with a limited class of compounds, it is often possible to develop models which may not be of general applicability to all kinds of materials, but could be adapted with a limited number of parameters to a given class of materials to yield useful predictions about the properties of these materials and to indicate which possible compounds might meet the requirements of the process.

There are many types of models available. For example, one can cite from the literature a large number of bonding models such as ionic bonding, covalent bonding, hybridization, electronegativity models, acid-base models, soft acids and hard acids, etc. which scientists are using to correlate properties of materials and to predict properties for materials which have not been studied. I would assert that a meaningful program of measurements of thermodynamic properties would be tied to one or more of such models in an effort to improve the models, to determine their limitations and to establish how far they may be safely used. Generally, then, this means trying to test the models under extreme conditions going to unusual conditions of temperature, pressure or composition to press each model to the limit to determine what its defects are and to determine its reliability. This often means carrying out measurements of materials that are unlikely, at least as far as we can tell today, to be of any practical importance. Nevertheless, these materials are important for testing available models and for sharpening up these models so that they can be used for predicting the properties of a wider range of materials which include many practical materials.



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## IMPORTANT NOTICE

Following the decision taken at the CODATA General Assembly at Tsakhadzor, U.S.S.R., in June 1974, the *CODATA Bulletin* will be expanded and distributed only on a subscription basis beginning in January 1975. In addition to Task Group reports, the new *Bulletin* will contain proceedings of CODATA conferences, reviews of new data publications, and articles on the methodology of data evaluation. The *Bulletin* will also serve as a medium for updating and expanding the *CODATA Compendium* through the inclusion of listings of data centers and other data sources for all the disciplines represented in CODATA.

The *Bulletin* will be edited by Bertrand Dreyfus, the Executive Secretary of CODATA. David R. Lide, Jr. and Edgar F. Westrum, Jr. will serve as Associate Editors, and an Editorial Board is being formed. The *Bulletin* will be edited and published by the CODATA Secretariat.

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# THE FUNDAMENTAL CONSTANTS, 1974 vs 1973

E. Richard Cohen  
Chairman, CODATA Task Group on Fundamental Constants  
Science Center/Rockwell International  
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The values of the fundamental physical constants recommended in the 1973 review of Cohen and Taylor were endorsed by the CODATA Task Group on Fundamental Constants in August and adopted by the 8th CODATA General Assembly in September 1973 at its meeting in Stockholm. The summary report of the Task Group has now been published as *CODATA Bulletin* No. 11,<sup>1</sup> and the full analysis appears in a recent issue of the *Journal of Physical and Chemical Reference Data*.<sup>2</sup>

As you know, the recent reanalysis was stimulated by the recognition of inadequacies in the 1963 recommendations of IUPAC which were based on the Cohen-DuMond analysis.<sup>3</sup> The fundamental difficulty in that study was the inconsistency of the data for the fine structure constant,  $\alpha \approx 1/137$ . At that time the measurement of the fine structure in hydrogen and deuterium, measured by Dayhoff, Triebwasser and Lamb at Columbia University led to a value of  $\alpha$  which was 20 ppm lower than the value deduced from the proton NMR (or hyperfine structure) frequency. This latter frequency is very accurately known; it is perhaps the most precise measurement in physics with an uncertainty (standard deviation) of less than 1 in  $10^{12}$ . In 1963 the theory of the measurement however was barely good to 1 or 2 parts in  $10^5$ . Since the theoretical interpretation of the experimental data therefore could not be counted on at the 1 ppm level, Cohen and DuMond were forced to exclude those data and based the value of  $\alpha$  entirely on the fine structure measurements. DuMond had emphasized the dangers in this procedure and had pointed out the critical role played by  $\alpha$  in determining the values of the fundamental constants.

The discovery of the ac Josephson effect by B.D. Josephson and the precise measurement of the ratio  $h/e$  by means of it by Parker *et al.* showed that the proton NMR data was in fact valid and the correct value of  $1/\alpha$  was much nearer to 137.036 than to the Cohen-DuMond value of 137.0388. This led Taylor, Parker and Langenberg in 1969 to carry out a new analysis.<sup>5</sup> A careful review of the theory of the proton hyperfine structure frequency and the work stimulated by the Cohen-DuMond discrepancy increased the reliability of the NMR data to approximately 5 parts in  $10^6$  and cast more doubt on the fine structure data.

Taylor, Parker and Langenberg, although resolving one discrepancy, were faced with a different one. This was the contradictory data on the ratio of the proton cyclotron frequency to the proton NMR frequency in the same field, which is the reciprocal of the ratio of the proton magnetic moment to the nuclear magneton. Basing their analysis on three well-documented and consistent values and rejecting two measurements which gave significantly higher values, Taylor *et al.* deduced a value which one now believes to be approximately 25 ppm too low. The changes in the numerical values over the past decade are shown in Table I and Fig. 1.

