

18 CODATA / NEWSLETTER

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SEPTEMBER 1977

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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.

SITE OF 6TH INTERNATIONAL CODATA
CONFERENCE CHANGED FROM TAORMINA TO
PALERMO, SICILY, ITALY

The 6th International CODATA Conference is scheduled for May 22-25 at the Hotel Zagarella and Sea Palace, Santa Flavia (16 km from Palermo) in Sicily, at the invitation of the Consiglio Nazionale delle Ricerche.

SCOPE OF THE CONFERENCE * * * * *

The following aspects will be covered:

- data evaluation methodology
- compilation procedures
- critical evaluation
- mathematical modelling data requirements
- correlation, extrapolation, and estimation procedures
- data systems analysis
- machine techniques for storage, retrieval, and dissemination of numerical data

It is hoped to devote part of the Conference to data relevant to the quality of life and the environment, in particular, preservation of natural ecosystems, prediction of natural disasters, and prevention of man-made hazards, bearing in mind the important data files already in existence.

It is tentatively planned to have public lectures of general interest on some of the topics with emphasis on the local seismic and volcanic environment.

CALL FOR PAPERS * * * * *

Users of data, as well as those involved in data compilation, data evaluation, and data handling are invited to submit papers on subjects within the scope of the Conference.

The title, together with a brief description of the contents of the paper should be submitted as soon as possible, but not later than October 1, 1977 to the Co-Chairman of the Program Committee, Prof. J.E. Dubois, Centre d'Informatique et de Documentation Automatique (CIDA), 1, rue Guy de la Brosse, 75005 Paris, France.

Authors of papers will be notified before December 1, 1977, about the acceptance of their papers and will receive instructions on providing an abstract at that time.

SCIENTIFIC PROGRAM COMMITTEE * * * * *

Professor M. Carapezza, Co-Chairman (Italy)
Professor J.E. Dubois, Co-Chairman (France)
Dr. Robert E. Harte (U.S.A.)
Dr. Alan Shapley (U.S.A.)
Professor V.V. Sytchev (U.S.S.R.)

FOR FURTHER INFORMATION WRITE:

CODATA Secretariat
51 Boulevard de Montmorency
75016 Paris, France

CANADIAN NATIONAL COMMITTEE FOR CODATA

Following the reorganization of the Canadian National Committee for CODATA, the membership is as follows:

Dr. C.F. Burk (Chairman)
Canada Centre for Geoscience Data
580 Booth Street
Ottawa, Ontario K1A 0E4

Mr. L.G. Côté
Canada Institute for Scientific and
Technical Information
National Research Council of Canada
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Professor B.G. Cumming
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New Brunswick E3B 5A3

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University of Lethbridge
Lethbridge, Alberta

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Geological Survey of Canada
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Department of Physics
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Dr. H. Preston-Thomas
Division of Physics
National Research Council of Canada
Montreal Road
Ottawa, Ontario K1A 0R6

*Re-election or continuation

TRANSPORT PROPERTIES TASK GROUP MEETS IN NEW YORK

The Task Group met on 21 and 22 March 1977 at the American Institute of Physics in New York. In attendance were Drs. R. Berman (U.K.), Dr. M. Minges (USA) and Dr. Y.S. Touloukian (U.S.A.). A certain number of items on the agenda were unhappily unable to be treated due to either inability on the part of IUFOST to submit a report on their work concerning Physical Properties of Foods or to a misunderstanding on the part of the IUGG consultant as to what the Task Group's terms of reference really were. Among the items of a scientific nature that were discussed, however, the Task Group dwelt at length on the international co-operation in the development of standard reference materials and noted the very encouraging results obtained so far. These results concern a series of measurements performed in various labs throughout the world on the thermal and electrical conductivities of tungsten, stainless steel and Poco graphite. Details are as follows:

I. Cryogenic and Low Temperature. Results obtained from tungsten and stainless steel samples, circulated to labs in round-robin fashion were sufficiently advanced to justify the announcement that a definitive technical report would be submitted to CODATA by mid-1977. The work will cover temperatures up to 90 K. Responsibility for the preparation of this report was entrusted to Dr. Berman.

II. Intermediate and High Temperatures. The problems discussed in the Task Group's last report were resolved in the interim period and samples of sintered tungsten are being distributed to a number of laboratories who volunteered to perform measurements. One laboratory has completed electrical and thermal transport property measurements and heat capacity determinations over the range from 1250 to 3050 K. Poco graphite as a standard reference material is not fully characterized yet. However work is underway at four laboratories (NBS-Boulder, NBS-Washington, Oak Ridge, Purdue) to characterize Poco graphite through measurements of its electrical and thermal conductivity as a function of density and temperature. NBS-Boulder has already completed the room temperature evaluation of the electrical and thermal conductivity of Poco graphite as a function of density, and the results look promising. Preliminary results from Oak Ridge National Laboratory corroborate the NBS measurements.

It is anticipated that adequate results on high-temperature measurements will become available by mid-1978 to enable the Task Group to prepare a second definitive technical report on reference standards at high temperature and available state-of-the-art capabilities among the cooperating laboratories. This report will be submitted to CODATA at the 1978 General Assembly. Dr. M. Minges will assume primary responsibility for this work.

The Task Group regrets that it does not have as yet a full international representation. It looks forward to contributing more substantively to the life and earth science areas in the years ahead.

FIRST MEETING OF NEWLY CONSTITUTED CHEMICAL KINETICS TASK GROUP

The newly formed CODATA Task Group on Chemical Kinetics held its first meeting under the chairmanship of Dr. J. Alistair Kerr in London on May 23, 1977. In attendance were Drs. D. L. Baulch, R.A. Cox, R.F. Hampson, J. Troe and R.T. Watson. Dr. P.J. Crutzen had sent his apologies for being unable to attend. Dr. R.F. Hampson was appointed Secretary of the Task Group, and the following notes are based on the report he prepared.

-The Task Group agreed to produce a list of recommended rate constants and photochemical parameters (photoabsorption cross sections and primary quantum yields) for atmospheric reactions with the intent of furnishing the kinetic data needed by atmospheric modelers.

-Data sheets on these reactions, intermediate in detail between those provided by the Leeds group and those of the NBS group, will be produced as back-up material to the above-mentioned list.

-Reactions to be considered are limited to neutral reactions occurring in the stratosphere and the natural (i.e. unpolluted) troposphere. No hydrocarbons of greater complexity than methane will be included. The reactions to be considered will be based on a list of about 150 reactions furnished by R.A. Cox with the addition of reactions of sulfur, bromine and fluorine.

-These reactions are classified according to catalytic cycles. Responsibility for assigning each reaction to its relevant class, according to these cycles, has been devolved to individual Task Group members as follows:

O _x	Association-Dissociation Rxns}	TROE
Association-Dissociation Rxns}		
HO _x		KERR
NO _x		HAMPSON
CH ₄		COX
S		BAULCH
Cl, Br, F		WATSON

-Reactions of vibrationally excited species and heterogeneous reactions will be considered at a later date.

-In connection with the various aspects concerning the publications procedure of its results, the Task Group agreed

--to produce initial drafts of data sheets by the end of 1977, the final version of these data sheets being scheduled to appear in 1978 and the Task Group's final recommendations being due sometime in 1979.

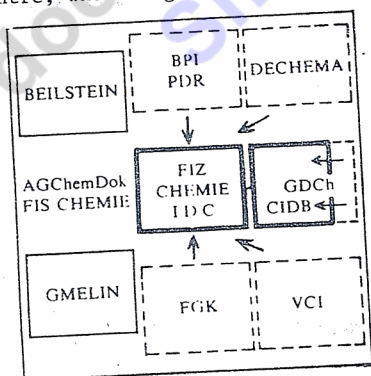
--to publish its final report in a refereed journal, such as the Journal of Physical and Chemical Reference Data or the International Journal of Chemical Kinetics.

--to publicize the activities of the Task Group by placing notices in appropriate professional society publications and newsletters.

FACHINFORMATIONSZENTRUM CHEMIE (FIZ CHEMIE) - TECHNICAL INFORMATION CENTRE CHEMISTRY ESTABLISHED IN GERMANY

Following the decision of the German Federal Government in 1973 to re-organize and co-ordinate the information and documentation activities in the entire field of science in the FRG, a joint Information and Documentation Program, consisting in the setting up of sixteen Technical Information Systems and four Interdisciplinary Information Bureaus, was launched in early 1974.

The first discipline chosen to be implemented was chemistry, and accordingly a press conference took place in Frankfurt/Main on 14 February 1977 to introduce the Technical Information Centre Chemistry (FIZ Chemie). This Centre, sponsored by the Federal Government, originates from the working pool for chemical documentation formed in 1968 by various scientific institutions under the acronym AGChemDok (Arbeitsgemeinschaft Chemedokumentation - Working Community for Chemical Documentation). It will be operated jointly by IDC (International Documentation Society for Chemistry, Frankfurt) and CIDB (Chemical Information and Documentation, Berlin, a division of GDCh, the Society of German Chemists), in cooperation with four other large chemical organizations: BPI (Bundesverband der Pharmazeutischen Industrie - Federal Union of Pharmaceutical Industries), DECHEMA (Deutsche Gesellschaft für Chemisches Apparatewesen - German Society for Chemical Equipment), FGK/DKI (Forschungsgesellschaft Kunststoffe, Research Society for Synthetic Materials and Deutsches Kunststoffinstitut, German Institute for Plastics, Darmstadt), VCI (Verband der Chemischen Industrie, Union of Chemical Industries). In addition, the two main chemical publications, Beilstein and Gmelin, are also contributing to the input into the Centre, whose organizational diagram is as follows:



Thanks to this multiple cooperation, the services provided by the Centre in the way of physical data on compounds, bibliographic references, information on substances, manufacturers, institutions, technical projects, etc., cover the entire area of chemistry, the chief domains being:

- Inorganic chemistry (IDC/CIDB)
- Organic chemistry (IDC/CIDB)
- Polymers (FGK/DKI)
- Pharmaceutical chemistry (BPI)
- Chemical technology, chemical engineering (DECHEMA)
- Chemical industries (VCI)
- Thermo-physical data on pure compounds and mixtures (DECHEMA. - see below article on DECHEMA Data Service)

The headquarters of the Centre are located in Frankfurt/Main, where three computers are installed (a Siemens 4004/151 and two Telefunken TR6), whereas the CIDB in Berlin has an IBM 360/20.

The financial endowment of the Technical Information Centre for 1977 is 27.5 million DM, of which 5.5 million comes from the Federal Government and 22 million from the six associated organizations, namely IDC, CIDB, BPI, FGK/DKI, VCI and DECHEMA.

DSD: DECHEMA DATA SERVICE -- A DATA BANK FOR CHEMISTRY AND CHEMICAL ENGINEERING

In 1973, the DECHEMA (Deutsche Gesellschaft für chemisches Apparatewesen) started setting up, with the financial support of the German Federal Ministry for Science and Technology, a computer-operated data bank designed to supply chemical engineers and industrialists with thermodynamic and thermophysical property data of important chemical compounds and mixtures for any given state in the fluid phase. Since the data found in the literature alone are not sufficient, the properties for the desired state have to be calculated by means of suitable computer programs. Therefore, three systems have been incorporated in the DECHEMA Data Service:

1. The Data Retrieval System (SDR), to store and retrieve literature data by means of a structured data bank capable of storing any data and data quantities along with the relevant programs and data files.
2. The Data Analysis System (SDA) for evaluation and analyzing measured values as well as literature values by means of programs for linear and non-linear regression, with plots of the functional relationships and residuals.
3. The Data Calculation System (SDC) for calculating data.

This Data Calculation System consists of two parts:

The "pure compound" program by means of which basic data for pure compounds are generated or approximated from the chemical structure and some other basic information, e.g. boiling temperature, critical properties, etc.,

and

the "mixture" data program, by means of which pure compound and mixture data are calculated for the fluid state, e.g.

