

# 32 CODATA / NEWSLETTER

**APRIL 1985**

## **INT'L OTTAWA CODATA CONFERENCE**

On CODATA's 20th anniversary (1966-1986), its Tenth International Conference will be held in Ottawa, Canada. The theme of the 14-17 July 1986 Conference is "Computer Handling and Dissemination of Data."

The conference will be organized around four multidisciplinary aspects:

- computerized databases--technology and management;
- computer techniques in data and systems analysis;
- international aspects--data needs and flow across national boundaries;
- data structures, validation, robustness, graphics, etc.,

and a dozen more definitively focussed symposia involving:

- numerical information systems in materials science, technology, and industry (biotechnology, resources, process control);
- numerical information processing in the biosciences (epidemiology, toxicology, etc.);
- numerical data processing and dissemination in the geosciences (space- and time-dependent data, modeling, exploration, resources);
- artificial intelligence, expert systems;
- data for advanced technology;
- environmental impact;
- trade-offs (mainframe, networking, PC's, etc.).

### **Call for Papers**

Users of data, as well as those involved in data compilation, data evaluation, and data handling are invited to submit contributions on subjects within the scope of the Conference. To facilitate discussion and interchange of ideas, all contributed papers will be presented as posters. In addition to the presentation of posters, workshops will be organized in which groups of related posters will be discussed with an appointed chairman after the poster sessions.

The titles of proposed posters should be submitted as soon as possible to the Program Committee Chairman, Prof. C.B. Alcock (Dept. of Metallurgy and Materials Science, University of Toronto, Toronto, Ontario, Canada M5S 1A4).

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## **HIGHLIGHTS**

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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 interdisciplinary basis, CODATA seeks to improve the quality, reliability, processing, management, and accessibility of data of importance to science and technology.



## Scientific Software Survey

The periodical, *Spectrochimica Acta*, Part A, has introduced an interesting new innovation—a Software Survey Section—to encourage the open exchange of information on software programs unique to their professional field. With the rapid penetration of computers into academic and industrial institutions has come a parallel increase in the number of scientists and researchers designing their own software. The existence of much of this software remains unknown to even those who could most benefit from its use. The editors believe that a professional journal is the best place to share such information.

Interested potential contributors should note that their information will reach thousands of colleagues who may benefit from their work—and may possibly offer suggestions for further enhancements to their software. They should contact: Professor J.I. Steinfeld, Editor, Department of Chemistry, 2-221, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139.

## IAMAP/IAPSO Assembly

The IAMAP/IAPSO Joint Assembly is sponsored by the International Association of Meteorology and Atmospheric Physics (IAMAP) and the International Association for the Physical Sciences of the Ocean (IAPSO) of the International Union of Geodesy and Geophysics (IUGG).

Subjects for discussion include: CO<sub>2</sub> in the Ocean/Atmosphere System; Monitoring the Ocean/Atmosphere System; Modeling the Global Ocean/Atmosphere Climate System; Heat and Water Budgets; Monsoon Circulations in Ocean and Atmosphere; Precipitation Session on Meteorology and Physical Oceanography; Formation of the Main Ocean Thermocline; Low Frequency Dynamics in Mid-Latitudes; Dynamics of the Mixed Layer; Variations of Sea Level; Physical and Chemical Structure of the Ocean; Dynamics and Thermodynamics of the Equatorial Ocean; Atmospheric Chemistry and Climate; Long-Range Transport and Distribution of Trace Substances in Remote Regions; Clouds and Radiation; Nowcasting; Planetary Boundary-Layer Physics; Role of Air/Sea Interaction in Mesoscale Development; Convective Processes and their Feedback onto the Large-Scale Motion; Weather Forecasting in the Tropics; Comparative Climatology of the Terrestrial Planets; Clouds in Planetary Atmosphere; Remote Sensing Over the Polar Regions; Polar and Midlatitude Weather Systems; Variability of Aerosol Optical Properties; Climate Effects of Nuclear War; Tracing Large-Scale Motions Over the Oceans by Measurements of Atmospheric Electricity.

## Turing Tackles Information Technology

The Turing Institute, a self-styled "center of excellence in advanced information technology" in Glasgow, Scotland, was formally opened in December by Mr. Geoffrey Pattie, UK Minister of State for Industry and Information Technology. With the help of start-up funds from the Scottish Development Agency and with working capital provided by subscribing industrial companies, the institute promises elaborate services, including intensive training, discounted use of commercial and non-commercial software, library and information services, a "confidential" quarterly newsletter, and consultancy.