## CHANGES IN PHYSICAL CONSTANTS

1963-1973

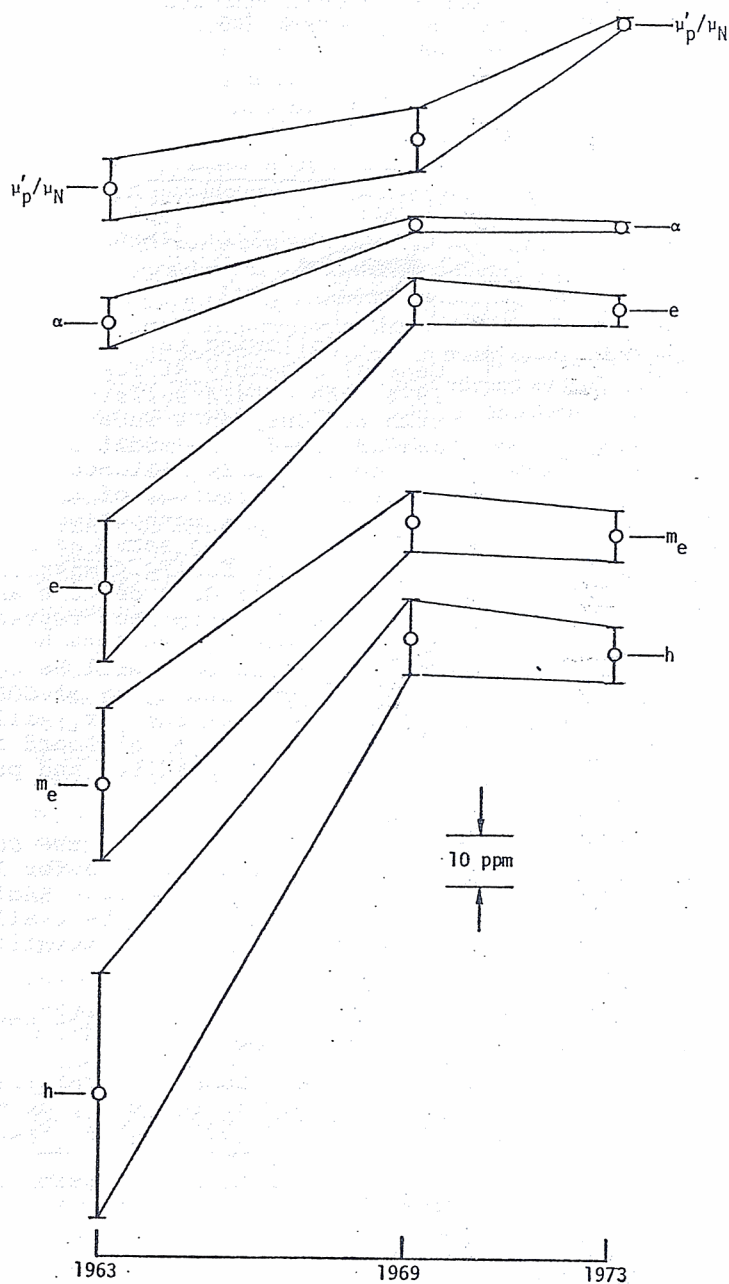


Figure 1



Some of the data on which the 1973 adjustment is based are shown in Figures 2 to 6. It is clear that there is a wide variation in the uncertainty assigned to different quantities. More significant is the variation in the uncertainty and numerical value of different measurements of the same quantity. The four measurements of the Rydberg constant shown in Fig. 2 which were used in the 1973 analysis have now been superseded by the recent (reported April 1974) measurement of Hänsch *et al.*<sup>6</sup> using laser saturation spectroscopy to resolve and measure the fine structure of the Balmer- $\alpha$  line in hydrogen and deuterium. The difference between the laser measurement  $R_\infty = 10973731.43 \pm 0.10 \text{ m}^{-1}$  and the 1973 recommendation,  $R_\infty = 10973731.77 \pm 0.83 \text{ m}^{-1}$  is  $0.34 \pm 0.84 \text{ m}^{-1}$  or 0.4 standard deviations. Hence the new value is quite consistent with, but approximately 10 times more precise than, the earlier data. The change in numerical value is only 0.03 ppm.