- critical data
- enthalpy of vaporisation
- vapor pressure
- boiling temperature
- ideal and real K-values (vapor-liquid equilibrium constants)
- activity coefficients
- specific heat capacity
- enthalpy
- thermal conductivity
- viscosity
- calorific value
- diffusion coefficients
- density
- adiabatic exponent

- compressibility factor
- pseudo-critical constants
- vapor-liquid equilibria; (according to the methods of Margules, van Laar, Wilson, NRTL, UNIQUAC, UNIFAC, Chao-Seader)
- boiling and dew temperatures and pressures
- liquid and vapor mole or weight fractions
- T-x diagrams

Ever since its creation in 1974, the Data Service has been used intensively to help users (i.e. firms, institutes, etc.) solve their problems. For calculation of vapor-liquid equilibria, a large data collection is now available. The constants of the correlation equations can be regressed from measured values by appropriate programs and are used for calculating phase equilibria with respect to the desired state. If there is no experimental information about the system in question, incremental methods can be applied (Gilmont, UNIFAC).

The development of the Retrieval System, and more particularly of the Calculation System, is followed up in cooperation with firms and university institutes (Development Group Data Compiler). The main developments are:

- phase equilibria
- mixture properties for the fluid state (equation of state)
- error minimization in data calculation

Furthermore, data compilations (DECHEMA Chemistry Data Series) are published at irregular intervals: the first volume (Vapor-Liquid Equilibria Data Collection of Aqueous-Organic Systems) has just come out (see the review of this volume on p. 18 of the present issue).

* * * * *

REORGANIZATION OF UNESCO'S INFORMATION PROGRAMMES

At the 19th session of its General Conference, Unesco decided to reorganize the activities previously covered by the programme sections "Scientific and technological information and documentation" (UNISIST) and "Documentation, libraries and archives".

The implementation of this decision has given rise to changes in the organizational structure inside Unesco. On 24 February 1977, the Director-General created a Division for the General Information Programme, covering the majority of the activities formerly coming under the two above-mentioned sections. This division, under the direction of Dr. Adam Wysocki, is attached to the Directorate and has been placed under the authority of the Director of the Bureau of Studies and Programming. UNISIST activities and goals for scientific and technological information exchange will remain unchanged.

BULLETIN OF THERMODYNAMICS AND THERMOCHEMISTRY, NO. 19, JULY 1976

EDITED BY E.F. WESTRUM, JR.

This Bulletin is the 19th annual survey of research in thermodynamics and thermochemistry prepared under the auspices of the Commission on Thermodynamics and Thermochemistry of the Division of Physical Chemistry of the International Union of Pure and Applied Chemistry. It is an annotated bibliography covering research reported during 1975. There are two major parts: Abstracts on current research and Indexes to published papers.

The Abstracts are excellent guides to the current status of thermodynamic and thermochemical research and to where experts on particular topics may be found. They contain a listing of 506 research groups in 31 countries, 360 of which have reported in this issue on measurements currently underway. Although most of these new measurements will be published, the delays may be extensive; thus the Abstracts remain for many years the only source of information on some work.

The Indexes to published work are comprehensive subject bibliographies having approximately 16,000 entries based on measurements reported in 4400 articles and the 360 abstracts of current research. Four separate indexes are provided: organic substances, organic systems (mixtures), inorganic substances, and biological and macromolecular systems, each index being arranged by chemical compound. Each index entry lists explicitly the substance (or system) studied, gives the property measured in terms of a category, e.g. P-V-T data, calorimetric heats of reaction, solubilities, etc., and a complete bibliographic citation. Each index section also contains a collection of entries devoted to correlations, descriptions of apparatus, and to properties of miscellaneous industrial materials and substances not readily identified by chemical formula.

The Bulletin is recommended as a useful research tool for all scientists and engineers who need to find new thermodynamic and thermochemical data.

Available from University of Michigan Publication Distribution Service, 615 East University Avenue, Ann Arbor, Michigan 48109, USA. Price \$20.00.

ERRATA IN CODATA BULLETIN 16

- 1) On page 11, the third sentence of paragraph 2. Generation and Presentation of Data, should be modified to read as follows:

In the former case, the data...in describing the main results of the research. Some of the data are not published at all when they are not essential for the description of the main results of the research or when they have been obtained solely as a by-product of the research. (The underlined words should be inserted.)

- 2) On page 11, in the second line of the right-hand column, the words "half-width values" should be replaced by "half-value widths".

A NEW FRENCH SERVICE IN CHEMICAL INFORMATION: DATA BANKS OF THE DARC PLURIDATA SYSTEM (DARC=Description, Acquisition, Retrieval, Conception)

Three of the seven data banks at present incorporated in the DARC PLURIDATA SYSTEM (DPDS) are now accessible to the public at the Centre d'Informatique et Documentation Automatique (CIDA) and will be accessible by the end of 1977 through the nodes of CYCLADES, the French Computer Network. The three physico-chemical data banks for Carbon-13 Nuclear Magnetic Resonance spectra, for Mass Spectra and for Crystallographic Data are described in the next column. Thanks to low processing costs on the mini-computer PDP-11/35, interrogation of the data banks, which is free for an initial promotional period, will remain very inexpensive.

The DARC PLURIDATA SYSTEM was created by CIDA at the University of Paris VII in pursuance of the policy of the Bureau National de l'Information Scientifique et Technique (BNIST) to encourage data bank development.

Relying on the general system of chemical informatics and using a mini-computer PDP-11/35, DPDS groups a coherent set of data banks in accordance with a simple scheme, namely the association of an Information Data Base (IDB) - containing numerical values, spectra, bibliographic data, etc. - with the Structural Data Base (SDB) containing the storage and retrieval data relative to the chemical compounds of the data bank.

DARC PLURIDATA SYSTEM possesses all the computer functions necessary for the creation, maintenance and interrogation of chemical data banks:

- Automatic input and registration of chemical structures
 - by direct acquisition of the structural diagram on a specialized device, the "Topocodeur".
 - by transcoding into the DARC code from other codes, such as the Chemical Abstract Service Connection Tables and the Wiswesser Linear Notation.
- Checking and non redundant merging of structural files originating in different sources.
- Interactive structural and substructural searching of the SDB by alphanumerical or graphical terminals. In the latter case the query is directly formulated in natural chemical language by direct drawing of the structure or substructure.
- Display of the 2-dimensional or 3-dimensional structural diagram on plotter or CRT terminals.
- Interactive searching of the IDB, directly or via SDB.
- Analytic display of spectra on CRT and synthetic display of numerical arrays.

These functions can be placed, totally or partially, at the disposal of any user desirous of creating his own data bank, under conditions negotiated in accordance with individual cooperative agreements.

Further information may be obtained from CIDA, 1, rue Guy de la Brosse, 75005 Paris, France, Telephone (01) 707-1165.

PLURIDATA: C-13 NMR DATA BANK

Origin

Compilation and indexing by the CIDA of the most well-known publications (1971-1977) plus French and foreign collections (1977)

Content

- Structural data: chemical structures indexed from JACS, JCS, JOM, J. Org. Chemistry, Tetrahedron Letters, J. Chim. Phys. and coded via "Topocodeur" input.
- Spectral data: unambiguously assigned chemical shifts of the NMR Spectra.
- Textual data: experimental conditions, bibliographic sources.

Volume: July 1977: 6 500 compounds and 7 000 spectra
growth rate: 300 new compounds/month

Retrieval software

- Graphical and alphanumerical interactive DARC software for structural, sub-structural searching.
- Interactive DARC software for bibliographic searching.
- NMR Spectra matching DARC software.

Objectives

- Documentation:
 - *Spectra Retrieval from structures, substructures and bibliography.
 - *Structure Retrieval from NMR spectra features.
- Computer Aided Design:
 - *Elucidation of an unknown structure from its NMR spectrum, computer aided correlation.

PLURIDATA: MASS SPECTRA DATA BANK

Origin

American National Institutes of Health (NIH)/Environment Protection Agency (EPA) (by lease from National Bureau of Standards - NBS).

-Chemical Abstract Service.

Content

- Structural data: chemical structures transcoded into DARC code from CAS RIII/SDF Connection Tables.
- Spectral data: mass-intensity pairs for each peak of the Complete low resolution spectrum.
- Textual data: origin of the spectra, experimental conditions.

Volume: July 1977: 25 560 chemical compounds.

Retrieval software

- Graphical and alphanumerical interactive DARC software for structural and substructural searching.
- NIH/EPA interactive software (adapted to PDP-11/35 for mass spectra searching).

Objectives

- Documentation
 - *Spectra retrieval from structure and substructures.
 - *Structure retrieval from mass spectral features.
- Computer Aided Design
 - *Elucidation of an unknown structure from its mass spectrum, computer aided correlation.

PLURIDATA: X-RAY CRYSTALLOGRAPHIC DATA BANK

Origin

Cambridge University Chemical Laboratory. CIDA is an affiliated center of the Cambridge Crystallographic Data Centre.

Content

- Structure data: chemical structures transcoded into DARC code from the Connection Tables of the Crystallographic Data Centre.
- Numerical data: crystallographic data (validation data, atomic X, Y, Z coordinates, bond lengths).
- Textual data: bibliographic sources, nomenclature.

Volume: July 1977: 15 000 chemical compounds.

Retrieval software

- Graphical and alphanumerical interactive DARC software for structural and substructural searching in natural chemical language.
- Crystallographic Data Centre software (adapted to interactive processing on PDP-11/35) for bibliographic searching.
- 3D display searching.

Objectives

- Documentation:
 - *Crystallographic data retrieval from structure, substructures and bibliography.
- Computer Aided Design:
 - *Computer aided correlation, structural elucidation, energy optimization.

SCIENTIFIC INFORMATION TRANSFER: THE EDITOR'S ROLE IN TOMORROW'S WORLD

The First International Conference of Scientific Editors, with representatives of 29 relevant national and international organizations, 18 nations, and a total participation in excess of 160 individuals met in Jerusalem, Israel, April 21 to 29. (Only the Soviet Union participants were conspicuous by their absence.)

Not only was the role of the editor in the publishing process, in science, in society, and in mechanization and computerization of the editorial process considered, but concerns for user reaction to innovations and the impact of the new techniques were also discussed.

Responsibilities of authors (creators), and of referees and editors (gatekeepers) and the relevance of standards, language and style in the publication process were intermixed with presentations on the financial, economic, organizational, and other national and international publishing and distributional problems.

Multilingual, social science, and agricultural problems were also reviewed as were developments in secondary information services and information transfer between primary and secondary services. Although some deficiencies in programming and organization were evident, it is interesting that with few exceptions, the slide and textual projections prepared by the speakers -- presumed to be experts in "informatics and communication" -- were as illegible as those of laboratory and theoretical scientists at conferences. The importance of graphical representation as well as the practicality of publishing in English for maximum research (as distinguished from educational) readership was reiterated frequently, especially by commentators from countries speaking languages other than French, German, or English.

CODATA concerns resided in the importance of data in information transfer: in such problems as numerical data flow among primary, secondary, and tertiary literature (by Professor Stephen Kertes); in the CODATA *Guide for the Presentation of Biological Numerical Data* (by Dr. Philip L. Altman) and in data indexing as well as in the presentation of numerical data in such form that it may be critically evaluated (by Prof. Edgar F. Westrum, Jr.).

Although the editor's role in tomorrow's world was the featured topic, editors themselves were not very much in evidence and statements made in discussion that not more than 15 to 30 bona fide editors were present went unchallenged. In view of the part-time (almost extra curricular) aspect of most scientific editorial endeavors and the fact that editors typically serve as such for less than a decade, the situation of a scientific editor is, of course, quite different from the professional status of a technical documentalist, for example. Attempts to achieve resolutions about international coordination were unsuccessful, but a second conference in about three years time is contemplated. Those interested in more information about conference plans or the anticipated availability of proceedings of the present conference may contact Dr. Miriam Balaban (Chairman of the Organizing Committee) in care of National Council for Research and Development, Jerusalem, Israel.