The Department of Trade and Industry (DTI) contributes about £ 250 million to industry's £ 100 million, and a government spokesman says that this is ample proof of DTI's eagerness to encourage this kind of research". It is debatable whether private institutions such as the Turing Institute and restricted retraining initiatives such as Journeyman are seriously analogous—despite department claims—to the substantial investment in artificial intelligence research and development in West Germany, Japan, and the United States; however, these provisions for accelerated "technology transfer" may mean that DTI is not content to rest on the United Kingdom's traditional excellence in the field of machine intelligence.

## Carbon Dioxide Role

The United Nations Environment Programme (UNEP), the World Meteorological Organization (WMO), and the International Council of Scientific Unions (ICSU) are undertaking a second joint assessment of the role of carbon dioxide in climate variations. (The first was in November 1980.) The second joint assessment meeting is planned for October 1985 in Villach, Austria, at the invitation of the Government of Austria. Participation is by invitation only. Participants will be limited to representatives of governments having major CO<sub>2</sub> climate research programs, invited experts, those associated with the UNEP/WMO-sponsored CO<sub>2</sub>-related research programs, and organizations involved in the World Climate Program.

The assessment will involve three working groups:

- the Carbon Cycle and future concentration of atmospheric CO<sub>2</sub>;
- physical impacts of increasing atmospheric CO<sub>2</sub> and the detection of climate change;
- impacts on terrestrial and marine ecosystems.

## Referral Data Base Task Group

Launched at Paris in February as an ad hoc committee, the Task Group met to establish a general approach and a realistic time scale for the creation of a prototype online version of the *CODATA Directory of Data Sources for Science and Technology* and the *Unesco/CODATA Inventory*. Building this prototype system will provide the opportunity to examine the various issues involved in satisfying the long-term objective of setting up and maintaining an online directory of data sources for science and technology.

Proposed approaches to automating these publications included D. Laurent's design for combining entities with their attributes and relationships in a DBMS approach and keying this to a free-field textual searching and F.J. Smith's advocacy of a more nearly total free-field approach and subsequent inversion.

The group concluded that any online system of the *Directory* and *Inventory* should have the capability to provide three major outputs: ease in preparing current and updated publications, online searching capabilities, and an automated distributable file. A common record for the prototype system will be established.

In order to better examine the relative merits of the two approaches (namely, a free-field approach on an inexpensive, transportable micro-computer versus a more highly structured approach on a larger machine), two experiments in building prototype systems will be run in parallel on a sample file appropriately formatted for each of these experiments. The sample will be loaded onto an IBM PC using a package for free-field searching (MICROVERT), and independently onto the Unesco DBMS (CDS/ISIS). The Task Group will analyze the results of typical queries (provided by NBS), using each approach, and examine other related issues, including the user friendliness, ease of use, the specialized coding for computer typesetting, the need/use/development of a thesaurus, and the relative cost and transportability of the systems and the database.

The composition of the Task Group has been designated as E.F. Westrum, Jr. (Chairman), D. Laurent, B.B. Molino, and F.J. Smith. In addition a group of consultants is being formed.

## Chihara Directs JAICI

Dr. Hideaki Chihara was named director of the Japan Association for International Chemical Information in 1971. Dr. Chihara is a professor of physical chemistry at Osaka University.



## Executive Committee Actions

A summary of the major actions taken at the 29th CODATA Executive Committee Meeting (Paris, 6-7 February 1985) would include:

- Plans for the program and local arrangements for the 10th CODATA Conference (14-17 July 1986) and 15th General Assembly (18-19 July 1986) were approved. The Conference will be held at the Westin Hotel, Ottawa, Canada, with rooms available at the hotel and university residences. The First Circular is to be mailed in March 1985; the Second Circular in September 1985; and abstracts will be due 15 December 1985. There will be 20-25 invited talks; all contributed papers will be presented as posters, with a workshop-type discussion to follow each poster session.

- A budget for 1985 was approved, which allocated \$74,500 for Task Group activities (actual expenditures for Task Groups in 1984 were about \$39,000.).

- A revised dues scale for Supporting Organizations was approved and the benefits provided in each category were clarified.

- It was agreed to continue with the present Pergamon Press contract for publication of the *Bulletin* in 1986.