MEASUREMENTS OF RYDBERG CONSTANT

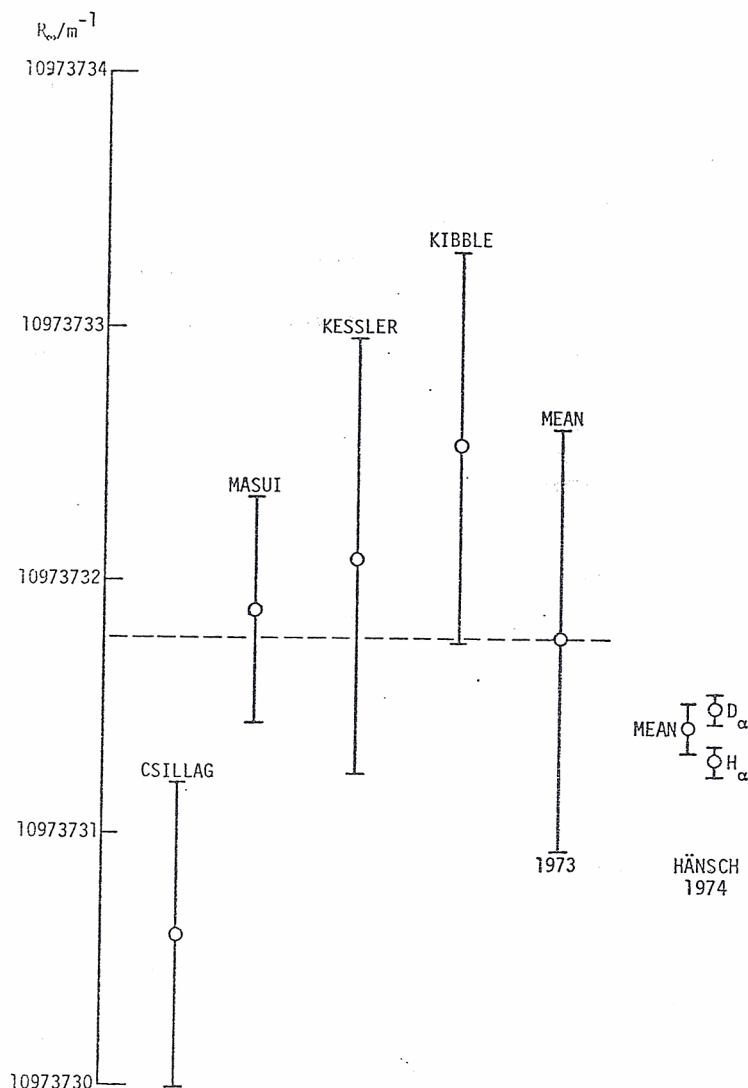


Figure 2

THE FARADAY CONSTANT AND THE GYROMAGNETIC RATIO OF THE PROTON

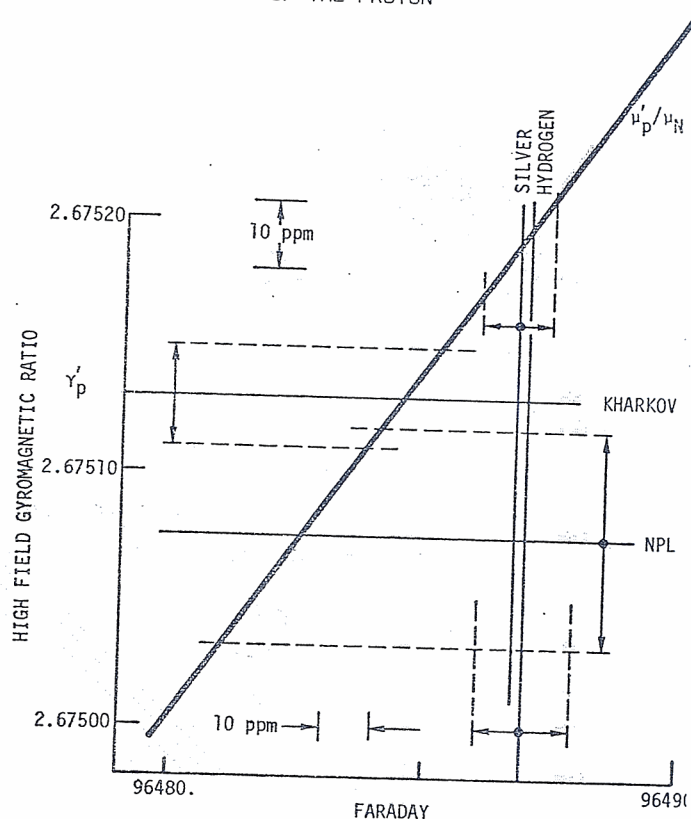


Figure 3

Figure 3 shows, in a different fashion the relationships among the data on the Faraday constant, the proton magnetic moment and the high field gyromagnetic ratio measurements. These three quantities are not independent since we may write

$$F = M_p \times (10^{-3} \text{ kg mol}^{-1}) \gamma'_p / (\mu'_p / \mu_N)$$

when both the Faraday and the gyromagnetic ratio are expressed in terms of BIPM realization of the ampere. It is clear from this figure that although the two determinations of the Faraday are mutually consistent they are not consistent with the somewhat less precise determinations of the gyromagnetic ratio. From this data alone one cannot decide which set of data is to be rejected. Other evidence (the overall consistency of all of the data) indicates that the Faraday measurements are in error. Unless some completely new experimental procedures in electrochemistry can be developed for the determination of the Faraday constant, one cannot expect to reduce the uncertainty of this measurement below 5 ppm. On the other hand programs at NPL and VNIIM to determine  $\gamma'_p$  should ultimately yield uncertainties of the order of 1 to 2 ppm or better. Combining a determination of  $\gamma'_p$  with the determination of the proton magnetic moment will then provide the best value of the Faraday.

Measurements of  $\gamma'_p$  in low field (i.e., in a magnetic field computed from a measured current and the measured geometry of the solenoid) should also be improved within the next few years. A comparison of  $\gamma'_p$  (high field) and  $\gamma'_p$  (low field) is equivalent to a direct determination of the laboratory realization of the ampere in SI units, the proton precession frequency serving as a means of transferring the high-field measurement in terms of force on a current-carrying conductor to the low-field measurement in terms of current and solenoid geometry. Here again significant reductions in uncertainty appear possible.

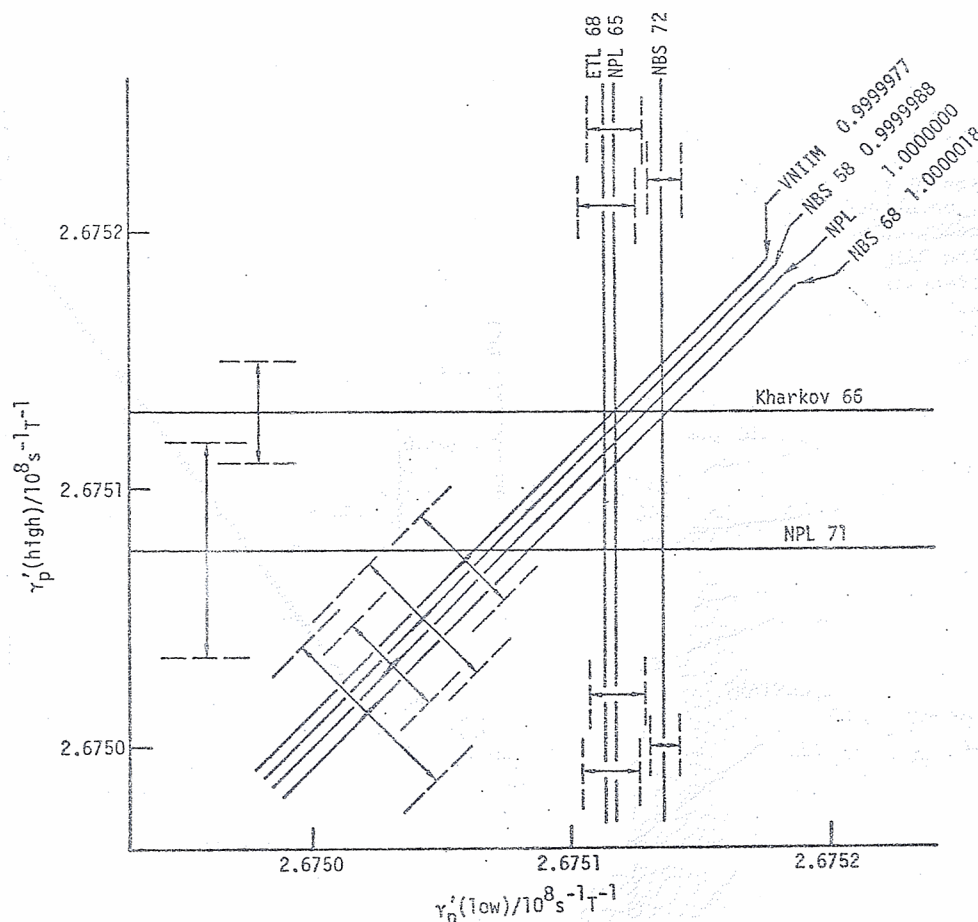


Figure 4

Figure 4 shows the relationships which exist between the direct measurement of the ampere conversion factor,  $K$ , and the two different experimental techniques for determining the proton gyromagnetic ratio. The relationship

$$\gamma_p'(\text{low}) = K^2 \gamma_p'(\text{high})$$

expresses the dependence of the gyromagnetic ratio measurements on the laboratory realization of ampere. It is clear from Figure 4 that when the precision of the high-field determination of  $\gamma_p'$  is increased to the level of the low-field measurement, the square root of the ratio will give a more accurate value of  $K$  than the "direct" measurements of this factor.