E.F. Westrum, Jr.
June 1977

INTERNATIONAL MEETING ON PHYSICAL DATA OF HIGH PRESSURE FLUIDS HELD IN KYOTO IN SEPTEMBER, 1976

Twenty scientists from seven countries met in Kyoto, Japan, when the International Meeting on Physical Data of High Pressure Fluids, sponsored by the Yoshida Foundation for Science and Technology and the Physico-Chemical Society of Japan, was held on September 11, 1976.

In the morning session, chaired by Prof. J. Osugi, four scientists (Dr. S. Angus, Dr. H.J. White, Jr., Prof. J. Kestin and Prof. E.U. Franck) spoke on the international cooperation in data evaluation activities, and five other scientists including Prof. B. Vodar joined the discussion.

The afternoon session was chaired by Prof. Y. Takezaki, who also gave a talk on "Present Status of the Data Evaluation carried out at the High Pressure Data Center of Japan". Then followed speeches by Dr. S. Angus and Dr. G.S. Kell, entitled "Weighting of Data in Constitution of State" and "Weighted Least Squares" respectively, with free talking and discussion by twelve of the participants.

Copies of the Proceedings of the meeting, transcribed from the sound tape, are available from Prof. J. Osugi, Faculty of Science, Kyoto University, Sakyo-ku, Kyoto, 606 Japan.

THE USE OF GENERALISED DATA MANAGEMENT SYSTEMS (GDMS) FOR HANDLING SCIENTIFIC INFORMATION

A specialist study carried on by an OECD/NEA Working Group on Nuclear Energy Information Specialist Study on Computing Techniques, jointly organized by OECD/NEA, US ERDA and NBS held the first of two scheduled meetings in Paris in January 1977. The second meeting will be held at Lawrence Berkeley Laboratory, Berkeley, California from 5-7 October 1977. A published report on the study is planned for early 1978.

The report will be aimed at programmers, scientists and managers concerned with scientific information, and in particular those whose problems include handling large amounts of numerical data in specialised information projects or data centres. Many readers will have little knowledge of GDMS before they read the report, and it is hoped to

- give a clear introduction to what GDMS (better known as DBMS) are, and why they may be useful;
- consider the special nature of scientific information and the limitations of existing GDMS in handling it;
- show by case studies of existing and potential GDMS applications to scientific data what may be involved in their use, and what the users think about this software;
- survey the directions taken by new developments in GDMS;
- consider the capabilities required by users from a GDMS for use with scientific information, and also the relative costs of GDMS use and traditional programming;

Attendance at the meeting is by invitation, but further information on the study may be requested from Dr. N. Tubbs, OECD/NEA, 38 Boulevard Suchet, 75016 Paris, France.

CAPTURE, EVALUATION AND STORAGE OF DATA -- AS SEEN BY CODATA

N. Kurti

Department of Engineering Science, University of Oxford

It is obvious that to deal with the whole subject "Capture, Evaluation and Storage of Data" one would need several lectures and not just a 20 minute talk -- hence the qualifying subtitle. This will be a very specific treatment, an attempt to explain what CODATA (the Committee on Data for Science and Technology of ICSU, the International Council of Scientific Unions) has done, and is trying to do, in this field. My lecture will contain no hard or particularly useful facts. Its rationale could be best characterised by the well known story about the two young Irishmen who one Sunday morning felt very contrite after a boisterous Saturday evening out. So they went to Church, and first one went in and confessed to having committed the mortal sin of fornication. But he would not divulge the name of the person he did it with, even though the priest tried to make it easier for him by mentioning the names of a few young ladies of the town who might have been his willing partners. So: no full confession, no absolution. He went out rather crest-fallen and his pal asked him, "Well, what happened, did you get absolution?" "No, but he gave me three good tips." Similarly I do not expect to get absolution for any past misdeeds or lack of deeds of CODATA but I hope that in the ensuing discussion you will be able to give me and through me CODATA a few good tips on how we can improve our ways and how we can be more helpful to the scientific community in general and to the chemists in particular.

As the chairman mentioned, CODATA was founded at a time when the amount of scientific data being collected was increasing rapidly, and when it was therefore felt that a co-ordination might be necessary. First in the field was the United States, where the National Bureau of Standards was asked to start a National Standards Reference Data System. A large amount of work was also being carried out in the USSR and when it was finally decided to set up an international co-ordinating body the United Kingdom entered wholeheartedly into this scheme and so CODATA was formed, with France, the Federal Republic of Germany, Japan, UK, USA and USSR as the six "founding" members. CODATA has at present 15 "national" members and they provide most of CODATA's funds. The rest of the membership consists of 12 scientific unions of ICSU and the ICSU Panel on World Data Centres.

What are the aims of CODATA? There is one thing it does not want to do and cannot do, namely to edit and publish large data collections, that is entirely beyond its means. CODATA's raison d'être is expressed in its constitution which says "CODATA working on an inter-disciplinary basis,

shall seek to improve the quality, the reliability and accessibility of data of importance to science and technology including not only quantitative information on the properties and behaviour of matter but also other experimental and observational data". It took incidentally, the better part of 4 hours to draft this passage, especially the last 19 words. The reason was as follows. CODATA was originally set up to improve the quality of data used mainly in chemistry and in physics, that is data obtained by physical measurements on pure or readily identifiable or readily reproducible substances. That was a fairly straightforward task and there was no difficulty about expressing it in the constitution. However, in about 1972, 6 years after CODATA's birth, the International Council of Scientific Unions asked CODATA that it should concern itself not only with data important for physics and chemistry, data on pure or readily identifiable substances, but also with data of importance to the earth sciences and to the life sciences. This widening of its scope has somewhat altered the character of CODATA. Although some people regret this departure from CODATA's original philosophy, I believe that this is a good development because CODATA is supposed to work on an interdisciplinary basis, and by concerning itself also with earth and life sciences, it can hope to establish in the field close co-operation between disciplines which deal with "immutable" data and disciplines concerned with data which depend on time and location. So I think from that point of view this was a good move.

What are the specific goals of CODATA? Well, the basic aim is -- I quote again from its constitution, "to promote the evaluation, and in general the quality control of data and the methods by which they are acquired". Another aim is to increase awareness amongst all scientists of the importance of data activities and in particular to encourage scientists to participate in them, and connected with it, to promote the improvement of the status and the training of data evaluators and of data compilers. And finally, CODATA wishes to encourage the application of new methods to data handling, storage, and retrieval, as well as to the evaluation, the presentation, and the organised production and dissemination of data. How can CODATA, a relatively small and far from wealthy organization perform these functions? It does so mainly through small specialist task groups consisting of anything between 4 and maybe 10 scientists all specialists in the particular field the task group is concerned with. These task groups have well defined terms of reference, are established for limited periods at a time and when their task is completed, they are dissolved or put into abeyance. I think that the activities of CODATA can be best explained by listing its Task Groups and describing briefly what each of them has been doing, is doing, or proposing to do in

Thermodynamic Data and the Methodology of Handling Space and Time Dependent Data, the latter being of particular interest to geologists and geographers.

But it is not enough to have good, critically evaluated data. It is important that they are widely disseminated and readily accessible. The CODATA Task Group on the *Accessibility and Dissemination of Data* has been grappling with this question for over 4 years with the generous support of Unesco-UNISIST. After the publication of its report (10) it turned its attention to the more specific question of Data Referral Centres. Many of the developed countries have such centres -- national or local -- to which people can turn for information about where data in a certain field may be obtainable. The Task Group studied the feasibility of a World Data Referral Centre which would link the national and local centres and recommended that such a centre be set up. Preparations are in hand to establish such a World Data Referral Centre (WDRC) in Paris, in the same building where the CODATA Secretariat (together with ICSU and a few other ICSU bodies) are housed, and it is hoped that the WDRC can be in operation sometime in 1978.

One of the first tasks of CODATA was the publication in 1969 of an International Compendium of Numerical Data Projects (11). While this is still a fairly useful book, some of the information is out of date and -- more important -- a very large number of projects are missing from it, either because they were started since publication of the Compendium or because they were concerned with the life and earth sciences which in the early days were outside CODATA's scope. It has therefore been decided to publish an entirely new Directory of Data Sources for Science and Technology. This will be published initially in parts -- each covering one more or less wide area -- as separate issues of the *CODATA Bulletin*, but the sections will eventually be consolidated into a single volume. The part on crystallographic data has been published as a *CODATA Bulletin* (12). Sections on biological sciences and on astronomy-astrophysics will follow soon after.

This brings me to the end of my review of CODATA's role in the capture, evaluation, storage and dissemination of data, and this is the right moment to pay tribute and give thanks to those scores of scientists who give their time and services freely in helping this good cause. Although for many who take part in these activities a considerable financial sacrifice is involved, CODATA's work still costs money -- our annual budget is about \$110,000 -- and for most of this we rely on the contributions from our National Members and from ICSU, and on contracts -- mainly from Unesco-UNISIST.

In order to expand our work we shall need more funds and this is where industrial firms, national or international data organizations, etc. could help. By becoming "Associate Organizations" they

would become involved in various CODATA activities, would have access to unpublished reports and memoranda, and would help CODATA financially. So, to echo the young Irishman's remark, "I'm waiting for a few good tips!"

References

1. Guide for the Presentation in the Primary Literature of Numerical Data Derived from Experiments. *CODATA Bulletin* No. 9, Dec. 1973.
2. The Presentation of Chemical Kinetics Data in the Primary Literature. *CODATA Bulletin* No. 13, Dec. 1974.
3. Recommendations for Measurement and Presentation of Biochemical Equilibrium Data. *CODATA Bulletin* No. 20, Sept. 1976.
4. Flagging and Tagging Data -- to indicate its presence and facilitate its retrieval. *CODATA Bulletin* No. 19, June 1976.
5. Key Values for Thermodynamics:
 - Tentative Set, Part I. *CODATA Bulletin* No. 2, Nov. 1970.
 - Final Set, Part I. *CODATA Bulletin* No. 5, Dec. 1971.
 - Tentative Set, Part II. *CODATA Bulletin* No. 6, Dec. 1971.
 - Tentative Set, Part III. *CODATA Bulletin* No. 7, Aug. 1972.
 - Recommended Values. *CODATA Bulletin* No. 10, Dec. 1973.
 - Recommended Values. *CODATA Bulletin* No. 17, Jan. 1976.
6. Recommended Consistent Values of the Fundamental Physical Constants, 1973. *CODATA Bulletin* No. 11, Dec. 1973.
7. A Catalogue of Compilation and Data Evaluation Activities in Chemical Kinetics, Photochemistry and Radiation Chemistry. *CODATA Bulletin* No. 3, Dec. 1971.
8. Automated Information Handling in Data Centres. 1st edition, *CODATA Bulletin* No. 1, Oct. 1969. 2nd edition, *CODATA Bulletin* No. 4, Nov. 1971.
9. Man-Machine Communication in Scientific Data Handling. *CODATA Bulletin* No. 15, March 1975.
10. Study on the Problems of Accessibility and Dissemination of Data for Science and Technology. *CODATA Bulletin* No. 16, Oct. 1975.
11. *CODATA International Compendium of Numerical Data Projects*. Springer Verlag, Berlin-Heidelberg, 1969.
12. CODATA Directory of Data Sources for Science and Technology.- Chapter 1: Crystallography. *CODATA Bulletin* No. 24, June 1977.

All the above publications can be obtained from the CODATA Secretariat (51 Boulevard de Montmorency, F-75016 Paris, France; Tel. 525-0496, Telex 630553 F), to which all enquiries concerning CODATA should be addressed.

