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.
Professor Takehiko Shimanouchi died suddenly of a heart attack at his home in Tokyo on 19th May 1980. His passing is a great loss to the scientific community, not only in Japan but throughout the whole world. He is survived by his wife Reiko and two daughters Michiko and Yuriko. He died two days before his sixty-fourth birthday. Prof. Shimanouchi's diminutive figure and abundant energy are well known to all active in CODATA. His joviality and cheerful personality gained him many friends.

His formal association with CODATA began in 1973 when he was appointed National Delegate and later, when he became a Co-Chairman of the Program Committee and Chairman of the Organizing Committee. He brought to these tasks his characteristic organizing abilities and infectious enthusiasm. Prof. Shimanouchi also partook very actively in the affairs of the Chemical Society of Japan and many other Japanese scientific organizations. He was also prominent in IUPAC in which he served as a Titular Member of the Commission on Molecular Structure and Spectroscopy and as Chairman of the Subcommittee on Storage and Retrieval of Spectroscopic Data.

Takehiko Shimanouchi was born in Tokyo in 1916. He took the B.Sc. degree at the University of Tokyo in 1941 and began graduate studies with Prof. San'ichiro Mizushima. He was appointed Associate Professor under Prof. Mizushima in 1946 and was awarded the doctorate degree of the University of Tokyo in 1949. Periods of study abroad followed during which he was a post-doctoral fellow at the University of Minnesota with Prof. Bryce Crawford and at the Thermodynamics Division of the U.S. National Bureau of Standards with Dr. David Mann. In 1959 he was appointed a full Professor at the University of Tokyo succeeding to that prestigious chair on the retirement of Prof. Mizushima.

Prof. Shimanouchi was among the earliest physical chemists to recognize the importance the electronic computer was to have in basic scientific research and scientific data management. In 1972 he was appointed Director of the Computing Center of the University of Tokyo. In this capacity he played a major role in developing a network of computerized chemical and spectroscopic data bases throughout Japan. On his retirement from the University of Tokyo he was appointed Dean of the College of Information Science at the new University of Tsukuba. Prof. Shimanouchi held this position until a few months before his death. Returning to Tokyo in March 1980 he joined Meisei University, an institution with which he had had a long association having attended the Meisei Highschool in his boyhood.

Prof. Shimanouchi during his long period at the University of Tokyo, first in association with Prof. Mizushima, and later on his own accord, continued and developed the traditions of this active and imaginative school of molecular spectroscopy. He gathered around him many promising young scholars who now occupy senior positions in the academic and industrial life of Japan. This school has also attracted to Tokyo numerous molecular spectroscopists from all parts of the world.

In 1977 his students published a Memorial Volume of his 293 papers and monographs in commemoration of his sixtieth-birthday. In a preface to this volume Prof. Shimanouchi summarized his area of scientific activity as follows: For the past 36 years I have been engaged in the study of molecular structures by means of vibrational spectroscopy. It has always given me much pleasure to examine the infrared and Raman spectra which I believe are the communications from the world of molecules. Decoding these messages provides the basis for practical utilization of the molecules for various purposes. With my colleagues I have tried to decode such messages from molecules of as many classes as possible.

Those of us who have had the privilege of close association with Prof. Shimanouchi will see in this succinct summary of his many-sided research activities the broad philosophical approach he brought to the day-by-day problems of the laboratory. However, his interests ranged much wider. In informal technical conversations he was always ready to bring out pencil and paper to explain to foreign visitors some of the intricacies of Japanese language and history.

Prof. Shimanouchi leaves with us all a fond memory of an outstanding scholar. A man whom we all admire not only for his academic achievements but also for his fortitude in overcoming physical handicaps.

R. Norman Jones
June 1980
IN MEMORIAM
STIG ARNE SUNNER

The sudden death of Professor Stig Sunner on 3rd June 1980, at the age of 63, has robbed interna-
tional science of one of its wisest counsellors. Born in Linköping, Sweden, Stig Sunner spent most
of his professional life in the ancient cathedral
and university city of Lund, in southernmost
Sweden. He received his doctorate from the Uni-
versity of Lund in 1949, was appointed Docent
(1949), became Head of the Thermochemistry Lab-
oratory there (1956), was appointed Associate Pro-
fessor (1958) and Professor (1966) under the
Swedish Natural Science Research Council and
finally University Professor (1977).

Stig Sunner was introduced to thermochemistry in
the 1940's by Lennart Smith, then Professor of
organic chemistry at Lund, and a specialist in
combustion calorimetry. This subject had recent-
ly undergone a renaissance, with two distinct
aspects: one, inspired by Frederick Rossini, in-
volved very precise measurements on hydrocarbons,
by attention to the details of calorimetry and
the chemistry of combustion; the other, in which
Smith was prominent, involved the extension of
combustion calorimetry to organic compounds whose
successful combustion required considerable arti-
fice by the experimenter. Stig's great contribu-
tion to thermochemistry was to conjoin these two
aspects, to produce precise thermochemical data
on a variety of compounds, so providing informa-
tion. He evened his doctorate from Lund. This
he achieved by ingenuity in the design of his
calorimeters and by insight into the highways and
byways of chemical reactions. With the aid of
many students and researchers who were attracted
to the Lund school of thermochemistry, Stig de-
developed and utilized a range of equipment for the
measurement of reliable thermodynamic data. Some
of the laboratory versions of this equipment were
later developed into production models. Indeed,
Sunner and his collaborators have been engaged in a number
of technical developments by Swedish industry. One
notable example, with only a tenuous connection
with thermochemistry, was the development of
"Tetrapak" sealed containers for the hygienic
dispensing of drinks.