An improved low-field value of  $\gamma_p'$  (when combined with the Josephson effect determination of  $2e/h$ ) gives a value of the fine structure constant which is independent of any quantum electrodynamic considerations. This can, in view of the serious difficulties associated with present atomic beam spectroscopy determinations of the fine structure constant, also provide the most accurate value of  $\alpha$ . The difficulties with the spectroscopic determinations lie in the problems associated with the width of the lines. In all of the experiments the quoted accuracy is achieved by utilizing a detailed theory of the line shape to determine the unperturbed transition frequency to an extremely small fraction of the observed line width. One must therefore place great reliance on the adequacy of the theory and the absence of any unknown and undetected perturbations or systematic errors. There is there-

fore a practical limit beyond which the mere accumulation of data cannot be utilized to reduce statistical uncertainty.

The experimental data on the fine structure separation  $2S_{1/2} - 2P_{3/2}$  is presented in Figure 5. It is possible here to show both hydrogen and deuterium data on the same scale because the isotope shift can be calculated accurately from theory with very little uncertainty. G.W. Erickson<sup>7</sup> gives this isotope shift as 1.6335 MHz and the two scales in Figure 5 are displaced by that amount so that the old Dayhoff-Lamb measurements in deuterium (to which the right-hand scale applies) can be directly compared with the more recent hydrogen measurements. The deuterium data which led in 1963 to the value  $\alpha^{-1} = 137.0388$  is however shown here only for comparison. It was not used in the 1973 adjustment because of the serious criticisms of the data pointed out by Taylor *et al.* in their 1969 analysis and because the newer measurements by Lamb *et al.* should be considered as a replacement for it. In the 1963 adjustment the total fine structure interval  $2P_{3/2} - 2P_{1/2}$  was determined by combining the Dayhoff measurement of  $2P_{3/2} - 2S_{1/2}$  with the Triebwasser determination of the Lamb shift in deuterium  $2S_{1/2} - 2P_{1/2}$ . This gave a fine structure interval  $10971.59 \pm 0.10$  MHz. Combining this with Erickson's theoretical calculation yields a "modernized" value for the fine structure constant,  $\alpha^{-1} = 137.0387(6)$ ; on the other hand if one uses only the  $2P_{3/2} - 2S_{1/2}$  interval shown in Figure 5 in conjunction with Erickson's calculations, one obtains  $\alpha^{-1} = 137.0371(4)$ .



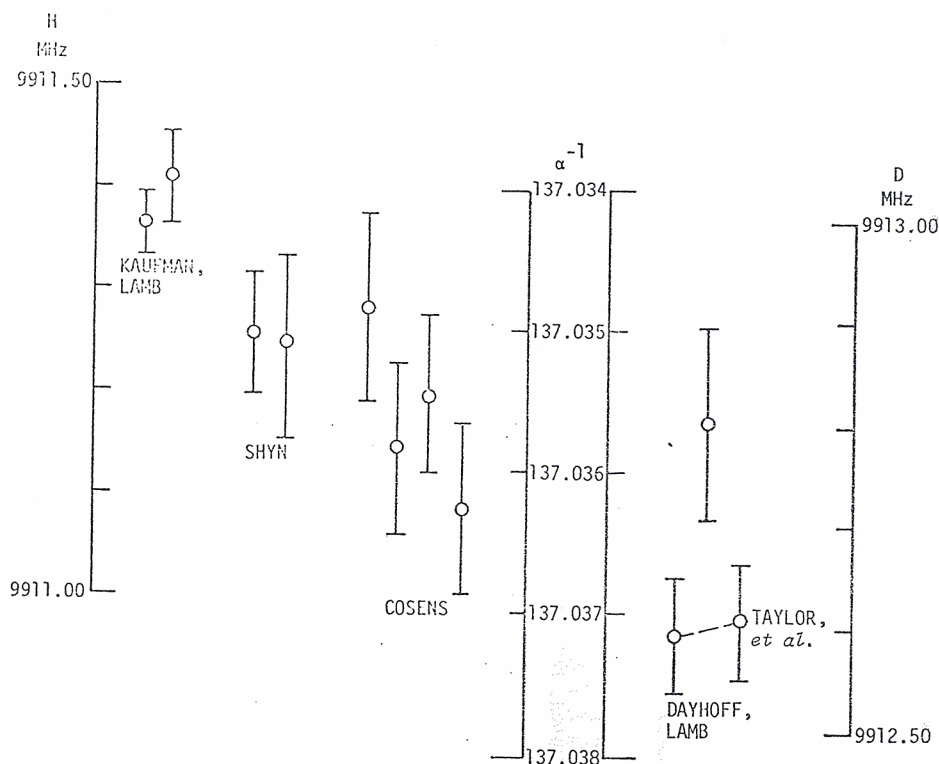


Figure 5

It is clear from this figure that the Kaufman-Lamb measurements are significantly higher than the Cosens or Shyn results. Unfortunately this conclusion is strongly influenced by the small uncertainty attached to the Kaufman data. If the uncertainty of that data were increased by a factor of 2, the disagreement between that data and the other measurements would be acceptable but the weight assigned to the Kaufman data would have been reduced correspondingly by 75%. On this basis then the total rejection of the data seems reasonable. This, however, is clearly an area where additional measurements would be extremely useful in future analyses.