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An Addendum

Owing to an unfortunate oversight, the following footnote explaining the origin of the contribution by N. Kurti, was omitted on page 8:

This article was presented at the International Symposium on Techniques for the Retrieval of Chemical Information held at The Royal Society, London (November 1976) and is reproduced here with the permission of IUPAC. Main lectures from the Symposium are in the press for publication in the Journal Pure and Applied Chemistry and as a separate Symposium volume by Pergamon Press, Oxford.

We apologize to those of our readers who may have been surprised at the informal tone of the article.

The above correction will be printed in the next Number of the CODATA Newsletter due to appear at the end of 1977 or early in 1978. It would have been impracticable to send this correction individually to all of our 5000-6000 readers, but during the next month or so we shall include in letters sent out by the Secretariat and by Officers one or several copies of this note in the hope that in this way a fair proportion of our readers will receive this information.

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THE ROLE OF SPACE AND TIME DEPENDENT DATA IN CHEMISTRY*

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The intrinsic chemical properties of the materials that make up our world are largely, if not completely, independent of both time and location. It is true, of course, that the chemical stability of different materials will vary with respect to their environment as also will their readiness to enter into chemical reaction with one another. Chemists however will normally define the properties of the materials in terms of strictly prescribed conditions such as temperature, pressure and the nature of the radiation and atmosphere to which the materials are exposed. These will be considered to be static and invariant with regard both to space and time. Indeed, in setting up conditions for accurate measurement of chemical properties, chemists take great pains to avoid such time- or location-dependent variation.

In the real world of our everyday life, chemical materials are constantly exposed to time- and space-dependent variations. However the main responsibility of the chemist is to define the properties of the materials in fixed environments. It is the sister disciplines such as the geo-sciences, agricultural science, forestry, meteorology, oceanography which use the basic information from the chemical data banks to interpret the chemical behavior of the materials under conditions of natural or man-induced change.

Perhaps I can make this point clearer by citing a specific example. We are all much concerned about the stability of our upper atmosphere, and particular about the effects of disturbance of its equilibrium resulting from real or potential human interaction. This is basically a problem for geo-scientists and meteorologists and it is a problem which is highly sensitive to time- and location-dependent variations. A powerful method to study it is to construct computer models and try to predict changes in the atmospheric composition as a result of controlled simulations in the model. In such models we need to have precise information about how the constituents of the atmosphere will react with one another under a wide range of conditions. The chemist quantifies the reactivity of materials under precisely defined conditions by the *rate constant* of the reaction. Such rate constants are functions of pressure, temperature, concentration and exposure to radiation of specific wavelengths. These rate constants must be entered into the computer calculations simulating the atmospheric conditions. If the rate constants are not sufficiently

accurate the results of the computation may be completely erroneous.

CODATA has a Task Group on Chemical Kinetics Data and at the CODATA General Assembly at Boulder last July, it was agreed that the generation, by chemists, of good evaluated rate constants for reactions occurring in the upper atmosphere was a matter of high priority. This, I think, well illustrates how important is the interaction between the hard data of the physical sciences with the inherently less precise time- and location-dependent data which plays such a large part in the problems of the astro-, bio- and geo-sciences.

It is interesting to look also at the influence of the time dimension on the science of chemistry at a somewhat more philosophical level. The nature of chemical processes extends over many orders of magnitude on the time scale. Looking first at the longest time scale, that of the universe itself, chemical events do not play a very great role. The changing character of stellar events on a time scale of cosmic evolution depends mainly on properties centered within the nucleus of the atom. We therefore hear much more about *astro-physics* than about *astro-chemistry*. Next on a diminishing time scale we enter into the realm of geological time. Geological events are much involved with chemical change though I think most chemists are prepared to concede that geo-chemistry plays the secondary role as an aid to geologists and mineralogists.

The problems of corrosion and the deterioration of man-made artefacts on a time scale of historical and other human events is a true field of chemical science. So also are biological events that take place on the scale of human, animal and plant life cycles. These constitute an active area of bio-chemistry. Perhaps we can quantify this as a time scale in the range from *mega seconds* to *seconds*.

When the chemist comes to study the structure and behavior patterns of individual molecules or small molecular aggregates such as occur in colloid science and in kinetic and spectroscopic studies involving the interaction of molecules with radiation and with one another, he enters a world where events occur on millisecond, microsecond, nanosecond, and picosecond time scales. Modern chemists, particularly physical chemists, are acquiring a facility in adjusting their thought processes to work selectively in these highly distinct time dimensions and to switch from one to another.

Thus, for example, in modern work in photochemistry, where pulses of visible or ultraviolet light are used to initiate chemical reactions, the events occur on the nanosecond time scale. In studies of the behavior and properties of liquids at the molecular level the chemist operates in a picosecond world. The picosecond world is a strange one since light travels a distance of only 0.3 mm in a picosecond.

*Excerpts from R.N. Jones' presentation at the meeting of the CODATA Task Group on Space- and Time-Dependent Data, Ottawa, February 17, 1977.

NEW PUBLICATIONS

ATOMIC AND MOLECULAR PROPERTIES

ELEMENTS DE METALLURGIE PHYSIQUE. (1976, Tome 1: Rappels, 234 p, 40 Francs; Tome 2: Physique du métal, 508 p, 40 F). Cet ouvrage collectif publié par le Commissariat à l'énergie atomique, comprendra 6 tomes dont les deux premiers viennent de paraître:
Tome 1: Rappels. Les bases de la thermodynamique macroscopique. Mécanique statistique. Mécanique quantique. Cristallographie. Elasticité et anélasticité. Déformation plastique d'un milieu homogène.
Tome 2: Physique du métal. Vibrations atomiques. Propriétés thermiques du réseau. La liaison chimique. Modèle de l'électron libre. Eléments de théorie des bandes. Les métaux de transition des terres rares et des actinides. Phénomène de transport. Propriétés magnétiques. Métaux liquides et alliages amorphes.

BIOLOGICAL SCIENCES

THE AROMATIC METABOLITES OF TRYPTOPHAN. (1977, 70 pp, \$10.00) by R.W.A. Oliver and M. Corrie. The metabolism of the essential amino acid tryptophan has been implicated in a very wide range of human diseases, e.g. breast cancer, schizophrenia and mental retardation. Because of this an International Study Group for the Metabolism of Tryptophan (ISTRY) was established in 1974 at a meeting held at the University of Padua. The second meeting of ISTRY is to be held this summer (1977) at the University of Wisconsin. The metabolism of tryptophan is so complex that a total of forty-four aromatic metabolites are formed. At the first ISTRY meeting it became clear that a molecular dictionary of these metabolites was needed which would list not only their physical properties but also the methods by which they could be separated from biological fluids. The present publication provides this information in convenient and compact form, being an evaluated data compilation of thin layer chromatographic, chromogenic reactions, ultra violet and mass spectroscopic data together with a comprehensive bibliography of references reporting their separation from biological fluids. The chromatographic data presented originates from the thin layer chromatographic systems developed within the authors' Biological Material Analysis Unit but the comprehensive bibliography, covering the period 1951-1976, also gives references to other methods of separation. The key spectroscopic properties listed are the ultra violet and visible spectra and the low resolution, electron compact mass spectra. All of these measurements have been made by the authors who have also carefully evaluated their results by comparison with published data. With the publication of this evaluated data compilation, investigators now have available an invaluable research tool enabling them to decide how best to separate and to unambiguously identify each of the aromatic metabolites of the essential amino acid. The book is available from: Dr. R.W.A. Oliver, Director of the Biological Materials Analysis Unit, Department of Chemistry and Applied Chemistry, University of Salford, Salford 5, Lancs., United Kingdom.

ATLAS OF PROTEIN SEQUENCE AND STRUCTURE, VOL. 5, SUPPLEMENT 2. (1976, XX+345 pp, \$15.00, National Biomedical Research Foundation, Silver Springs, MD 20901, U.S.A. - ISBN 0-912466-05-7) by Margaret O. Dayhoff and five co-authors, contains 350 protein sequences covering the literature between June 1972 and August 1974, and 50 RNA sequences published between June 1972 and January 1975, as well as revisions to previously published experimental sequences received through early 1976. The illustrations include 37 stereo-pair drawings and 17 molecular architecture drawings, while the tables provide a list of the 68 newly added protein families and the 33 newly added protein superfamilies. In addition to this new material, this Supplement also incorporates sequence information from Volume 5 and its supplements: superfamily list (hierarchical organization of 116 superfamilies, 197 families, 328 subfamilies and 493 entries); 17 evolutionary trees; mutation rate list for 42 protein families; biological distribution of protein sequence entries; 48 alignments; 43 difference matrices; 5 alignment score tables; composition of protein families; lengths of sequences from each protein family; families with largest percentages of each amino acid; list of known tRNA sequences; cumulative index of protein sequences; and computer program descriptions.

BACTERIOLOGY ILLUSTRATED. Fourth edition (1976 247 pp, 170 illustrations, £11, Churchill Livingstone, Edinburgh. Distribué en France par Editions André Leson, 10 rue de l'Eperon, 75006 Paris. - ISBN 0-443-01445-0), par R.R. Gillies et T.C. Dodds, est la plus récente révision d'un célèbre manuel rédigé principalement à l'intention des étudiants en médecine et des techniciens de laboratoire. Après une introduction d'une quarantaine de pages dans laquelle sont rappelées les principales notions concernant la morphologie des bactéries, les différentes techniques de coloration, les milieux de culture, les réactions sérologiques et les procédures utilisées dans l'identification des microorganismes, la deuxième partie de l'ouvrage passe en revue 20 groupes ou espèces de bactéries, en décrivant chaque fois les caractéristiques suivantes: aspect microscopique, aspect des cultures, réactions biochimiques, caractères sérologiques, typage par bactériophages, inoculation aux animaux de laboratoire, infections provoquées chez l'homme. La troisième partie expose les méthodes et procédures utilisées pour le diagnostic bactériologique à partir des spécimens recueillis (sang, urine, crachats, liquide céphalo-rachidien, matières fécales, pus, etc.). Les deux dernières parties traitent brièvement des principales affections dues aux protozoaires et aux champignons. Par l'abondance de ses illustrations, dont plus de la moitié sont des photos en couleurs, soit de bactéries individuelles soit de colonies, ce livre constitue autant un atlas qu'un manuel et, à ce titre, mérite d'être considéré comme un ouvrage de référence.

CHEMICAL WEEK PESTICIDES REGISTER. (1976, 346 pp, \$95.00, McGraw-Hill), compiled by Robert P. Ouellette and John A. King, is designed to help both pesticide producers and pesticide users abide by the new regulations recently laid down by the Environmental Protection Agency and going into force

as of mid-1977. These regulations make it mandatory for producers to re-register their materials and formulations with the EPA, and enunciate the limits to pesticide use as well as the penalties incurred for violation. The Register is the only complete source of technical, safety and marketing information needed for such registration. The users searching for a pesticide for a specific application will find in the Register a very useful ingredient application index, both from the chemical and from the legal standpoints. A highly practical and informative book for the agricultural community.

THE NUTRIENT REQUIREMENTS OF FARM LIVE-STOCK. 4. Composition of British feedingstuffs. Technical review and tables (1976, VII+710 pp, £15.00, Agricultural Research Council, London. ISBN 0-7084-0027-2).

PICTORIAL ATLAS OF PATHOGENIC MICRO-ORGANISMS. (Volume I: 1974, 53 pp+89 plates, DM 124. Volume II: more than 100 plates (in preparation). Volume III: 1969, 171 plates, DM 142. Gustav Fischer Verlag, Stuttgart), edited by G. Henneberg, provides some 400 photographic plates of the most characteristic forms and structures of the various kinds of bacteria, both as regards their individual features and their macroscopic organization. Volume I is mostly devoted to the morphology of bacterial colonies, either in the course of normal development or reacting to an invasion of bacteriophage. Volume II (in preparation) will deal with the heteromorphism of bacteria. Volume III devotes 141 plates to the most important fine-structure features of bacteria as observed by electron microscopy. The English translation of the three volumes is by A. Mayr-Harting of the University of Bristol.