Stig's attendance as an observer at the 17th Con-
ference of the International Union of Pure and Ap-
plied Chemistry (IUPAC) held in Stockholm in 1953,
was the start of his involvement in international
science. A visit shortly afterwards to Dr. Guy
Waddington at the Bartlesville station of the U.S.
Bureau of Mines led to the rapid emergence of the
rotating-bomb calorimeter as the preferred instru-
ment for measuring the energies of combustion of
organic compounds containing sulphur and the
halogens. Stig was appointed to IUPAC's Commis-
sion on Thermodynamics and Thermochemistry in 1957,
serving as its Chairman from 1969 to 1973. He
served on the Physical Chemistry Committee of
IUPAC from 1969 to 1979, becoming successively the
Secretary, Vice-President and President. Amongst
the more tangible outcomes of the IUPAC Commis-
sion's work during Stig's long service may be men-
tioned the production of a series of definitive
monographs on experimental thermochemistry and ther-
mochemistry and the organizing of a series of
international conferences on chemical thermo-
dynamics.

His strong belief in international scientific co-
operation took Stig to Arnoldshain, FRG, in 1968
for the First International CODATA Conference. He
was there appointed Chairman of the Task Group on
Key Values for Thermodynamics. By the time of his
retirement from the Chairmanship in 1974, the Task
Group had come to grips with its assignment and
had produced its first data tables. Thereafter the
Task Group continued to benefit from his advice,
and indeed we held our 1977 meeting in Lund, with
Stig as our local host. Within his own country,
Stig acted as Chairman of the National CODATA
Committee from 1971-77.

Amongst the honours which Stig received were the
Gold Medal of the Royal Swedish Academy of Engi-
neering Sciences and the Nordsted-Ekstrand medal of the
Svenska Kemistamfundet. He received the 1970
Huffman Memorial Award of the (US) Calorimetry Con-
ference and was to have delivered the keynote Ros-
sini lecture at the forthcoming 6th International Confer-
ence on Chemical Thermodynamics, in Merseburg,
GDR. But the honour which he probably prized most
was the warm esteem in which he was held by chemists
around the globe, esteem gained in his many travels
(his was one of the first foreign scientists to visit the
People's Republic of China) and during visits to
Lund by thermodynamicists from East, West and the
Third World; such a visitor was invariably ac-
corded the most genuine hospitality by Stig and his
wife, the chemist Gerd Olofsson.

Finally, how shall we remember Stig Sunner? Some
will recall his thoughtfulness over little
things, like the provision of his visitors with
pocket-sized compendia of the fundamental constants
and units for thermodynamics. Many will remember
evening telephone calls from the Sunners' country
cottage. All will recall his deep concern for the
well-being of others.

J.D. Cox
IN MEMORIAM

SIR GORDON SUTHERLAND

Sir Gordon Sutherland who died on the 27th June 1960 at the age of 73 was a "founder" and the first Secretary-Treasurer of CODATA. He had a very special relationship with CODATA shared by very few others; he was from its earliest days continually associated with CODATA in one way or another.

When in 1965 the International Council of Scientific Unions (ICSU) set up an ad-hoc committee to examine how it might help in the field of scientific data generation, evaluation and dissemination, Sutherland was the United Kingdom's representative. When, a year later, CODATA was established by the 6 founding National Members, France, Federal Republic of Germany, Japan, U.K., U.S.A., and U.S.S.R., he became CODATA's first Secretary-Treasurer. He gave up this office in 1970 but remained U.K. delegate and Vice-President until 1972. During the next years he retained his contact with CODATA as chairman of the British National Committee on Data for Science and Technology and in 1974 became U.K. delegate once again.

What were the special qualities, scientific and personal, that led to Gordon Sutherland's assuming such an almost unique position in CODATA? A sketch of his life, his interests, his achievements and his personality may provide the answer.

Gordon Brims Black M'Ivor Sutherland was born on 8 April 1907 at Wattens in Caithness, Scotland - a truly Highland Scot who to the end of his life retained his soft native accent. After undergraduate studies at the University of St. Andrews he went to Cambridge where, working in Professor (later Sir Eric) Rideal's group he acquired an expertise in infrared spectroscopy and developed his life-long interest in and fascination with the use of I.R. Spectroscopy for determining molecular structures. Having obtained his Ph.D. he spent 2 years (1931-33) as a Commonwealth Fund Fellow at the University of Michigan, Ann Arbor, an important centre for infrared studies and then returned to Cambridge. The next 6 fruitful years brought forth what was perhaps his most significant discovery, namely the elucidation of the structure of the hydrogen peroxide molecule. By applying quantum mechanics to the carefully measured spectrum of H$_2$O$_2$, Sutherland, in collaboration with W.G. (later Lord) Penney was able to show that contrary to previous ideas the four atoms of hydrogen peroxide were not co-planar: the first example of determining a molecular structure in this way.

During the 1939-1945 war he was one of the pioneers in the use of infrared spectroscopy for chemical analysis, for instance of mixtures of hydrocarbons, a development of great national importance.

In 1949 Sutherland became Professor of Physics at the University of Michigan where during the next 7 years he built up a successful I.R. spectroscopy group with interests extending into biology.

Then, in 1956 he returned to England to become the Director of the National Physical Laboratory (NPL) where he stayed until 1964. He was the last Director of the NPL while it was still relatively free of direct governmental control and before, as a result of the reorganization of the Scientific Civil Service, it was placed under Government Departments, first the Ministry of Technology and, now, the Department of Industry. The 8 years of Sutherland's directorship thus marked the end of an era at the NPL and was a period worthy of its distinguished past. New research was started, the scientific staff was substantially increased and new facilities - some of them of great industrial importance, were established.

Sutherland's stewardship at the NPL reflected his whole philosophy about the desirable aims and functions of such an establishment - views he often and forcefully expressed at meetings of the British National Committee on Data. He passionately believed that a National Laboratory should help Government, Industry and the Academy World alike, especially in areas such as standards and data, where tradition, continuity and esprit de corps are prerequisites of success. He also believed that the morale of a scientific establishment depends to a great extent on its being involved in the advancement of science and that, therefore, basic research in areas relevant to the laboratory's work should be encouraged.