Another weak area in the present adjustment is the Avogadro constant,  $N_A$ . Its assigned uncertainty (5.1 ppm) could be significantly improved when measurements of  $\gamma_p$  and the ampere achieve the level of 2 ppm. In SI units one can write

$$N_A = \frac{M_p \mu_0}{8(\mu_p'/\mu_N)} \sqrt{\frac{c^3 (2e/h)^3 (\mu_p'/\mu_B) \gamma_p'}{R_\infty}}$$

so that the primary source of uncertainty in  $N_A$  is due to the uncertainty in  $\gamma_p$  and in the conversion factors from laboratory standards of the ampere and volt to SI units. Experiments presently under way in several standards laboratories (DAMW, VNIIM, NPL, NSL, NBS) should yield significant improvements in our knowledge of  $A_{B169}/A$  and  $\gamma_p$  within the next few years.

An alternative attack on the value of  $N_A$  comes from the work with the x-ray optical interfero-

meter. This instrument makes possible the direct measurement of crystal lattice spacings in terms of optical wavelengths. R.D. Deslattes and his co-workers at NBS<sup>8</sup> have now achieved a precision of 0.3 ppm in determining the lattice spacing,  $d_{220}$ , of a silicon single crystal. When combined with a determination of the density and isotopic composition of the same crystal, this should lead to a value of  $N_A$  with an uncertainty that should approach 2 ppm.

The last area of improvement which I wish to discuss is the theoretical basis for interpreting the hyperfine and fine structure measurements. Here significant improvements in theory are desperately needed before full advantage can be taken of much excellent experimental data. Measurements of hydrogen hfs, with a precision of parts in  $10^{12}$ , are limited by our knowledge, primarily, of internal structure of the proton and of the relativistic proton "recoil" terms which contribute corrections to the theoretical expression of the order of a few parts per million. The muonium hfs, although free of problems associated with internal structure (since the muon is sufficiently understood as a heavy structureless electron) suffers from larger recoil corrections because the "nucleus" has a relative atomic mass of only 0.11. The experimental precision is now almost a factor of ten better than the present uncertainties in theory. The experimental data on  $\alpha^{-1}$  is presented in Figure 6. The experimental uncertainty is shown by the solid error bars while the total uncertainty, including the contribution from the shortcomings of the present theoretical calculations is shown by the broken bars. It is clear that there is an important area here for future activity.

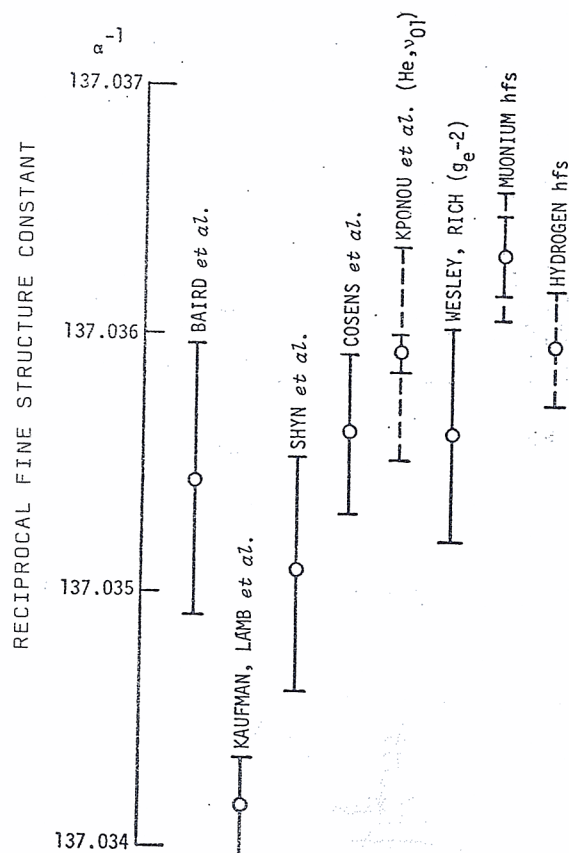


Figure 6

In conclusion, the presently available data, excellent as they are, and in spite of the significant improvements in accuracy and precision which have been achieved in the last five years, are still capable of further improvement. The field of fundamental precision measurement has continued to

be extremely active. These improvements will aid not only the field of metrology and standards, but will also increase our knowledge and understanding of the fundamental physical quantities and our knowledge of the world in which we live.

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## ATOMIC AND MOLECULAR PROPERTIES

**CRITICAL EVALUATION OF CHEMICAL AND PHYSICAL STRUCTURAL DATA** (1974, XII + 616 pp, \$26.25, The National Academy of Sciences, Washington, D.C. 20418) David R. Lide, Jr. and Martin A. Paul, eds, reports the proceedings of a conference held at Dartmouth College in June 1973 and sponsored by the Committee on Chemical Crystallography of the National Research Council with support from the National Science Foundation. The idea underlying the conference was to alleviate the difficulties now experienced by investigators in many disciplines when they seek to utilize structural information derived from experimental techniques other than their own. The extensive scope of the book is indicated by its table of contents:

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**IX THEORETICAL METHODS.** Studies of Molecular Properties Pertaining to Electronic Charge Distribution: A Comparison between Theory and Experiment, *Robert Ditchfield*; Status of *ab initio* Molecular Structure Predictions, *Henry F. Schaefer III*. (45 p.)

## BIO SCIENCES

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**BIOLOGY DATA BOOK**, 2nd edition (1974, 3 volumes at \$30.00, Federation of American Societies for Experimental Biology, Bethesda, Md. 20014). Philip L. Altman and Dorothy S. Dittmer, eds, is an expanded and updated edition of the original version of the *Biology Data Book* first published in 1964 as part of the Biological Handbooks series. In its present form, the *Biology Data Book* has been broken down in 3 volumes, comprising 13 sections. *Volume 1* (Sections I through V, 541 pp + tables) covers Genetics and Cytology - Reproduction - Development and Growth - Properties of Biological Substances - Materials and Methods - Appendices. *Volume 2* (Sections VI through IX, 700 pp + tables) covers Biological Regulators and Toxins - Environment and Survival - Parasitism - Sensory and Neuro-Biology. *Volume 3* (Sections X through XIII, 607 pp + tables) covers Nutrition, Digestion and Excretion - Metabolism - Respiration and Circulation - Blood and Other Body Fluids.