STAPHYLOCOCCI AND STAPHYLOCOCCAL DISEASES. (1976, 1200 pp, 513 figures, DM 248, Gustav Fischer Verlag, Stuttgart. ISBN 3-437-10436-5), edited by J. Jeljaszewicz, contains the proceedings of the Third International Symposium on Staphylococci and Staphylococcal Infections held in 1975 in Warsaw, Poland. Its contents include a comprehensive and detailed description of research on the taxonomy of micrococcaceae, coagulase-negative staphylococci with special reference to their biology, phage typing and infections, metabolism of staphylococci, genetics of staphylococci, cell envelope and associated phenomena, staphylococcal extracellular products, experimental staphylococcal infections, non-specific and specific resistance to staphylococcal disease, staphylococcal epidemiology and ecology, and staphylococcal infections and antistaphylococcal drugs.

TOXIC METALS 1976: POLLUTION CONTROL AND WORKER PROTECTION. (1976, 349 pp, \$39, Noyes Data Corporation, ISBN 0-8155-0636-8) by Marshall Sittig. This is a practical book about those metals and their compounds that are most likely to cause poisoning either in industry or in the general environment. Each of the 18 metals discussed (antimony, arsenic, barium, beryllium, boron, cadmium, chromium, copper, indium, lead, manganese, mercury, molybdenum, nickel, selenium, tin, vanadium, zinc) is surveyed from the points of view of: toxicity, exposure, detection and determination, environmental standards, handling procedure and precautions, removal from the air, removal from water, solid waste disposal, and economic impact of controls.

Specific data are given on permissible intake, acute and chronic toxicities, also on sensitization and the resulting hypersensitivities. In addition, some mention is made of possible carcinogenicity and other immunologic pathogenesis, such as occurs in beryllium poisoning, but the harmful effects likely to be caused by ionizing radiation from radioactive isotopes are not discussed.

CHEMICAL KINETICS

* THERMOMETRIC TITRATIONS. (1975, 209 pp, \$19.95, Wiley-Interscience, ISBN 0-471-05448-8), by Josef Bartels, reviews the range of applications afforded by thermometric titration from thermometric methods mostly used in analytical work to calorimetric methods used for the precise determination of thermodynamic data in equilibrium processes. Contents: Theoretical basis for an analysis of thermograms. Methods of thermometric titration. Acid-base titrations in aqueous solutions. Titrations in nonaqueous solvents. Thermometric precipitation titration. Thermometric redox titrations. Formation of compounds and complexes -- problems of complexometric titration. Instrumentation in titration calorimetry by R. Wachter. Index.

* CHEMICAL KINETICS: A MODERN SURVEY OF GAS REACTIONS. (1976, 241 pp, \$19.50, Halsted, Division of Wiley. - ISBN 0-470-63686-6) by John E. Nicholas, is an intermediate-level textbook directed at undergraduate students. The emphasis is clearly on the environmental side of gaseous reaction chemistry: most of the systems discussed are either industrial (internal combustion engines) or atmospheric (ionic processes in the higher atmosphere, stratospheric ozone) or at the intersection of these two domains (photochemical smogs). Each chapter is supplemented by a bibliography and a set of exercises. - Contents: Basic kinetic laws. Molecular activation. Experimental methods: slow reactions, fast reactions. Theories of reaction rates. Radical reactions, non-chain and straight-chain reactions. Branched-chain reactions. Molecular dynamics. Molecular beams. Chemiluminescence, hot-atom reactions, ion-molecule reactions. Appendix. Index of names. Index of subjects.

CHEMISTRY

* THE BEILSTEIN GUIDE: A MANUAL FOR THE USE OF BEILSTEIN'S HANDBUCH DER ORGANISCHEN CHEMIE. (1976, 95 pp, \$4.90, Springer-Verlag. - ISBN 0-387-07457-0) by Oskar Weissbach is the English translation, by H.M.R. Hoffman, of the system of rules presiding over the arrangement of the compounds listed in the 150 volumes now comprised in this famous handbook. - Contents: Coverage of Beilstein. Organization of Beilstein. How to find an article in Beilstein. Formula indexes. Name indexes. Filing procedures. Fundamental terms of the system: principal compounds and derivatives. Classification of principal compounds. Classification of derivatives. Filing of tautomers. Appendix. German-English-French vocabulary. Subject index.

BEILSTEIN HANDBOOK OF ORGANIC CHEMISTRY. BEILSTEIN'S HANDBUCH DER ORGANISCHEN CHEMIE. Volume 18, Part 8. HETEROCYCLIC COMPOUNDS. Amines: Monoamines, diamines, triamines, tetraamines, hydroxyamines (Springer Verlag, 1977, 812 pp, \$470).

CHEMISTRY (CONTINUED)

GMELIN HANDBOOK OF INORGANIC CHEMISTRY
GMELIN HANDBUCH DER ANORGANISCHEN CHEMIE
(Text in German with a German-English table of contents)
System
No.

3. OXYGEN: WATER DESALTING - SAUERSTOFF:
WASSER-ENTSALZUNG. (Springer Verlag, 1974,
62 Figures, xx+ 339 pp, \$228.80.)

11. TELLURIUM - TELLUR. Supplement, Part B1.
Compounds with H₂, O₂ and N₂ (Springer Verlag,
1976, 60 Figures, xx+153 pp, \$148.30.)

14. CARBON - KOHLENSTOFF. Part D3: Simple
Carbon-Halogen Compounds: XCO radicals and
ions. Carbonyl halides COX₂. Halogen deriv-
atives of urea (e.g. (NX₂)(NH₂)CO, (NX₂)₂CO).
Carbamoyl halides, NH₂C(O)X. Halogen iso-
cyanates, XNCO, the cyclic dimer (ClNCO)₂,
the trihaloisocyanuric acids (XCNCO)₃.
Halogen cyanides, XCN, halogenisocyanides,
XNC. Cyanuric halides (XCN)₃. The radical
F₂CN. Halogenated cyanamides, NF₂CN, NHC1CN.
(Springer Verlag, 1976, 13 Figures, xxxiv+
294 pp, \$272.40)

Part D4: The
Carbon-Sulfur Compounds: Tricarbon disulfide.
Carbon monosulfide. The CS⁺ ion. Carbon
disulfide CS₂. The CS₂⁺ ion. The CS₂⁺⁺ and
CS₂⁺⁺⁺ ions. The CS₂. Thiocarbonic acids
and thiocarbonates. Substituted thiocarbonic
acids and thiocarbonates. (Springer Verlag,
1977, 19 illustrations, xxvi+271 pp, \$261.80.
Text in German, with a German-English table
of contents.)

21. SODIUM - Natrium. Supplement, Section 6.
Halides: Preparation, properties, chemical
reactions. Na halide systems with water.
Na halide systems with aqueous solutions.
Na halide-D₂O systems. Non-aqueous Na hal-
ide systems. Na halides in binary solvents.
Na polyhalides. (Verlag Chemie GmbH, 1973,
85 Figures, xxii+402 pp, \$235.90.)

Supplement, Section 7.
Halides: Systems, solutions. (Verlag Chemie
GmbH, 1973, 143 Figures, xxiv+351 pp, \$209.50.)

Index. Alphabetic
subject index. Formula index. (Verlag
Chemie GmbH, 1973, viii+167 pp, \$99.50.)

31. RADIUM - Radium. Supplement, Vol. 1.
History. Cosmochemistry. Geochemistry.
(Springer Verlag, 1977, xiv+131 pp, \$131.20.)

39. RARE EARTH ELEMENTS - SELTENERDELEMENTE.
Part B1. Chemistry of the rare earth metals.
History. Atomic weight; isotope distribution.
Comparison of properties of atoms and ions
along the lanthanide series (text in English).
Preparation and technical separation from
raw materials. (Springer Verlag, 1976, 15
Figures, xvi+184 pp, \$168.10)

Part B2. Sc, Y, La and lanthanides. Separa-
tion of the rare earth elements: preliminary
procedures, technical procedures. Preparation
of the metals; refining procedures; purity
tests. Uses and applications. Toxicology.
(Springer Verlag, 1976, 6 Figures, xx+283 pp,
\$257.40.)

Part B4. Properties of nuclei, atoms, ions
and molecules. Data concerning the external
electrons (optical terms, ionization energies,
electron affinities, scattering factors).
Data concerning the inner shells (binding
energies of electrons, effective cross sec-
tions, level widths, emission of X-rays and
Auger electrons, absorption of X- and gamma
rays). Atomic and ion radii. (Springer
Verlag, 1976, 60 Figures, xi+427 pp, \$348.10.)

Part C3. The chemical compounds of Sc, Y,
La and the lanthanides: Fluorides. Oxyfluor-
ides. Hydroxyfluorides. Nitride fluorides.
Alkali fluorometallates. (Springer Verlag,
1976, 98 Figures, xxxiv+439 pp, \$349.40.)

44. THORIUM - THORIUM. Part C2. Ternary and
polynary oxides of Thorium. (Springer Verlag,
1976, 114 Figures, xviii+145 pp, \$151.00.)

46. TIN - ZINN. Part C4. The compounds of Sn
with zinc, cadmium, mercury, aluminum, gallium, indium,
thallium, the rare earth metals, titanium, zirconium,
hafnium, thorium and germanium. (Springer Ver-
lag, 1976, 139 Figures, xxii+247 pp, \$215.20.)

47. LEAD - BLEI. Part A2a. Occurrence:
The cosmochemistry and geochemistry of
lead. Total content of Pb in the solar system.
Occurrence and isotope ratios of Pb in meteor-
ites and moon rocks. Description of the coor-
dinations of Pb occurring in 297 minerals. Iso-
tope geochemistry and the history of the Earth.
Abundance of Pb on Earth and its relation to
Uranium during the formation of our planet.
Behavior of Pb during Earth's formation: respec-
tive abundances found in the Earth's mantle,
crust and atmosphere. (Springer Verlag, 1976,
7 Figures, xiv+280 pp, \$255.70.)

Part A2c. Occurrence:
Sedimentary sequence. Metamorphic sequence.
Hydrosphere. Atmosphere. (Springer Verlag, 1975,
4 Figures, xii+185 pp, \$175.20.)

53. MOLYBDENUM - MOLYBDÄN. Supplement, Part B1.
The compounds: Compounds of Mo with the noble
gases, hydrogen and oxygen, anhydrous antimony,
bismuth and the alkali molybdates. (Springer
Verlag, 1975, 97 Figures, xvi+241 pp, \$224.00.)

Supplement, Part B2.
The anhydrous Mo-O₂ compounds. The anhydrous
molybdates of Sc, Y, La and the lanthanides.
Compounds of the M₂(MoO₄)₃ type with M=Pr through
Ho. Complex molybdates of alkaline metals.
(Springer Verlag, 1976, 119 Figures, xliiv+320 pp,
\$300.10.)

55. URANIUM - URAN. Supplement, Part C3. Ter-
nary and polynary oxides of Uranium. (Springer
Verlag, 1975, 151 Figures, xx+360 pp, \$253.90.)

56. MANGANESE - MANGAN. Part C2. The com-
pounds: Oxomanganic ions. Permanganic acid.
Compounds and phases with metals of the main
groups 1 and 2 of the periodic table. (Springer
Verlag, 1975, 66 Figures, xviii+302 pp, \$214.30.)

Part C3. The com-
pounds: Compounds of Mn with oxygen and the
metals of groups 3 to 6 of the periodic table.
(Springer Verlag, 1975, 140 Figures, xx+307 pp,
\$260.50.)