Perhaps towards the end of his Directorship Sutherland began to doubt whether his ideas will continue to be put into practice at the NPL. Be it as it may he was certainly happy to accept in 1964 the Mastership of Emmanuel College, Cambridge, which he held until his retirement in 1977.
The foregoing sketch of Sutherland's scientific career shows that in view of his involvement in the field of standards field, both in university and government research, he was the obvious person to represent the U.K. on the ICSU Committee already mentioned. What were the other qualities which made Sutherland such a useful, respected and much-liked member of many scientific organizations, among them CODATA? He had the ability and the patience to dissect and to analyze knotty problems, he was meticulous in listening and weighing up arguments, he was fair and unbiased and as a result his decisions commanded respect; even those who may have disagreed with him were disarmed by his urbanity, his gentleness and his sense of humour.

Indeed, this sense of humour was one of Sutherland's most endearing qualities. Watching his quizzical smile as he was about to speak at some meeting or gathering one never knew what was coming - a humorous aside or an important statement. More often than not it was a combination of the two.

He also had the gift of self-mockery, of laughing at his own expenses. It was after the dinner of the 3rd CODATA Conference in Le Creusot that Gordon was asked to say a few words. He did so reluctantly and expressed his concern that if the story he was going to tell became known in his native Scotland he would be shunned by his fellow countrymen. Earlier that year while crossing the Atlantic he was offered a head-set so that he may enjoy the film to be shown. The idea of spending £2.50 on what was likely to be a second-rate film did not appeal to him, but, purely out of politeness he asked what they were going to show. "City Lights with Charlie Chaplin" answered the stewardess and Gordon, being a Chaplin fan, paid for the head-set - only to realize a little later that "City Lights" was a silent film. He finished the story, chuckling merrily, with the remark that he was certainly the first and only Scotman to spend £2.50 on a head-set to watch a silent film.

He was a Scotman to the core and, as such, was enthusiastic about golf. There is a story - it may be apocryphal - that the choice of St. Andrews as the venue for the 2nd CODATA International Conference arose out of a conversation between Lewis Branscomb, U.S.A. Delegate to CODATA, a keen golfer and Sutherland. When Branscomb remarked that his great and as yet unfulfilled ambition was to play a round of golf on St. Andrews' famous "Royal and Ancient" course Sutherland replied "You will do so at the next CODATA Conference." Whatever the truth of this story, it is significant that at St. Andrews formal sessions were held only in the mornings and in the evenings after dinner, so that in the afternoons participants could engage, according to taste, in informal discussions or in a round of golf on one of St. Andrews' superb links.

Those who attended the 3rd CODATA Conference in Le Creusot may remember Gordon, notebook and pencil in hand, walking in the park surrounding Marie Antoinette's chateau accompanied by some of Le Creusot's city dignitaries advising them on the lay-out of a golf course.

Sutherland was elected a Fellow of the Royal Society in 1949, was a Vice-President in 1961-63, and Chairman of the Royal Society's Committee to study the causes and effects of the "Brain Drain" i.e. the loss of many able British scientists to the U.S.A. during the 1950's. The Sutherland Report is a shining example of what such a report should be. A compact, lucid exposition with just enough statistical data to give the reader confidence but not so much as to bore him.

He was a Vice-President of the International Union for Pure and Applied Physics, President of the Institute of Physics and Physical Society and a member of the Council for Scientific Policy in Britain and a Foreign Honorary Member of the American Academy of Arts and Sciences. But his interests and activities ranged far outside science, science policy and education. Probably through the influence of his Swedish-born wife née Gunborg Wahlström who had artistic inclinations Gordon became quite a connoisseur of Chinese art; he was also a Trustee of the National Gallery.

He was a man of many achievements and considerable influence but wore his greatness with genuine modesty. When the sad news broke in the national press - The Times obituary ran to 1300 words, a rare occurrence - the little boy of the Sutherlands' next door neighbours rushed up to Lady Sutherland exclaiming "It's in the papers, you know! We did not know he was that important!" What better sentence to keep fresh the memory of Gordon, the renowned scientist, the loyal colleague, the dear and reliable friend, the man with the warm and unforgettable smile.

Nicholas Kurti
CODATA ELECTIONS

Following the elections at the 12th CODATA General Assembly in Kyoto, Japan on 13-14 October 1980, the composition of the CODATA Executive Committee is as follows:

President:
Professor MASAO KOTANI
Science University of Tokyo, Kagurazaka 1-3, Shinjuku-ku, Tokyo 162, Japan

Vice-Presidents:
Professor JACQUES-EMILE DUBOIS
ITODYS, 1, rue Guy de la Brosse, 75005 Paris, France
Professor V. V. SYTCHEV

Secretary General:
Professor EDGAR F. WESTRUM, JR.
Department of Chemistry, University of Michigan, Ann Arbor, Michigan 48109, U.S.A.

Treasurer:
Dr. DAVID G. WATSON
University Chemical Laboratory, Lensfield Road, Cambridge CB2 1EW, U.K.

Members:
Professor A. BUSSARD
Chef du Service d'Immunologie Cellulaire
Institut Pasteur, 75015 Paris, France

Professor ANDRZEJ BYLICKI
Institute of Physical Chemistry
Polish Academy of Sciences, P.O. Box 49 ul. Kasprzaka 44/52, 01-224 Warsaw, Poland

Dr. DOROTHY L. DUNCAN
Oakfield, Horam, Heathfield, East Sussex TN21 OHA, U.K.

Dr. DAVID R. LIDE, JR.