## CHEMISTRY

**THE CHEMICAL DURABILITY OF GLASS** (1972, 211 pp, 500 Belgian Francs, Secretariat of Sub-committee A1, Institut National du Verre, 34 rue Michel-Ange, 75016 Paris, France). A bibliographic review of literature compiled by Sub-committee A II of the International Commission on Glass, under the direction of Jaime Robredo, with the assistance of Fabio Nicoletti and of Marie-Thérèse Carregal.



## EARTH SCIENCES

**CATALOGUE OF TERRESTRIAL CRATERIFORM STRUCTURES. PART 1: CANADA** (1972, 45 pp, ESRO SP-92, European Space Research Organisation, 92-Neuilly, France), R.J. Fryer and C. Titulaer, eds, is primarily aimed at astronomers and planetary scientists in an attempt to provide them with an inventory of crateriform structures existing on the surface of the Earth. Such an inventory, undertaken at the initiative of the International Astronomical Union, is designed to help astronomers compare these terrestrial structures with similar features observed and photographed on the Moon, Mars and Mercury. In the future, other large geographical regions will be similarly covered and the corresponding catalogue published, until the entire surface of the Earth is fully mapped for craters. In this first volume, thirty-nine crateriform structures discovered in Canada are described, each one being characterized by its geographic coordinates, its horizontal dimensions, depth, probable age, etc. These quantitative data are followed by a topographic description and a summary of suggested modes of origin. The sources of all quoted information are listed and full references can be found in the bibliography. The volume is presented in loose-leaf binding in order to facilitate future updatings.

**CATALOGUE OF TERRESTRIAL CRATERIFORM STRUCTURES. PART 2: INDONESIA** (1972, 62 pp, ESRO SP-93, European Space Research Organisation, 92-Neuilly, France), compiled by Neumann van Padang and edited by R.J. Fryer and C. Titulaer, is the second volume in the series of regional inventories of crateriform structures. In sharp contrast to the first volume of the series (Canada), which contained mainly meteoric impact features, the present volume is comprised exclusively of crateriform structures having a volcanic origin but not listed in the *Catalogue of Active Volcanoes of the World*. In other words, the authors have restricted their choice to calderas. The same basic layout as in the Canada listing has been adopted, with Section I containing the numerical data and Section II a descriptive summary on "Form and Structure". Section III on "Probable Origin" not being required in this instance has been replaced by maps and diagrams for 17 of the 23 calderas listed. A list of 54 references ranging from 1855 to 1970 is appended.

**MICROWAVE SPECTRA OF MOLECULES OF ASTROPHYSICAL INTEREST - V. WATER VAPOR** (1974, Journal of Physical and Chemical Reference Data, vol. 3, No. 1, Reprint No. 45, \$3.00) by Frank C. De Lucia, Paul Helminger and William H. Kirchhoff. The available data on the microwave spectrum of water vapor are critically reviewed for information applicable to radio astronomy. Molecular data such as rotational constants, centrifugal distortion constants, hyperfine coupling parameters, and dipole moments are tabulated. A detailed centrifugal distortion calculation has been carried out for the most abundant isotopic form of this molecule  $H_2^{16}O$  as well as for  $H_2^{18}O$  and  $HD^{16}O$ . Transitions have been predicted and tabulated for the frequency range 1 MHz to 800 GHz. All predicted transitions include 95 percent confidence limits; estimated error limits have been reported for all measured transitions. Observed transitions of  $H_2^{17}O$  are also listed.

**MICROWAVE SPECTRA OF MOLECULES OF ASTROPHYSICAL INTEREST - VI. CARBONYL SULFIDE AND HYDROGEN CYANIDE** (1974, Journal of Physical and Chemical Reference Data, vol. 3, No. 1, Reprint No. 46, \$3.50) by Arthur G. Maki. All available data on the microwave spectra of carbonyl sulfide and hydrogen cyanide are critically reviewed and tabulated. Molecular data such as rotational constants, dipole moments, hyperfine coupling constants, and structural parameters are also tabulated. All rotational transitions from 100 MHz to 300 GHz that are deemed likely to be of interest to radio astronomers are calculated and tabulated along with their estimated 95 percent confidence limits. Microwave measurements

are tabulated for most isotopic species and for many of the lower vibrational states. For both carbonyl sulfide and hydrogen cyanide a bibliography is given which includes nearly all the spectroscopic work reported in the literature. For each molecule a bibliography of related astrophysical papers is also given.

**MICROWAVE SPECTRA OF MOLECULES OF ASTROPHYSICAL INTEREST - VII. CARBON MONOXIDE, CARBON MONOSULFIDE, AND SILICON MONOXIDE** (1974, Journal of Physical and Chemical Reference Data, vol. 3, No. 1, Reprint No. 47, \$3.00) by Frank J. Lovas and Paul H. Krupenie. The available data on the microwave spectra of carbon monoxide, carbon monosulfide, and silicon monoxide are critically reviewed for information applicable to radio astronomy. Molecular data such as rotational constants, centrifugal distortion parameters, dipole moments, hyperfine coupling constants, and structure are tabulated. Observed rotational transitions are presented for all measured isotopic forms of these molecules. All of the available data has been analyzed in order to predict all rotational transitions of these molecules up to 300 GHz. Error limits have been taken from the original literature for each measured transition frequency. All predicted transition frequencies are given with estimated uncertainties which represent the 90 percent confidence limit.

**MICROWAVE SPECTRA OF MOLECULES OF ASTROPHYSICAL INTEREST - VIII. SULFUR MONOXIDE** (1974, Journal of Physical and Chemical Reference Data, vol. 3, No. 1, Reprint No. 48, \$3.00) by Eberhard Tiemann. The available data on the microwave spectrum of sulfur monoxide (SO) is critically reviewed and tabulated. Molecular data such as rotational constants, hyperfine coupling constants, electric dipole moment, and magnetic  $g$ -factors are given. All rotational transitions up to 350 GHz for the isotopic species  $^{32}S^{16}O$ ,  $^{34}S^{16}O$ , and  $^{32}S^{18}O$  in the ground vibrational state are calculated and tabulated along with their estimated 95 percent confidence levels. The line strengths of all tabulated transitions have been determined. A bibliography of SO is given which includes results from microwave spectroscopy as well as from electron paramagnetic resonance.