56. MANGANESE - MANGAN, (Continued) Part C6
The compounds: Compounds of Mn with sulfur,
selenium and tellurium. 5Springer Verlag,
1976, 127 Figures, xl+360 pp, \$336.60.)

61. SILVER - SILBER, Part B6. The compounds:
Complexes formed with neutral ligands or with
ligands forming inner complexes: Silver (I).
Complexes with ligands containing N and O
atoms. (Springer Verlag, 1975, 49 Figures,
xvi+356 pp, \$264.50.)

Part B7. The compounds:
Complexes formed with neutral ligands or with
ligands forming inner complexes: Silver (I).
Complexes with ligands containing S, Se, Te,
P, As, Sb, Bi, Si, B or Ge; Silver II and III;
Subject index; Index of ligands for Silver
B1 to B7. (Springer Verlag, 1976, 49 Figures,
xvi+430 pp, \$345.90.)

NEW SUPPLEMENT SERIES

Volume No.

16. ORGANONICKEL COMPOUNDS - NICKEL -
ORGANISCHE VERBINDUNGEN, Part 1. (Springer
Verlag, 1975, 44 Figures, xiv+419 pp, \$305.40.)

18. ORGANONICKEL COMPOUNDS, INDEX FOR PARTS
1 AND 2 - NICKEL-ORGANISCHE VERBINDUNGEN,
REGISTER FÜR TEIL 1 UND TEIL 2, (Springer
Verlag, 1975, ix+129 pp, \$87.20.)

19. BORON COMPOUNDS - BOR VERBINDUNGEN,
Part 3. The compounds of Boron with the non-
metals S, Se, Te, P, As, Sb, Si and with metals.
(Springer Verlag, 1975, 9 figures, xx+201 pp,
(with 66 pages in English), \$151.00.)

20. TRANSURANIUM ELEMENTS - TRANSURANE,
Part D1. Chemistry in solution. (Springer
Verlag, 1975, 24 Figures, xix+176 pp (75 pp
in English, 101 pp in French), \$129.20.)

21. TRANSURANIUM ELEMENTS - TRANSURANE,
Part D2. Chemistry in solution. (Springer
Verlag, 1975, 212 Figures, xiv+278 pp (147 pp
in English, 80 pp in French), \$197.20.)

22. BORON COMPOUNDS - BOR VERBINDUNGEN,
Part 4. Compounds with an isolated trigonal
Boron atom and a covalent B-N bonding.
(Springer Verlag, 1975 13 Figures, xx+360 pp,
(31 pp in English), \$257.90.)

23. BORON COMPOUNDS - BOR VERBINDUNGEN,
Part 5. Boron-pyrazol derivatives. Spectro-
scopy of trigonal B-N compounds. (Springer
Verlag, 1975, 28 Figures, xvi+277 pp (82 pp
in English), \$198.50.)

24. PERFLUOROHALOGENOORGANO COMPOUNDS OF
MAIN GROUP ELEMENTS - PERFLUORHALOGEN-
ORGANO-VERBINDUNGEN DER HAUPTGRUPPEN-
ELEMENTE, Part 3. (Springer Verlag, 1975,
4 Figures, xviii+233 pp, \$172.50.)

25. PERFLUOROHALOGENOORGANO COMPOUNDS OF
MAIN GROUP ELEMENTS - PERFLUORHALOGEN-
ORGANO-VERBINDUNGEN DER HAUPTGRUPPEN-
ELEMENTE, Part 4. Compounds with elements
of main groups 1 to 4 (except carbon).
(Springer Verlag, 1975, 2 Figures, xvi+213 pp,
\$207.30.)

26. ORGANOTIN COMPOUNDS - ZINN-ORGANISCHE
VERBINDUNGEN, Part 1. Tin-tetraorganyl
compounds SnR_4 . (Springer Verlag, 1975,
1 Figure, xiv+182 pp, \$132.50.)

27. BORON COMPOUNDS - BOR VERBINDUNGEN,
Part 6. Carborane 2. Electronic properties of
closocarboranes, hetero- and metallocarboranes,
and polymeric carborane compounds. (Springer
Verlag, 1975, 48 Figures, xvi+150 pp (82 pp
in English), \$149.20.)

28. BORON COMPOUNDS - BOR VERBINDUNGEN,
Part 7. Boron oxides. Boric acids. Borates.
(Springer Verlag, 1975, 84 Figures, xx+237 pp,
\$217.80.)

29. ORGANOTIN COMPOUNDS - ZINN-ORGANISCHE
VERBINDUNGEN, Part 2. Tin-tetraorganyl
compounds $\text{R}_2\text{SnR}'$. (Springer Verlag, 1975,
2 Figures, xv+480 pp, \$346.80.)

30. ORGANOTIN COMPOUNDS - ZINN-ORGANISCHE
VERBINDUNGEN, Part 3. Tin tetraorganyls
 $\text{R}_2\text{SnR}'_2$, $\text{R}_2\text{SnR}'\text{R}''$, $\text{RR}'\text{SnR}''\text{R}'''$. Heterocycles and
spiranes. (Springer Verlag, 1976, xv+164 pp,
\$143.90.)

31. TRANSURANIUM ELEMENTS - TRANSURANE,
Part B1. The metals. Discussion of the elements
Np (No. 93), Pu (No. 94), Am (No. 95), Cm (No.
96), Bk (No. 97), Cf (No. 98), Es (No. 99) and
Fm (No. 100) with regard to their preparation,
crystal structure, mechanical, thermal, elec-
trical and magnetic properties. (Springer
Verlag, 1976, 29 Figures, xii+84 pp, \$82.30.)

32. SULFUR-NITROGEN COMPOUNDS - SCHWEFEL-
STICKSTOFF VERBINDUNGEN, Part 1. Compounds
with sulfur of oxidation number VI. Cyclic com-
pounds. Compounds with (respective) S:N ratios
>1, 1:1, 2:3, 1:2, 1:3, 1:4. Derivatives of
hydrogen aside. Derivatives of hydrazine.
Derivatives of hydroxylamine. (Springer Verlag,
1977, 6 Figures, xii+268 pp, \$233.70.)

33. BORON COMPOUNDS - BOR VERBINDUNGEN,
Part 8. Tetrahydroborate ion and derivatives.
(Springer Verlag, 1976, 15 Figures, xxii+220 pp,
(135 pp in English), \$201.10.)

34. BORON COMPOUNDS - BOR VERBINDUNGEN,
Part 9. Boron-halogen compounds: Part 1.
Partially halogenated derivatives of BH_3 .
Partially halogenated diboranes and oxyhalo-
boranes. Organylhaloboranes. Organyldihalo-
boranes. Diorganylhaloboranes. (Springer Ver-
lag, 1976, 7 Figures, xviii+332 pp (37 pp in
English), \$293.50.)

35. ORGANOTIN COMPOUNDS - ZINN-ORGANISCHE
VERBINDUNGEN, Part 4. Organotin hydrides.
(Springer Verlag, 1976, 1 Figure, xix+134 pp,
\$136.90.)

36. ORGANOIRON COMPOUNDS - EISEN-ORGANISCHE
VERBINDUNGEN, Part B, Section 1. Mono-
nuclear compounds 1. Compounds with 1L ligands.
Carborates. Compounds containing up to three
CO groups. (Springer Verlag, 1976, 18 Figures,
xv+209 pp, \$189.70.)

37. BORON COMPOUNDS - BOR VERBINDUNGEN,
Part 10. Boron compounds with coordination
number 4. Neutral μ -derivatives of diboranes.
Adducts of μ -diborane derivatives. Boronium
salts. Tetrahaloborate ions (BX_4)⁻. Carbonyl-
boranes. Data on boron compounds with rare
gases. (Springer Verlag, 1976, 11 Figures,
xx+272 pp, (183 pp in English), \$273.30.)

38. TRANSURANIUM ELEMENTS - TRANSURANE. Part B2. Binary alloy systems 1. Binary alloys of Ne. Alloys of Pu with: alkali metals; alkaline earth metals; rare earth elements; Ac, Th, Pa, U, Ti, Zr, Hf, V, Nb, Ta, Cr, Mo, W, Mn, Te and Re. The alloys are described with regard to their preparation, crystal structure, mechanical, thermal, electrical and magnetic properties. (Springer Verlag, 1976, 191 Figures, xxiv+241 pp, \$241.60.)
39. TRANSURANIUM ELEMENTS - TRANSURANE. Part B3. Binary alloy systems 2. Binary alloys of Pu with Fe, Co, Ni, the platinum metals, Cu, Ag, Au, Be, Mg, Zn, Cd, Hg, Al, Ga, In, Tl, Sn, Pb, Sb and Bi. Alloys of Am and Cm. Transcurium alloys. Description includes formation, crystal structure, mechanical, thermal, electrical and magnetic properties. (Springer Verlag, 1977, 204 Figures, xxviii+275 pp. \$271.50.)
40. ORGANOTITANIUM COMPOUNDS - TITAN-ORGANISCHE VERBINDUNGEN. Part 1. Mononuclear compounds 1. Compounds in which the organic ligand is bound to the Ti atom by one to five C atoms. (Springer Verlag, 1977, 6 Figures, xiv+212 pp, \$211.70.)
41. ORGANOIRON COMPOUNDS - EISEN-ORGANISCHE VERBINDUNGEN. Part A. Ferrocene 6. (Springer Verlag, 1977, 24 Figures, xiv+316 pp, \$282.50)
- FORMULA INDEX TO THE GMELIN HANDBOOK - FORMELREGISTER ZUM GMELIN HANDBUCH.
- | | | |
|----------|---------------------------------|--|
| Volume 1 | Ac-Au | Springer Verlag, 1975, xii+253 pp, \$190.10. |
| Volume 2 | B-Br ₂ | Springer Verlag, 1975, xiv+313 pp, \$263.20. |
| Volume 3 | Br ₃ -C ₃ | Springer Verlag, 1976, xv+259 pp, \$237.20. |
| Volume 4 | C ₄ -C ₇ | Springer Verlag, 1976, xv+255 pp, \$229.30. |
| Volume 5 | C ₈ -C ₁₂ | Springer Verlag, 1977, xvi+268 pp, \$264.70. |

ORGANOSILICON COMPOUNDS, Fall 1976 (1976, 14 pp, Silar Laboratories, 10 Alplaus Road, Scotia, N.Y., 12302 U.S.A.). This commercial catalog lists 228 organosilicon compounds readily available. Each entry includes the chemical formula, the molecular weight, the boiling point, the density, and the refraction index.

EARTH SCIENCES

- * INTERNATIONAL STRATIGRAPHIC GUIDE; A GUIDE TO STRATIGRAPHIC CLASSIFICATION, TERMINOLOGY AND PROCEDURE. (1976, 200 pp, \$9.50, Wiley-Interscience, ISBN 0-471-36743-5), edited by Hollis D. Edberg, has been prepared for the International Subcommittee on Stratigraphic Classification of IUGS. Contents: Principles of stratigraphic classification. Definitions and procedures. Stratotypes. Lithostratigraphic units. Biostratigraphic units. Chronostratigraphic units. Relation between litho-, bio-, chrono-, and other kinds of stratigraphic units. Bibliography (1500 items listed). Index.

MICROFACIES ET ORDINATEUR. (1976, 228 pp, 188 Figures, 95 F, Editions Technip, 27 rue Ginoux, 75015 Paris. Text in French), by Jean Charollais

et Eric Davaud, is a practical guide designed to provide geologists with a method for describing observations performed on thin sections of sedimentary rocks through the microscope, the ultimate objective being to enter all the data in a computer system so as to allow classification, storage and retrieval of the significant information. Such a method implies that the identifying parameters be selected very carefully and thoroughly. This is done in Chapter 1. The two other chapters are devoted, respectively, to the preparation of individual cards and to the actual utilization of various computer programs. Numerous worked examples and many illustrations.