Dr. MAURICE MENDACHE
7, rue de Reims, 75013 Paris, France

Professor C. N. R. RAO
Solid State & Structural Chemistry Unit, Indian Institute of Science, Malleswaram, Bangalore 560012, India

Professor WOLFGANG SCHIRMER
Zentrallinstitut für Physikalische Chemie Rudower Chaussee 5, 1199 Berlin-Adlershof, G.D.R.

Complete CODATA membership can be found on page 15.

Other decisions at the General Assembly included approval for continuance of the Task Groups on:
- Fundamental Constants
- Chemical Kinetics
- Accessibility and Dissemination of Data (ADD)
- Computer Use (hereafter: Computerized Data Handling)
- Data for the Chemical Industry
- Internationalization and Systematization of Thermodynamic Tables
- Thermophysical Properties of Solids
- Biothermodynamic Data
- Space and Time-Dependent Data

and the establishment of new Task Groups on:
- Critical Interdisciplinary Survey of Property Data on High Pressure Phases (Professor B. VODAR, Chairman) and
- Standardization of Data Bases for NMR and Photoelectron Spectroscopy (Professor C.N.R. RAO, Chairman).

The General Assembly also decided to have the CODATA Bulletin published by Pergamon Press beginning with 1981 and accepted the invitation from Poland to hold the 1982 Conference and General Assembly in Poland and the invitation from Israel to hold the 1984 Conference in Jerusalem.

CODATA NAMES IN THE NEWS

Professor Masao Kotani, President of CODATA, has received the prestigious "Order of Cultural Merit" from the Emperor of Japan.

Professor V.V. Sytchev, Vice-President of CODATA, has been named Deputy Chairman of the U.S.S.R. State Committee for Science and Technology.

Dr. W.W. Hutchison, former Member of the Executive Committee and IUGS Delegate to CODATA, named Director General of the Geological Survey of Canada.

Professor E. Guthreud, U.K. Delegate to CODATA and former Member of the CODATA Executive Committee, elected Fellow of the Royal Society.

Professor C.N.R. RAO, Indian Delegate to CODATA and Member of the Executive Committee, named Foreign Member of the Yugoslav Academy of Sciences.
8TH INTERNATIONAL CODATA CONFERENCE -
CALL FOR PAPERS

The 8th International CODATA Conference is scheduled for 3-7 October 1981 in Kozubnik, Poland (70 km from Cracow) at the invitation of the Polish Academy of Sciences.

SCOPE OF THE CONFERENCE

DATA ON NATURAL RESOURCES - Their Use for the Development of Society.

The Conference is intended to touch some aspects of data on natural resources and their utilization for the benefit of society.

A prime focus of the Conference will be on the relevance of scientific data for:
- estimation of world raw material resources, especially those needed for the development of the chemical industry, metallurgy and energy production
- utilization of coal, oil, and petrochemicals and other raw materials for the chemical and metallurgical industries
- properties of materials, particularly thermodynamic
- environmental protection including biological problems.

The following will be covered:
- analysis of data needs in selected fields of science and technology
- compilation, generation and preprocessing of data
- data evaluation methodology
- critical evaluation and role of data accuracy
- computer use for storage, retrieval and networking of data; data compression
- technical and organizational aspects of data banks including demonstrations
- materials information systems
- data systems analysis
- correlation, extrapolation and estimation procedures
- mathematical modelling data requirements.

CALL FOR PAPERS

Scientists involved in the methodology of data evaluation, estimation, generation, critical compilation, treatment, etc. - and also users of data - are invited to submit papers on the subject within the scope of the Conference.

Since poster sessions are planned at the Conference, the paper may be presented as a poster.

The title, together with a brief description of the contents of the paper should be submitted as soon as possible, but not later than December 1, 1981, to the Chairman of the Program Committee, Professor A. Bylicki, Institute of Physical Chemistry, Polish Academy of Sciences, P.O. Box 49, ul. Kasprzaka 44/52, 01-224 Warsaw, Poland.

Authors of papers will be notified before February 15, 1982 about the acceptance of their papers and will receive instructions on providing an abstract at that time.

SCIENTIFIC PROGRAM COMMITTEE

Professor A. Bylicki, Chairman (Poland)
Professor R. Sinding-Larsen, Vice-Chairman (Norway)
Professor V.V. Sychev, Vice-Chairman (U.S.S.R.)
Dr. J.H. Westbrook, Vice-Chairman (U.S.A.)

- Professor Z. Dembowski (Poland)
- Professor J.B. Dubois (France)
- Professor A.S. Kertes (Israel)
- Dr. David R. Lide, Jr. (U.S.A.)
- Professor Y. Mashiko (Japan)
- Professor C.N.R. Rao (India)
- Professor W. Schirmer (G.D.R.)
- Professor M. Szulcowski (Poland)

ADD TASK GROUP MEETING

The CODATA Task Group on Accessibility and Dissemination of Data (ADD) met in Paris on 18-20 March 1981 under the chairmanship of Madame Antoinette David. Dr. Sherman Flvosinsky of the National Bureau of Standards (U.S.A.) was appointed Secretary of the group. Other members of the Task Group are Dr. C.F. Burk, Jr. (Canada), Prof. A.S. Kertes (Israel), Dr. A.D. Koslov (U.S.S.R.), Prof. S.P. Spragg (U.K.), and Dr. I. Wesley-Tanaskovic (Yugoslavia).

The Task Group is concerned with trying to improve the access to and dissemination of evaluated scientific and technological data. Such improvements include the publication of recommended practices, educational activities for university students and information specialists, activities which promote and publicize existing data, and a variety of practical endeavors aimed at helping the user to find the required data. The aims of the Task Group are broad since it takes into consideration all the tools of accessibility to data in all the disciplines.