**GLACIOLOGICAL NOTES** (No. 55, Spring 1974, 70 pp, WDC-A, Glaciology - U.S. Geological Survey, Tacoma, Washington, U.S.A.). *Glaciological Notes* is a quarterly announcement bulletin of publications received by WDC-A, Glaciology. The publication also includes periodical listings of catalogued aerial glacier photography and acquisitions of maps and charts.

## MATHEMATICAL METHODS AND COMPUTER PROGRAMS

**INITIATION A L'APPRECIATION DES INFORMATIONS CHIFFRÉES** (1972, Association de Coordination Technique Agricole, 149 rue de Bercy, 75012 Paris, France, 15 FF, 6 volumes, 111.): Comment Résumer Une Série de Données (48 pp & erratum); Comment Lire les Résultats d'Essais. 1. (75 pp); Comment Lire les Résultats d'Essais. 2. (48 pp); Comment Apprécier les Données Chiffrées (28 pp); Aide-Mémoire (29 pp); Schémas et Tableaux (28 pp).

**COMPUTER PROCESSING OF METEOROLOGICAL DATA** (c1971, 210 pp, \$15, distributed by International Scholarly Book Services.) by S.L. Belousov et al. Translated from the Russian by A. Barouch. Jerusalem: Israel Program for Scientific Translations, 1973. Initial computer processing of meteorological data. Theoretical foundations of objective analysis of meteorological fields. Objective analysis methods and their application under operational conditions. Objective analysis for data-sparse areas. Automatic data processing in numerical weather forecasting.



**TABLES DE RÉSISTANCE A LA CORROSION DES ALLIAGES CUIVREUX DE FONDERIE DANS DIFFÉRENTS MILIEUX** (1972, 83 + XV pp, 39 FF, Editions techniques des industries de la fonderie, 12 avenue Raphaël, 75016 Paris) is the translation in French of an original German publication on the "Resistance to corrosion of cuprous alloys in various environments", produced jointly by the Deutsches Kupferinstitut and the Gesamt Verband Deutscher Metallgiessereien. It provides qualitative and semi-quantitative information on the behavior of cuprous alloys, and of copper itself, in various solutions of inorganic and organic salts, acids, and bases, in several types of soils and in sea water. The corrosion is expressed in mm/year, i.e. the thickness of superficial material actually removed over a period of one year. Electrochemical potentials are also given for a series of copper alloys when immersed in sea water and in ordinary water as found in water mains.

**THE EXACT OVER-WIRE MEASUREMENT OF SCREWS, GEARS, SPLINES, AND WORMS** (1973, 230 pp, \$19.95, The Wayne State University Press, Detroit, Mich., U.S.A.) by F.W. Vogel is a very useful treatise "providing for the first time universal exact equations of the best pin measurement applicable to general screws and the first exact equations for the ball measurement of internal threads." In addition, approximation procedures are described which lead to very appreciable shortcuts in the measurement of both square threads and backlash. A chapter on finding exact solutions by means of a digital computer is appended.

## SOLUTION PROPERTIES

**MOLTEN SALTS: VOLUME 4, PART 1, FLUORIDES AND MIXTURES, ELECTRICAL CONDUCTANCE, DENSITY, VISCOSITY, AND SURFACE TENSION DATA** (1974, Journal of Physical and Chemical Reference Data, vol. 3, No. 1, Reprint No. 41, \$6.50) by G.J. Janz, G.L. Gardner, Ursula Krebs. Data on the electrical conductance, density, viscosity, and surface tension of fluoride mixtures have been systematically collected and evaluated. Results are given for 44 binary mixtures over a range of compositions and temperatures. Values of the above properties for the single salts have been updated in accord with previously advanced recommendations.

## SPECTRA COLLECTIONS

**TABLES OF MOLECULAR VIBRATIONAL FREQUENCIES. PART 8** (1974, Journal of Physical and Chemical Reference Data, vol. 3, No. 1, Reprint No. 49, \$4.00) by T. Shimanouchi. The compilations of fundamental vibrational frequencies of molecules previously published in the NSRDS-NBS publication series and in this journal are here extended by 49 additional molecules. 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. The selection of vibrational fundamentals has been based on careful studies of the spectral data and comprehensive normal-coordinate analyses. An estimate of the accuracy of the selected values is included. The tables provide a convenient source of information for those who require vibrational energy levels and related properties in molecular spectroscopy, thermodynamics, analytical chemistry, and other fields of physics and chemistry.

## THERMODYNAMIC PROPERTIES

**IDEAL GAS THERMODYNAMIC PROPERTIES OF EIGHT CHLORO- AND FLUOROMETHANES** (1974, Journal of Physical and Chemical Reference Data, vol. 3, No. 1, Reprint No. 42, \$3.50) by A.S. Rodgers, J. Chao, R.C. Wilhoit and B.J. Zwolinski. The structural data, vibrational assignments, enthalpies of vaporization and formation for chloromethane, dichloromethane, trichloromethane, tetrachloromethane, fluoromethane, difluoromethane, trifluoromethane, and tetrafluoromethane were critically reviewed. Based on the selected best values, the thermodynamic properties for each of these eight chloro and fluoromethanes were calculated by statistical thermodynamic methods using the rigid-rotor harmonic-oscillator approximations. The derived entropies and heat capacities are compared with the available third law entropies and vapor heat capacities. The calculated values of  $C_p^\circ$ ,  $S^\circ$ , and  $\Delta H_f^\circ$  at 298.15 and 700 K are compared with those reported in the other major compilations.