HANDBOOKS FOR BROAD FIELDS OF SCIENCE & ENGINEERING

HANDBOOK OF SOVIET ALLOY COMPOSITIONS - First supplement. (1976, 225 pp, \$7.50, Metals and Ceramic Information Center, P.O. Box 8128, Columbus, Ohio 43201, U.S.A.). The objective of the Handbook of Soviet Alloys is to provide a tool by which engineers, metallurgists, and others can identify the chemical compositions of a wide variety of metals and alloys used in the USSR. Both recent alloys as well as earlier developed alloys are included in the Handbook along with their designations. Also, wherever possible, this document includes the U.S. equivalent of the Soviet alloys. Data on compositions, designations, and other miscellaneous information are compiled in 25 tables. An Index (Index of Alloys), which lists the location within the tables of specific alloys and metals by their alphabetical-numerical designation, is provided to aid in the use of the Handbook. The tables and index of alloys were generated by computer. The first supplement adds many new alloy compositions, expands on some of the data in the Handbook and corrects some of the errors or omissions in the original book. Also, a new index is included. Present plans are to issue updates to the Handbook at approximately two-year intervals.

INDEX OF CHEMICALS USED IN THE TREATMENT OF METAL SURFACES. (1974, XXIV+632 pp, DM 210, Carl Hanser Verlag, Munich. ISBN 3-446-10278-1), compiled by Hans Benninghoff gives the main properties and relevant data for 1034 substances currently employed in the chemical or electrochemical treatment of metallic surfaces. Each substance is described in the space of a half-page according to a standard format whereby the name of the substance, as given in conformity with the IUPAC recommendations, is followed by its chemical formula, molecular weight, melting point, boiling point, solubilities in water, acids and various solvents, its chief reactions, the maximal permissible concentrations when in actual use, and the categories of risks encountered in transportation. Most of the numerical data given have been verified. The text is entirely trilingual: German, English and French. The alphabetical index provided at the end of the book includes popular designations of chemicals, as well as incorrect or misleading names, thus making this index a regular chemical dictionary. A very useful reference work.

MECHANICAL AND ENGINEERING DATA

SPECIALTY STEELS 1977: RECENT DEVELOPMENTS.

(1977, 270 pp, \$39, Noyes Data Corporation, ISBN 0-8155-0649-X) by G.B. Rothenberg. This book describes the preparation, properties and uses of special purpose steels. It presents formulation and evaluation data for all types of carbon steels, high strength-low alloys steels, tool steels, stainless steels, heat resisting steels, low carbon structural steels and magneto-electric steels. 203 processes in all, emphasizing the latest advances in steel production, are described.

NOMENCLATURE, SYMBOLS, UNITS, STANDARDS & CONSTANTS

THESAURUS ISO - ISO THESAURUS. (1976, Volume 1: Liste alphabétique structurée, 281 pp; Volume 2: Index bilingue par mots vedettes, 193 pp; Volume 3: Table de correspondance anglais-français, 125 pp; Les 3 volumes, 1500 F, AFNOR, Tour Europe Cédex 7, 92080 Paris-La Défense). Conçu dans le cadre des activités du réseau ISONET, ce thesaurus multidisciplinaire couvre l'ensemble des domaines dans lesquels s'exerce la normalisation, c'est-à-dire pratiquement la totalité des branches de la technologie: mécanique, métallurgie, transports, construction, génie civil, électricité, énergie nucléaire, industries chimiques et parachimiques, agriculture et alimentation, banque, unités de mesure, optique, équipements audiovisuels, documentation, informatique, matériel médico-chirurgical, etc. Ceci a été rendu possible grâce à une liste de 9000 notions qui ont été finalement retenues, en conformité avec la norme ISO sur l'élaboration des thesaurus, après que 13 000 documents nationaux ou internationaux, aient été eux-mêmes indexés. A lui tout seul, ce thesaurus peut presque se substituer, ou en tout cas servir de point de départ, à un grand nombre de thesaurus spécialisés avec lesquels il demeure compatible. En particulier il est entièrement compatible avec le Thesaurus of Scientific and Technical Terms de l'Engineers Joint Council. L'ouvrage est entièrement bilingue, soit français-anglais, soit anglais-français, les deux éditions ayant été simultanément mises sur le marché. En outre, une édition sur microfiches est disponible. L'ensemble constitue un outil de travail absolument remarquable.

NUCLEAR PROPERTIES

WORLD SURVEY OF MAJOR FACILITIES IN CONTROLLED FUSION RESEARCH - 1976 Edition.

(1976, 868 pp, \$48, Special supplement of Nuclear Fusion, ISBN 92-0-139076-6). This is the third, updated and revised edition of the "World Survey of Major Facilities in Controlled Nuclear Fusion Research", published as a special supplement to "Nuclear Fusion". The purpose of this survey is to provide a broad and current outline of the research in controlled thermonuclear fusion (CTR). Thus, the scope of this third edition has been expanded to include fusion reactor design groups, fusion data centres, and more information on laser- and electron-beam fusion programmes. Only information received officially from contributing countries in response to a questionnaire has been considered for publication. All contributions

have been brought up to data, the information being as correct as possible up to June 1976. The survey consists of three parts: Part I - Detailed Information; Part B - Summarized Information; and Part C - Personnel Index. The latter, a new feature of this supplement, lists about 3500 names of researchers and is intended as a "Who's Who" in nuclear fusion. Entirely in English.

SOLUTION PROPERTIES

- * CHEMICAL TABLES. (1975, 476 pp, \$27, Halsted Division of Wiley, ISBN 0-470-63161-9). Compiled by Béla A. Nemeth. Contents, abridged: Atomic weights of the elements. Density of solutions of acetic acid; chloric acid; silver fluoride; caesium iodide; lithium iodide; sodium iodide; zinc chloride. Buffer mixtures of hydrochloric acid and glycine. Degree of dissociation of acids. Saturation pressure of water vapour. First aid measures for accidents.

SPECTRA COLLECTIONS

- * ORGANIC ELECTRONIC SPECTRAL DATA, Volume 11: Year 1969. (1975, 1057 pp, \$42, Wiley-Interscience, ISBN 0-471-68802-9), edited by John P. Phillips et al. Annual collection, published in formula order, of all the UV spectra of organic compounds reported in 89 journals. Approximately 25 000 entries. Lists of abbreviations used, journals abstracted and references quoted supplement the tables proper.

TABLES OF WAVENUMBERS FOR THE CALIBRATION OF INFRARED SPECTROMETERS. 2nd Edition. (1977, 220 pp, \$18.00, £9.00, Pergamon, Oxford), edited by A.R.H. Cole for the Commission on Molecular Structure and Spectroscopy of IUPAC. In 1961 the Commission on Molecular Structure and Spectroscopy published a volume of calibration data for infrared spectrometers which covered the region from 4300 cm⁻¹ down to 600 cm⁻¹. In 1973 coverage was extended from 600 cm⁻¹ down to 1 cm⁻¹. Now the collection has been further revised, making the best use of high resolution results, and integrating the far infrared data with the higher frequency values. As before, the material has been organised in two parts -- Part I for the moderately high resolution spectrometers used by physical chemists and physicists, and Part II for the smaller commercial instruments employed by organic and inorganic chemists. Much of Part II remains unchanged from the first edition, but the diagrams and tables of Part I have been completely replaced with improved material. The tables have been approved as standards by the Inter-Union Commission on Spectroscopy of ICSU, on which the International Unions of Astronomy, Chemistry and Physics are represented. Contents: Tables for the Calibration of High to Medium Resolution Spectrometers. Tables for the Calibration of Medium to Low Resolution Spectrometers. Appendices: i) Calibration program, ii) Refractive index of air. References. Author Index. Compound Index.

THERMODYNAMIC PROPERTIES

A NEW CORRELATION METHOD FOR THERMODYNAMIC DATA

applied to the vapour pressure curve of Argon, Nitrogen and Water (1976, 130 pp, £4, IUPAC Thermodynamic Tables Project Centre, London), by W. Wagner. [English translation of "Eine neue Korrelationsmethode für thermodynamische Daten angewendet auf die Dampfdruckkurve von Argon, Stickstoff und Wasser", a shortened version of the author's Habilitationsschrift, published in full in Fortschr. Ber. VDI-Z., Reihe 3, Nr. 39, 1974]. In spite of recent progress in the use of empirical equations to represent the thermodynamic properties of fluids, little advance has been made in the twin problems of selection of individual terms in an equation of state and other thermodynamic functions, and of the high correlation often found between them. The method proposed here by the author, when applied to vapour pressure equations of pure fluids, successfully overcomes the weaknesses of the more common regression techniques through the use of rigorous statistical tests. This new regression method now makes it possible to establish from comprehensive provisional formulae those terms most important in the representation of experimental data. It also makes available a powerful and highly objective means of establishing the "best" forms of correlating functions. The results of Dr. Wagner's work are not limited to the area of thermodynamics alone and should find application in many other branches of science. By translating this important work into English, it is hoped that it may be brought to the notice of a much wider audience than might otherwise have been possible. The translation is available in A4 format as a paper-back reproduction of typescript, from: IUPAC Thermodynamic Tables Project Centre, Chemical Engineering Dept., Imperial College of Science and Technology, London SW7 2BY, U.K.

STEAM AND AIR TABLES IN SI UNITS; including data for other substances and a separate Mollier chart for steam (1976, 127 pp, \$5.85, Hemisphere Publishing, Washington, D.C. ISBN 0-89116-004-3) compiled by Thomas F. Irvine, Jr. and James P. Hartnett, provides data from a variety of sources but all converted uniformly into SI units. Contents: Steam: properties at saturation temperatures; pressures; of superheated vapor; at the critical point. - Steam: density, specific heat, thermal conductivity, and viscosity. Thermal conductivity of water vapor. - Ammonia: properties at saturation temperatures. - Thermodynamic properties of various refrigerants. - Freon 11: properties at saturation temperatures. - Moist air: properties at saturation. Properties of air at low pressures. - Mercury: properties at saturation temperatures. - Conversion tables. Nomenclature. Mollier enthalpy and entropy chart for steam.

THE THERMODYNAMIC PROPERTIES OF WATER UP TO 1200 K AND 3000 BAR. (1976, £3, IUPAC Thermodynamic Tables Project Centre, London), by R. Pollak [English translation of Dr. Pollak's Ph.D. thesis "Die thermodynamischen Eigenschaften von Wasser - dargestellt durch eine kanonische Zustandsgleichung für die fluiden homogenen und heterogenen Zustände bis 1200 Kelvin und 3000 bar" University of the Ruhr, Bochum, 1974.] Methods of constructing empirical equations of state of high accuracy, such as are needed in steam power cycle design, have improved greatly since the International Skeleton Tables for Steam were constructed in 1963, and in this thesis Pollak applies

the most recent methods to water, the most difficult fluid of all to handle, and includes with the input data important experimental results obtained since 1963. The result is an equation for the Helmholtz free energy as a function of density and temperature which represents the liquid, the gas and the saturation region from the triple point to 1200 K, 3000 bar. The thesis discusses in detail the statistical methods used, the accuracy (and hence the weighting) of the experimental data, and compares the predictions of the resulting equation with the data for many different properties. The work is important to designers concerned with steam, since it replaces the existing "piece-wise" formulation by a single equation, with the facility that integration through the two-phase region produces values on either side of the saturation boundary which are thermodynamically consistent, and offers a substantial reduction in "look-up" time in computer calculations. The work is important to those concerned with other fluids, since it demonstrates the capabilities of the "extended BWR" type of equation when allied to the power of Wagner's method of statistical analysis of the significance of terms in the equation. The translation has been made jointly by the Thermodynamic Tables Project Centre and the U.K. Central Electricity Generating Board and has been edited by R. Pollak and Dr. S. Angus. The format is A4, paper-back reproduction of typescript and is available from: IUPAC Thermodynamic Tables Project Centre, Chemical Engineering Dept., Imperial College of Science and Technology, London SW7 2BY, U.K.