At its meeting the group evaluated the results of the training course in data dissemination given in Tsukuba, Japan in October 1980 and encouraged the continuance of such courses. It discussed its input into the CODATA/Unesco Preliminary Inventory of Data Referral Sources which is scheduled for completion during the summer of 1981. The group also decided to update CODATA Bulletin No. 16 "Study on the Problems of Accessibility and Dissemination of Data for Science and Technology."
SOLUBILITY DATA PROJECT

The more than 150 editors, compilers and evaluators involved in this massive endeavor have now reached the 104 mark in the production of the 80-100 volumes promised over the next 10-15 years of activity. This ambitious project of the Analytical Chemistry Division of IUPAC (Commission V.8) intends ultimately to provide a reliable basis for the rational prediction of solubilities in uncharted areas as well as the critically evaluated and clearly defined best values of gas/liquid, solid/liquid, liquid/liquid, gas/solid, and solid/solid equilibria as functions of both temperature and pressure. Each system consists of two essential parts:

- critically evaluated/recommended values with discussion on reliability
- data sheets with concise graphical presentation, adjuvant information on experimental procedures.

Fundamental to the philosophy of the project is the recognition that the basic element of strength is the active participation of career scientists. Consolidation of data from the primary literature and the production of a truly critically-evaluated set of numerical data are tasks worthy of the time of experienced scientists.

Reviews of the eight or so volumes already published by Pergamon Press in 1979-80 are still few, but those identified are listed below.

- Fluid Phase Equilibria 4 (1980), 313-317
  Volume 1: M. J. Bria
  Volume 2: R. F. Weiss
  Volume 3: U. N. Dash
- L. H. Gevartman, Bulletin of Chemical Thermodynamics 22 (1979), 496.

The average price for the extant volumes approximates $100 each, although reduced prices are available upon subscription. Biennial cumulative indexes are contemplated. The succinct evaluative commentary is designed to be appropriate for scientific and technological fields as diverse as agriculture, biology, chemistry, engineering, geology, materials science, medicine, metallurgy, oceanography, and pharmacology.

COMMISSION ON EQUILIBRIUM DATA - V.6

The IUPAC Analytical Chemistry Division's Commission on Equilibrium Data - V.6 announces the availability of the following publications:


For further information write to the Chairman of the Commission on Equilibrium Data, Professor G.R. Kanciolas, Dept. of Chemistry, State University of New York, Binghamton, N.Y. 13901, U.S.A.

SELECTED VALUES OF CHEMICAL THERMODYNAMIC PROPERTIES

Tables of the thermodynamic properties of inorganic substances and C1 and C2 organic compounds at 298.15K are prepared and published by the National Bureau of Standards. The properties covered are enthalpy of formation ($\Delta H_f$), Gibbs energy of formation ($\Delta G_f$), entropy ($S$), and heat capacity ($C_p$), all at 298.15K, $\Delta H_f$ (0), and $H$ (298) - $H$ (0).

Eight publications have been issued: NBS Technical Notes 270-1 through 270-8 which cover the compounds of all elements except those of the transuranics. The latest volume, issued in May 1961 by D.D. Wagman, W.R. Evans, V.B. Parker, R.B. Schumaa, and R.L. Nuttall covers the compounds of uranium, proteactinium, thorium, actinium, and the alkali metals. A later publication will contain data on compounds of the transuranic elements.

Information about the thermodynamic properties of specific inorganic compounds may be obtained from the NBS Chemical Thermodynamic Data Center. Inquiries should be addressed to Dr. David Garvin, Manager, Chemical Thermodynamics Data Center, Room 4H2, Chemistry Building, National Bureau of Standards, Washington, D.C. 20334. (Telephone 301) 921-2773.)
NEW GEODETIC REFERENCE SYSTEM

During the XVII General Assembly of the International Union of Geodesy and Geophysics in Canberra, the following Resolution was adopted:

Recognizing that the Geodetic Reference System 1967 adopted at the XIV General Assembly of IUGG, Lucerne, 1967 no longer represents the size, shape and gravity field of the Earth to an accuracy adequate for many geodetic, geophysical, astronomical and hydrographic applications and

Considering that more appropriate values are now available,

Recommends

a) that the Geodetic Reference System 1967 be replaced by a new Geodetic Reference System 1980, also based on the Earth's gravity field; the geodetic equatorial ellipsoid, defined by the following conventional constants:

- equatorial radius of the Earth: \( a = 6378 \, 137 \, \text{m} \)
- geocentric gravitational constant of the Earth (including the atmosphere):
  \[ GM = 3986 \, 004 \times 10^9 \, \text{kg m}^2 \]
- dynamical form factor of the Earth, excluding the permanent tidal deformation:
  \[ J_2 = 108 \, 263 \times 10^{-8} \]
- angular velocity of the Earth:
  \[ \omega = 7292 \, 115 \times 10^{-11} \, \text{rad s}^{-1} \]

b) that the same computational formulas, adopted at the XV General Assembly of IUGG in Moscow 1971 and published by IAG, be used as for the Geodetic Reference System 1967, and

c) that the minor axis of the reference ellipsoid, defined above, be parallel to the direction defined by the Conventional International Origin, and that the primary meridian be parallel to the zero meridian of the BIH adopted longitudes.

SEMINAR ON "GEOSCIENCE NUMERIC AND BIBLIOGRAPHIC DATA"

A seminar on "Geoscience Numeric and Bibliographic Data" was held 30 March–1 April 1981 under the auspices of the Australian Mineral Foundation.