**IDEAL GAS THERMODYNAMIC PROPERTIES OF SIX CHLOROETHANES** (1974, Journal of Physical and Chemical Reference Data, vol. 3, No. 1, Reprint No. 43, \$3.50) by J. Chao, A.S. Rodgers, R.C. Wilhoit and B.J. Zwolinski. The thermodynamic properties:  $C_p^\circ$ ,  $S^\circ$ ,  $H^\circ - H_0^\circ$ ,  $-(G^\circ - H_0^\circ)/T$ ,  $\Delta H_f^\circ$ ,  $\Delta G_f^\circ$  and  $\log K_f$  for chloroethane, 1,1-dichloroethane, 1,1,1-trichloroethane, 1,1,1,2-tetrachloroethane, pentachloroethane, and hexachloroethane in the ideal gaseous state in the temperature range from 0 to 1500 K and at 1 atm were evaluated by statistical thermodynamic methods based on a rigid-rotor harmonic-oscillator model. The internal rotation contributions to thermodynamic functions were calculated by using a partition function formed by summation of internal rotation energy levels. The internal rotation barrier heights (in kcal mol<sup>-1</sup>) employed for generation of the energy levels for each of the above six chloroethanes are: 3.69, 3.54, 5.08, 10.38, 14.43, and 14.7, respectively. The calculated heat capacities and entropies are compared with available experimental data. The derived values of  $C_p^\circ$ ,  $S^\circ$ , and  $\Delta H_f^\circ$  at 298.15 and 700 K are compared with those reported in the other major compilations.

**CRITICAL ANALYSIS OF HEAT-CAPACITY DATA AND EVALUATION OF THERMODYNAMIC PROPERTIES OF RUTHENIUM, RHODIUM, PALLADIUM, IRIIDIUM, AND PLATINUM FROM 0 TO 300 K. A SURVEY OF THE LITERATURE DATA ON OSMIUM** (1974, Journal of Physical and Chemical Reference Data, vol. 3, No. 1, Reprint No. 44, \$4.00) by George T. Furukawa, Martin L. Reilly and John S. Gallagher. The literature sources of heat-capacity data on ruthenium, rhodium, palladium, osmium, iridium and platinum have been compiled and the data critically analyzed. Except for osmium where data are lacking, best values of thermodynamic properties have been evaluated between 0 and 300 K from the analyses. The literature values of heat capacity, the electronic coefficient of heat capacity ( $\gamma$ ) and the zero K limiting Debye characteristic temperature [ $\theta_D(0)$ ] are compared. The sources of data are tabulated chronologically along with the temperature range of measurements, purity of sample, and the pertinent experimental procedures used. A bibliography of the reference is listed.

**LA MESURE DES TEMPERATURES DE SURFACE** (Cahiers de la thermique, Série A, No. 3, March 1973, 230 pp, 86 FF), H. Poncin, ed, comprises a dozen lectures on the various methods and devices now being used for the measurement of surface temperatures: liquid crystals, thermochromic paints, photoluminescent coatings, and optical pyrometers. A few chapters are devoted to more specific problems, e.g., the measurement of very low temperatures (down to 4 K) or rotating machinery (up to 4000 rpm), or the medical and industrial applications of infrared thermography. Available from the Institut Français des Combustibles et de l'Energie, 3 rue Henri-Heine, 75016 Paris, France.

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## CODATA PUBLICATIONS

### International Compendium of Numerical Data Projects

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

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

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

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

### CODATA Newsletter (twice a year) :

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

### CODATA Bulletin (irregular):

- No. 1 (Oct. 1969), 12 pp, *Automated Information Handling in Data Centers*  
(Report of the CODATA Task Group on Computer Use, June 1969), superseded by Bulletin No. 4.
- No. 2 (Nov. 1970), 6 pp, *Tentative Set of Key Values for Thermodynamics - Part I*  
(Report of the CODATA Task Group on Key Values for Thermodynamics, Oct. 1970), superseded by Bulletin No. 5.
- No. 3 (Dec. 1971), 28 pp, *A Catalog of Compilation and Data Evaluation Activities in Chemical Kinetics, Photochemistry and Radiation Chemistry*  
(Report of the CODATA Task Group on Data for Chemical Kinetics, Sept. 1971).
- No. 4 (Dec. 1971), 12 pp, *Automated Information Handling in Data Centers*  
2nd Edition (Report of the CODATA Task Group on Computer Use, Nov. 1971).
- No. 5 (Dec. 1971), 6 pp, *Final Set of Key Values for Thermodynamics - Part I*  
(Report of the CODATA Task Group on Key Values for Thermodynamics, Nov. 1971), superseded by Bulletin No. 10.
- No. 6 (Dec. 1971), 8 pp, *Tentative Set of Key Values for Thermodynamics - Part II*  
(Report of the CODATA Task Group on Key Values for Thermodynamics, Nov. 1971), superseded by Bulletin No. 10.
- No. 7 (Aug. 1972) 4 pp, *Tentative Set of Key Values for Thermodynamics - Part III*  
(Report of the CODATA Task Group on Key Values for Thermodynamics, June 1972), superseded by Bulletin No. 10.
- No. 8 (Dec. 1972), 32 pp, *Geological Data Files: Survey of International Activity*  
(Report of COGEODATA, Committee on Storage, Automatic Processing and Retrieval of Geological Data of the International Union of Geological Sciences (IUGS)).
- No. 9 (Dec. 1973), 6 pp, *Guide for the Presentation in the Primary Literature of Numerical Data Derived from Experiments*  
(Report of the CODATA Task Group on Publication of Data in the Primary Literature, Sept. 1973).
- No. 10 (Dec. 1973), 12 pp, *CODATA Recommended Key Values for Thermodynamics, 1973*  
(Report of the CODATA Task Group on Key Values for Thermodynamics, Nov. 1973).
- No. 11 (Dec. 1973), 8 pp, *Recommended Consistent Values of the Fundamental Physical Constants, 1973*  
(Report of the CODATA Task Group on Fundamental Constants, August 1973).
- No. 12 (Sept. 1974), 12 pp, *Energy Data Accessing and/or Retrieval*  
(Report on Data Tagging, compiled by a Panel of Experts at the Energy R&D Data Workshop held at Gaithersburg, Md., May 6-7, 1974).
- No. 13 (Dec. 74), 8 pp, *The Presentation of Chemical Kinetics Data in the Primary Literature*  
(Report of the CODATA Task Group on Data for Chemical Kinetics)

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