VAPOR-LIQUID EQUILIBRIUM DATA COLLECTION:

Aqueous-Organic Systems. (1977, 698 pp, DM 120, DECHEMA, Frankfurt/M, Federal Republic of Germany), by J. Gmehling and U. Onken, is the first volume of a new and ambitious chemical data series undertaken by DECHEMA to provide chemists and engineers with data for process design and development, in particular the necessary numerical values enabling them to predict the binary parameters representing the vapor-liquid equilibrium (VLE) of liquid mixtures. The present book is only Part 1 of Volume I and covers aqueous organic binary and ternary systems. When completed, Volume I will be comprised of 8 parts dealing with organic-organic systems, such as alcohols, aldehydes, ketones, ethers, esters, hydrocarbons, halides, sulfur and nitrogen compounds. The book consists of a very thorough and comprehensive introduction where the fundamentals of VLE calculations are outlined, following which the relevant data are given for 73 binary and 53 ternary compounds. These data include both experimentally-determined values taken from the literature and values calculated by some of the current correlation equations (Margules, van Laar, Wilson, NRTL, UNIQUAC). The parameters for these tables are also tabulated, as are the constants of the Antoine vapor pressure equation for the pure compounds. Whenever possible, the tables of data are accompanied by an equilibrium diagram from which the type of system can be perceived at once. The reliability of the data is indicated by the results of two different thermodynamic consistency tests. Volumes II and III in this series will appear later, being devoted respectively to "Critical Data of Pure Chemical Compounds" and "P-V-T Data of Liquids".

MISCELLANEOUS

COMPUTER-READABLE BIBLIOGRAPHIC DATA BASES:
A DIRECTORY AND DATA SOURCEBOOK. (1976, 814 pp, \$68.00, American Society for Information Science,

Washington, D.C.) compiled and edited by Martha E. Williams and Sandra H. Rouse, is a directory of 301 commercially available bibliographic data bases. The description of each data base includes: name of the data base, producer, distributor, generator, availability, size, frequency, scope, subject matter, types of documents covered, data elements, etc. Entries are arranged by alphabetical order of their acronyms. Four indexes are appended to allow easy consultation: subject, name (including acronym and synonym), producer, and processor. - The edition comes in a loose-leaf binder to accommodate future bi-annual updatings.

DE LA METROLOGIE FONDAMENTALE A SON APPLICATION INDUSTRIELLE. (1976, XV+328 pp, 120 FF, Editions A. Blanchard, 9 rue de Médecis, 75006 Paris). This introduction to theoretical metrology by Jean-Claude Engrand is intended for those non-specialists (students, technologists, engineers, etc.) who are likely to have to design, maintain or use measuring equipment. The first part of the book is devoted to measuring instruments and their characteristics. The second part defines the fundamental quantities and units, stresses the importance of dimensional analysis in metrology and lays down the rules for presenting results of measurements. The third and last part of the volume is a critical analysis of a set of results from a typical measurement operation: the overall accuracy is studied, the use of statistics in metrology is explained and illustrated, and the data supplied by the instruments are analyzed. - The book ends with a few examples of worked-out problems and a bibliography.

NEW JOURNALS

NATURAL RESOURCES FORUM is a new international quarterly published on behalf of the United Nations by D. Reidel Publishing Company, Dordrecht, Holland. It is primarily addressed to policymakers in an effort to acquaint them with the economic, scientific, technological, managerial and social aspects of energy, minerals and water resources development. In this endeavor to help those actively engaged in the management of natural resources, the *Forum* will examine ways and means of increasing supply by exploration, investment and the development of new technologies; simultaneously it will look at the possibilities of reducing demand, when desirable, through conservation, substitution and appropriate technology. The first issue of the *Forum*, dated January 1977 and comprising 88 pages, carries the following articles: J. Zwartendyk: Problems in interpretation of data on mineral resources production and consumption; Peter A. Rona: Plate tectonics and mineral exploration; Daniel A. Harkin: Systematic mineral exploration; Raymond F. Mikesell: Rate of exploitation of exhaustible resources; B.F. Bratchenko: Basis for the development of the coal industry of the USSR; D.G. Fallen Bailey: The bio-gas system: serious energy source or environmental fad; V.A. Ovcharenko: Prospects for more effective utilization of fuel through MHD.

PHYSIK DATEN / PHYSICS DATA. This bilingual publication was created under the aegis of ZAED, the Central Agency for Documentation in Nuclear Energy of the Federal Republic of Germany, to

facilitate user's access to all sorts of data collections or compilations, most of the time either unavailable or out of date or out of print or simply out of reach. The present series, *Physik Daten / Physics Data*, was conceived with the specific objective of relieving this shortcoming by periodically publishing data compilations from a variety of fields, all relevant to Physics. Periodicals devoted to data are sufficiently rare that the appearance of *PD/PD* be greeted with a special salute solely deserved so far by the *Journal of Physical and Chemical Reference Data* of the National Bureau of Standards. The data published in *PD/PD* may be experimental or theoretical. Each data compilation is published as a separate booklet and, in the case of large data collections, may also be obtained as a magnetic tape. - A special mention must be made of Issue No. 3 of the series which, by exception, does not contain data but gives a survey of all existing data compilations in the field of Physical Sciences. Each entry of *Data Compilations in Physics* contains full bibliographic details and, after having appeared in the main list by alphabetical order of its title, is cross-referenced in six successive indexes, viz. conferences, authors, subjects, report numbers, corporate sources and journals.

This Issue No. 3 of *PD/PD* will quickly find its place on the desks of Reference Librarians between the *International Compendium of Numerical Data Projects* of CODATA and the *Annotated Accession List of Data Compilations* of the NBS Office of Standard Reference Data. The Editors-in Chief for the whole series are H. Behrens and G. Ebel of ZAED. The individual issues published so far are as follows: *Physics Data*, 1-1, 1975: Survey Index of Pion-Nucleon Scattering Data, by K. Augenstein, G. Höhler, E. Pietarinen and H.M. Staudenmaier, 53 pp, September 1975; *Physics Data*, 2-1, 1976: Stopping Cross Sections of Elements with $Z=2$ to 87 for Li Ions with Energies between 80 keV and 840 keV, by W. Neuwirth, W. Peitsch and U. Hauser, 6 pp, 1976; *Physics Data*, 3-1, 1976: Data Compilations in Physics, by H. Behrens and G. Ebel, xii + 200 pp, 1976; *Physics Data*, 4-1, 1976: Compilation of Coupling Constants and Low-Energy Parameters, reprinted from *Nuclear Physics*, B-109 (1976), 90 pp, 1976; *Physics Data*, 5-1, 1976: Gases and Carbon in Metals (Thermodynamics, Kinetics and Properties). - Part 1: Alkali Metals, Alkaline Earth Metals, Light Metals, by E. Fromm, H. Jehn and G. Hörz, 26 pp, 1976; *Physics Data*, 6-1, 1976: Shapes of Beta Spectra, by H. Behrens and L. Szybisz, 43 pp, 1976.

PHYSICS AND CHEMISTRY OF MINERALS, a new quarterly journal published by Springer Verlag in co-operation with the International Mineralogical Association, aims at bridging the gaps between the various theories or techniques currently encountered in mineralogy and allied disciplines. - The nine articles making up the first issue deal, respectively, with the Kinetics and mechanism of transformations in iron-rich pyrrhotites (by G.V. Novikov et al.); Observation of growth defects in spodumene crystals by X-ray topography (by A. Authier and A. Zarka); Molecular orbitals of $\text{Si}_2\text{O}_7^{6-}$, etc. applied to clusters and X-ray spectroscopy data of silicates (by Yu.P. Dikov et al.); Compositional dependence of the hyperfine interaction of Fe-57 in anthophyllite (by F. Seifert); Tetrahedral bond length variations in sulfates (by S.J. Louisnathan et al.); Phase transitions and associated domains in Hexacelsian (by W.F. Müller); Temperature, pressure and composition: structurally analogous variables (by R.M. Hazen); Effects of shock pressures on calcic plagioclase (by R.V. Gibbons and T.J. Ahrens); Calculation of sub-solidus phase relations in carbonates and pyroxenes (by A. Navrotsky and D. Loucks).

* Grateful acknowledgement for the reprint of this review is given to *New Technical Books*, The New York Public Library, Fifth Avenue and 42nd Street, New York, NY 10018, USA.

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 x 210 mm, DM 30.—, US \$ 15.—, FF 75.—.

CODATA Newsletter

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 ; No 13 (Sept. 1974), 20 pp ; No 14 (June 1975), 12 pp ; No 15 (Nov. 1975), 16 pp ; No 16 (Mar. 1976), 16 pp ; No 17 (Feb. 1977), 20 pp ; No 18 (Sept. 1977), 20 pp.

CODATA Bulletin : Annual subscription : US \$ 20 or 100 French Francs.

No 1 (Oct. 1969), 12 pp, *Automated Information Handling in Data Centers*, US \$ 1.50, superseded by Bulletin No 4.

No 2, 5, 6, 7 and 10, superseded by Bulletin No 17.

No 3 (Dec. 1971), 28 pp, *A Catalog of Compilation and Data Evaluation Activities in Chemical Kinetics, Photochemistry and Radiation Chemistry*, US \$ 3.50.
(Report of the CODATA Task Group on Data for Chemical Kinetics).

No 4 (Dec. 1971), 12 pp, *Automated Information Handling in Data Centers*, US \$ 1.50 2nd Edition.
(Report of the CODATA Task Group on Computer Use, Nov. 1971).

No 8 (Nov. 1972), 32 pp, *Geological Data Files : Survey of International Activity*, US \$ 3.50.
(Report of COGEOGDATA, 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*, US \$ 1.50.
(Report of the CODATA Task Group on Presentation of Data in the Primary Literature, Sept. 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*, US \$ 1.50.
(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*, US \$ 1.50.
(Report of the CODATA Task Group on Data for Chemical Kinetics).

No 14 (Feb. 1975), 180 pp, *Proceedings of the Fourth International CODATA Conference on the Generation, Compilation, Evaluation and Dissemination of Data for Science and Technology* (Tsakhkadzor, U.S.S.R., June 1974), US \$ 17.00.

No 15 (March 1975), 32 pp, *Man-Machine Communication in Scientific Data Handling*, US \$ 5.00.
(Proceedings of the Symposium sponsored by the CODATA Task Group on Computer Use, Freiburg im Breisgau, F.R.G., July 1973).

No 16 (October 1975), 32 pp, *Study on the Problems of Accessibility and Dissemination of Data for Science and Technology*
(Report of the CODATA Task Group on Accessibility and Dissemination of Data), US \$ 5.00.

No 17 (Jan. 1976), 12 pp, *Key Values for Thermodynamics, 1975*, US \$ 1.50.
(Report of the CODATA Task Group on Key Values for Thermodynamics).

No 18 (April 1976), 44 pp, *Abstracts - Fifth International CODATA Conference*, US \$ 5.00.

No 19 (June 1976), 22 pp, *Flagging and Tagging Data*, US \$ 5.00.
(Report of the ICSU AB/CODATA Joint Working Group).

No 20 (Sept. 1976), 16 pp, *Recommendations for Measurement and Presentation of Biochemical Equilibrium Data*, US \$ 5.00.
(Report of the ICSU Interunion Commission on Biothermodynamics).

No 21 (Oct. 1976), 122 pp, *Proceedings of the Plenary Sessions Fifth International CODATA Conference*, US \$ 7.50.

No 22 (March 1977), 8 pp, *Key Values for Thermodynamics 1976*, US \$ 1.50.
(Report of the CODATA Task Group on Key Values for Thermodynamics).

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

No 24 (June 1977), 42 pp, *CODATA Directory of Data Sources for Science and Technology, Chapter 1 : Crystallography*, US \$ 10.

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