The principal speaker at the seminar was Dr. C.F. Burck, Jr., of the Canada Centre for Geoscience Data. He presented a 20-page compilation comprising lists of databases, of database directories, of publications concerning standards for data, of newsletters and periodicals and of related publications. He groups the databases in two categories namely "reference" databases and "source" databases - a helpful distinction. The latter, referred to in the title as "numeric" databases, are structured compilations which give the questioner the required information directly - usually in numeric form. The former, described in the title of the seminar as "bibliographic" refers the questioner to likely sources of answers to his inquiry. The list of geoscience databases in which each is indicated as "reference" or "source" has 111 entries, of these 46 are in the "reference" category and 65 in the "source" category. The distribution among the various subdisciplines is as follows: General Geoscience-18, Minerals-24, Fuels-22, Geology-21, Geochemistry-14, Geophysics-12. The names of the following randomly selected databases give an idea character of the compilation:

- MINING TECHNOLOGY (MINTEC) (Canada, Reference)
- PETROLEUM DATA SYSTEM (USA, Source)
- ROCK MECHANICS INFORMATION SERVICE (UK, Reference)
- NATIONAL URANIUM RESOURCE EVALUATION PROGRAM (NUREG) (USA, Reference)
- EARTHQUAKE DATA FILE (USA, Source)
- SEISMIC DATA ANALYSIS SYSTEM (SEDAS) (USA, Source).

Copies of the paper are available from Dr. C.F. Burck, Jr., Canada Centre for Geoscience Data, 580 Booth Street, Ottawa K1A 0E4, Canada.

CODATA/UNESCO TRAINING COURSE ON DATA MANAGEMENT IN THE GEOSCIENCES

A training course covering the general aspects of data accessibility dissemination and utilization, with emphasis on data in petrology and mineralogy is planned to be held at the Federal University of Ouro Prêto in Brazil on 7–12 December 1981, under the auspices of Unesco and CODATA.

The objectives of the course are:

- to review the current and future role of numeric databases in science and technology, with emphasis on those in geoscience and petrology and mineralogy
- to describe the availability of data resources and services currently available worldwide
- to analyze the particular problems of numerical data dissemination and how they differ from problems encountered in the dissemination of other kinds of information: formats, units of measurement, copyrights, costs
- to provide guidelines and references for the creation and utilization of data by means of database management systems and communication networks
- to encourage the formation of regional, topical, computer-based information and data centers, with particular emphasis on data generation and data exchange in petrology, mineralogy and geoscience
- to teach the use of databases for problem solving by computer.

Applications forms are available from:

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c/o Geological Department

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BOOKS OF SPECIAL INTEREST

DATA NEEDS: MECHANICAL PROPERTIES FOR
METALS AND ALLOYS

A U.S. National Research Council report has
been published that assesses the status of data
reporting, collecting, appraising, and disseminating
of mechanical properties for metals and alloys. The
report surveys comprehensively and documents
concisely issues and problems that must be address-
ed if data needs are to be adequately met in the
future.

The report explains the complexities of dealing
with identification of materials and appraisal of
their mechanical properties in contrast to
evaluating physical and chemical properties of
pure substances. It discusses: Data Uses and
Dissemination; Data Sources, Collection, and
Appraisal; Activities in Development of Test
Methods for Measuring Mechanical Properties;
Computerizing a Mechanical Properties Data System;
International Aspects; and, in an appendix, Some
Mechanical Properties Data Sources.

The study is the result of a request from the
U.S. National Bureau of Standards' Office of
Standard Reference Data to the Numerical Data
Advisory Board of the National Research Council/
National Academy of Sciences. A panel was
convened representing a broad range of interests
from industry, professional societies, standards
activities, energy technologies, and design of
critical parts, and was chaired by Jim Graham
from Deere & Co., and representing the Metals
Properties Council.

One conclusion of the report is that a major pre-
requisite to data activities is not yet adequately
in place, namely, that of standard test methods,
standardized nomenclature, and uniform data
reporting methods. Data in the literature or in
reports cannot be adequately compared, assessed,
and appraised ("evaluated") until such a
measurement basis becomes further developed and
utilized. This is particularly true when those
data are to be applied to critical structures
such as suspension bridges, nuclear reactor ves-
sels, containers for hazardous materials, and
aircraft. The panel identifies this problem as being
international and identifies several organizations
whose missions relate to this problem including
NBS, CODATA, ISO, and ASTM.

A second identified shortcoming is the absence of
uniform methods of property data appraisal. This
again is a topic that should be addressed on an
international level, the report notes.

Once these standard practices are adequately in
place, compatible evaluated databases can be
developed by any private or public concern. A
method of computerizing such a database, including
examples of data entry forms is described in the
report.

A number of other issues and problems are identi-
ﬁed and described in the report, several of
which are relevant to CODATA.

C.G. Carter

THE TECHNOLOGICAL IMPORTANCE OF ACCURATE
THERMOPHYSICAL PROPERTY INFORMATION
(NBS Special Publication 590).

There are doubts expressed nowadays in many
quarters about the completeness of generating and
evaluating data unless there is an actual need.
It is, therefore, a reassuring sign that the
National Bureau of Standards should have
published as an NBS Special Publication the
papers concerned with the technological importance
of data information given at a meeting of the
American Society of Mechanical Engineers (ASME).

It is true that there is the usual disclaimer that
the views expressed by the authors are not neces-
sarily those of the NBS, but the fact that the
proceedings have been published in this series
indicates the NBS's interest in the subject and
in the aim of ASME's Committee on Thermophysical
Properties which organized the special session.
It should also be noted that the introductory
survey on the role of data accuracy in applica-
tions of thermophysics was written by a member of
the NBS Thermophysics Division, Dr. Max Klein.

His splendid article may be likened to Hamlet:
it's "full of quotations" - rather, full of
passages worthy of becoming "quotations". How
better to express the rationale of data gathering
for industry than with the two well-worded anti-
thetical sentences: "Thus with the exception of
those very few substances whose utility is broad
and long term, e.g. steam, the probability is
quite small that a need will exist at any given
time for some particular subset of thermodynamic
properties for a particular substance or mixture
chosen at random. On the other hand, at any
particular time, the probability is quite large
that a need exists for thermodynamic data of
some kind for some substance and that this need
was not previously predictable". Or, when refer-
ing to the transfer of ethylene near its critical
point, he says: "Because of very large uncertain-
ties in data correlation near the critical point,
the resulting error estimate for the metering
process as to quantity transferred approached
total uncertainty". A delightfully diplomatic
way of saying: "They hadn't a clue as to what they
were doing".

1Mechanical Properties Data for Metals and Alloys:
Status of Data Reporting, Collecting, and
Disseminating. Panel on Mechanical Properties Data
for Metals and Alloys: Numerical Data Advisory Board
Assembly of Mathematical and Physical Sciences.
Available from Numerical Data Advisory Board,
National Research Council, 2101 Constitution
Avenue, N.W., Washington, D.C. 20418.
Another good example of the consequences of insufficient data is the case of the firm which suspected that all was not well with their way of metering ethylene. So they decided to evacuate completely a salt dome, used for storage, and measure the amount of the ethylene removed. They found that "much more ethylene had been removed than had been stored", a clear indication of the inadequacy of the thermophysical data on which the conversion of flow parameters to quantity of material is based.

These are just a few telling examples culled from a wealth of similar material contained in this introductory article. The remaining five papers deal with specific subjects, as the abstract shows: "The areas covered included aerospace sciences, where such data have played a central role for a number of years; and geosciences, where first steps are being taken towards using accuracy in describing systems in terms of thermophysical properties; so included were a discussion of the economic value of accuracy in the chemical process industry, a description of the role of data centers, and a description of several high-quality data compilations. An example of a specific problem in the design of heat exchanger for geothermal applications was also presented with the design uncertainties produced by data inaccuracies illustrated".

The authors are R.C. Hendricks, H.E. Khalifa and J. Kestin, M. Klein, P.E. Liley, N.A. Olien, H.P. Stephens, and S. Sinnoch.

All in all a good and timely publication which should be recommended reading matter for those who have the health and competitiveness of industry at heart.

N. Kurti

CONCRETE AND CRYOGENICS - F.H. Turner
(Cement and Concrete Association 1979, 100 pp., £10.00, ISBN 0 7210 1124 1).

Cryogenics, i.e. the art, science and technology of producing, distributing and conserving at low temperatures - say below -150 °C (120 °K) - has developed rapidly in the last 5 or 6 decades. The main reasons for this upsurge were the widespread use of oxygen (obtained from the atmosphere by low temperature fractional distillation) in many industrial processes, the use of liquid hydrogen (and of liquid oxygen) in rocket propulsion, the advent of liquid natural gas (LNG) and the possibilities of large scale use of liquid helium in the generation and transmission of electricity with the help of superconductors. The most commonly used constructional material in industry is steal in its various forms, but, for low temperature use, it has the great disadvantage of becoming brittle unless it has high nickel content. It is for this reason that prestressed concrete is finding more and more applications in cryogenics.

One would be justified in asking why a book addressed to specialists in concrete technology should be reviewed in a periodical serving the "Data Community". However it is felt that, even though large, comprehensive data-banks can answer the questions of specialists, there is also a need for well-chosen data collections designed to help the specialised engineer and, and that such a collection should be an integral part of any textbook or manual.

The book under review performs this desirable function well. It contains, in the form of tables or graphs, the essential low temperature data likely to be needed by the designers of low temperature equipment made of concrete. They include the thermophysical properties of fluids ranging from water (boiling point 373 °K) to hydrogen (B.P. 20 °K), low temperature data of prestressed concrete, such as elastic modulus, strength, thermal conductivity, permeability and, also, on a more general level, data for safety assessment.

The author should be commended for giving data not only in "Imperial Units" so beloved by engineers, particularly in the U.S., but also in SI (Système International) and sometimes in CSS (called "metric" in this book) units. There are extensive tables of conversion and it seems that the designer of a container, e.g. LNG, will find all he needs in these handsomely produced glossy pages. But one can't help wondering whether the needs of the designer would not have been better served if this book had been published not only as a library tome but also as a modestly sized and modestly priced volume within the reach of the individual engineer.

The introduction describes the manifold applications of low temperatures, but it is a pity that the credibility of this otherwise good review might be endangered by the mention of: "centres for low-temperature storage of human bodies ..... opened in the U.S.A., in which corpses can be stored until medical technology had advanced sufficiently to be able to revive them". The recent discoveries of rotting corpses have exposed this particular area of cryotechnology as a cruel confidence trick which has probably lined some pockets and has certainly created misery through giving hope, followed by bitter disappointment.

N. Kurti
NEW PUBLICATIONS

CHEMICAL KINETICS


CHEMISTRY


COMPUTER SCIENCE


EARTH SCIENCES

CATALOGUE OF INSTRUMENTALLY-MEASURED WAVE DATA, Issue No. 1 (1979, 276 pp.) Marine Information and Advisory Service (MIAS) which is the U.K.'s Responsible National Oceanographic Data Centre (RNODC), designated by the IOC (International Oceanographic Commission) to act on instrumentally measured wave data. Address: MIAS, Institute of Oceanographic Sciences, Wormley, Godalming, Surrey GU6 5UB, U.K.). A world-wide list of about 350 measuring centres (coastal stations, lighthouses, etc.), with details about measuring techniques, types of data, extent of collections.

covering the U.S., its dependent territories, and certain parts of Canada and Mexico. In addition to the usual information such as addresses, etc., each entry gives full information about the categories of information available (e.g. surface water quantity/quality, ground water quality, etc.) and the number of sites from which data in each of the above categories are collected.

HANDBOOKS


MECHANICAL AND ENGINEERING DATA


This report is concerned with the application of computational fluid flow technology to aircraft design. To test and to improve the various computational methods an Experimental Data Base was established to cover the following cases: 2-dimensional (2-D) configurations (airfoils) 3-D configurations (wing and wing-body), body-alone configurations.

THERMODYNAMIC PROPERTIES


A very extensive, thorough, and critically done evaluation for both individual substances and binary mixtures.


The latest volumes in this excellent series of ternary and quaternary data on systems containing water, hydrocarbons, alcohols, ketones, ethers, esters, organic acids, amines, nitriles, halogenated and sulphur-containing hydrocarbons and other non-polymeric organic compounds. The data are correlated with the Hertz and UNIQUE equations.

MOLYBDENUM: PHYSICO-CHEMICAL PROPERTIES OF ITS COMPOUNDS AND ALLOYS, (1980, 754 pp., 1000 Austrian Schillings, International Atomic Energy Agency, Vienna) edited by L. Breuer. This is the seventh volume in an IAEA series on important materials in reactor technology. The first six volumes treated plutonium, niobium, tantalum, beryllium, thorium and zirconium. The present volume is concerned with the critical evaluation and documentation of the following data on molybdenum: thermodynamic properties, densities, crystallographic structures, equilibrium diagrams and diffusion rates in the condensed state.

SUMMARY OF ON-LINE OR INTERACTIVE PHYSICO-CHEMICAL NUMERICAL DATA SYSTEMS, (1980, 24 pp., $1.75, National Bureau of Standards Technical Note 1122, Govt. Printing Office, Washington, D.C.) by Joseph Hilsenrath. A brief description is given of 51 interactive physico-chemical numerical data systems, most of which are on-line on international computer networks. The systems are listed under five headings: those useful for identification of substances from spectroscopic data; those providing thermodynamic and transport properties of pure components and mixtures; those which perform metallurgical calculations and draw phase diagrams, systems producing complete tables of thermodynamic properties of individual substances; and those for chemical process simulation, optimization, and design. References to published descriptions of the systems, where they exist, are also given.

THERMODYNAMIC PROPERTIES OF METHANE (TERMODINAMICHESKIE SVOISTVA METANA), (in Russian, 1979, 349 pp., 2 rubles 70 Kopecks, available from "Znak Pochta" Izdatelstvo Standartov, Novopresnenskij per. 3, Moscow D-557) by V.V.
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SECOND INTERNATIONAL CONFERENCE ON PRECISION MEASUREMENT AND FUNDAMENTAL CONSTANTS

The Second Precision Measurement and Fundamental Constants Conference was held on 8-12 June 1981 at the National Bureau of Standards in Gaithersburg, Maryland. Information may be obtained from: Dr. B. N. Taylor, National Bureau of Standards, Building 220, Room B258, Washington, D.C. 20234, U.S.A.

The following speakers presented review talks:


The CODATA Task Group on Fundamental Constants under the chairmanship of Dr. E. Richard Cohen met directly afterwards. A report of their meeting will appear in the next Newsletter.
SPECIAL OFFER FOR SUBSCRIBERS TO THE CODATA NEWSLETTER

DATA FOR SCIENCE AND TECHNOLOGY

Proceedings of the 7th International CODATA Conference, Kyoto, Japan, 8-11 October 1980
Edited by P S Glaeser, CODATA Secretariat, Paris

The scope of this book ranges from the role of data in basic scientific research to applications focusing on major problems facing society. Aspects receiving special emphasis are the formation of new scientific concepts and the solution of problems using existing data; the need for new evaluated data to test new working hypotheses; the critical evaluation of data; and the promotion of data reliability in scientific applications. The 130 contributions, from some of the world’s leading producers and users of scientific data, cover many areas of science, including chemistry, physics, astronomy, geoscience, bioscience, information science, nuclear science, engineering and industry.

Available June 1981
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No 18 (April 1976), 44 pp, Abstracts - Fifth International CODATA Conference, US $5.00.


No 23 (May 1977), 42 pp, Selected Papers Relevant to Energy Presented at the 5th International CODATA Conference, US $5.


*Proceedings of the Joint French-Israeli Interdisciplinary Symposium, Jerusalem, Israel, 5-6 March 1980.*
Data Handling for Science and Technology
AN OVERVIEW AND SOURCEBOOK

Sponsored by CODATA and UNESCO


Price in the U.S.A./Canada: US $25.00. In all other countries: US $29.25/Dfl. 60.00

This book is intended to provide an introductory survey of the basic aspects of handling scientific and technical data, and to indicate to the reader, selected sources from which more details can be obtained. It is in this sense that the title carries the name “Sourcebook”. The text is addressed to a varied body of users, including people who generate, publish, abstract, collect, evaluate, repackage, disseminate, and apply data, as well as to those who provide training courses in the handling of data, and those who administer the funding for all these activities.

Immediately following the Introduction, there is an examination of how and why data are generated, with a discussion of the differing degrees to which data have an “absolute” aspect (in the sense that they can be determined independently of any environmental conditions or measurement techniques) and a brief overview of systems for measuring and recording data. A two-part chapter is devoted to data-related aspects of the biosciences and geosciences.

There is also a survey of statistical analysis and interpretation of data. The following four chapters examine four important systematic aspects of data handling: presentation in the primary literature, means of finding data in the primary literature, the critical operations of compilation and evaluation of data, and the standards and guidelines which give structure to data handling. A chapter is devoted to a brief overview of how computers are used in laboratory science to handle data. The final chapter offers a cross-cut analysis of the formal and informal mechanisms by which data are disseminated, involving the interactions between suppliers and users of data.

The book therefore addresses itself to producers and users of data as well as to information specialists increasingly called upon to provide numerical data to scientific users. It should prove invaluable in scientific libraries and other information centres in both developed and developing countries. It is a book which by its very nature is timely and necessary, and yet will clearly require periodic revision since it is concerned with a rapidly developing field.


In Memoriam
This volume is dedicated to the memory of Stephen A. Rossmassler, whose scholarly approach to complex problems, his conscientious service to many organizations, and his urbane but gentle wit will be remembered by all.

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