- An ad hoc group was established to advise the Executive Committee on the need for a formal Commission dealing with data dissemination and/or training activities. The members of this group are: D.G. Watson (Chairman), E. F. Westrum, Jr., H. Behrens, and W. Schirmer. The group will report at the February 1986 Executive Committee Meeting. Please send any comments to the group.

- A similar ad hoc group consisting of J.E. Dubois (Chairman), Y. Kamboyashi, J.R. Rumble, and another person to be selected, was established to advise on the need for a Commission to deal with broad problems of computer handling of data. Comments should be sent to the group. The Executive Committee will consider the reports of this group and the dissemination/training group and make a formal recommendation to the General Assembly in 1986.

- The Executive Committee agreed to accept the suggestion of the newly-formed International Council for Scientific and Technical Information (ICSTI) that CODATA become a member of ICSTI and vice versa. CODATA will apply for admission to ICSTI as a Class A Member and ICSTI will apply to become a Coopted Member of CODATA, with no financial exchange involved.

- A Working Group chaired by J.H. Westbrook was set up to prepare a brief glossary of terms and acronyms used in scientific and technical data handling.

- It was agreed to explore having a workshop on nucleic acid and protein sequence data banks to be held in mid-1986. Dr. Rita Colwell was appointed chairman of the Organizing Committee, and she will work closely with the Protein Sequence Task Group. Joint sponsorship will be sought from the interested Unions and other bodies.

- The report of the Hybridoma Data Bank (HDB) Task Group was reviewed, and the Executive Committee agreed that CODATA should retain an association with the HDB during its two-year transition (1986-1987) from a prototype project to a fully operational one.

- After extensive discussion of the need for a formal advisory structure (i.e., Commissions) in the biosciences, geosciences, and other disciplinary areas, the Executive Committee decided that this is not required at the present time. Suggestions and criticisms from the relevant Unions in these areas will continue to be encouraged.

## CODATA CALENDAR

1985

<b>April</b>	
15-16	Materials Data Systems for Engineering. Paris, France.
<b>May</b>	
9-10	Task Group on Phase Equilibrium Data. Paris, France.
<b>June</b>	
24-29	Regional Meetings on Protein Sequence Data Banks. Tokyo, Osaka, and Kyoto, Japan.
17-22	Software for Protein Sequence Data Banks. Georgetown, U.S.A.
---	Working Group on Data for Surveillance of Active Volcanoes. Tokyo, Japan.
<b>August</b>	
15-16	Task Group on Geothermodynamics. State College, PA and Reston, VA, U.S.A.
<b>September</b>	
5-7	Vapor-Liquid Equilibria in 1-Alkanol and n-Alkane Mixtures. Paris, France.
5-7	Task Group on Critically Evaluated Phase Equilibrium Data. Paris, France.
5-8	Task Group on Data for the Chemical Industry. Paris, France.
9-10	Chemical Thermodynamic and Thermophysical Properties Data Bases. Paris, France.
11-13	Critical Evaluation and Prediction of Phase Equilibria in Multicomponent Systems. Paris, France.
---	Workshop on Materials Data Systems for Engineering. F.R.G.
---	Working Group on Data for Surveillance of Active Volcanoes. Catania, Italy
<b>December</b>	
9-11	Task Group on a Hybridoma Data Bank. Nice, France.

1986

<b>May</b>	
---	Workshop on Standardization of Environmental Data (Tentative). Toronto, Canada.
<b>July</b>	
14-18	10th International CODATA Conference. Ottawa, Canada.
18-19	15th General Assembly. Ottawa, Canada.

## CODATA Personalities in the News...

Professor **PAUL MELCHIOR** has been designated Director of l'Observatoire Royal de Belgique by His Royal Majesty the King upon the proposal of the National Minister of Education. Professor Melchior was CODATA's President from 1974 to 1978. We congratulate him on his promotion.



## CODATA Task Group on Geothermodynamic Data

Prof. I.L. Khodakovsky of the V.I. Vernadsky Institute of Geochemistry and Analytical Chemistry (Moscow, U.S.S.R.) organized in 1984 a Task Group on Geothermodynamic Data for the purpose of developing plans for the creation of key values and international tables of the thermodynamic properties of minerals and mineral-forming substances.

**Members of the Task Group include:**

- Dr. B.S. Hemingway (Geological Survey, Reston, VA, U.S.A.)
- Dr. C. Monnin (Laboratoire de Mineralogie, Toulouse, France)
- Dr. B.R. Staples (Bureau of Mines, Albany, OR, U.S.A.)
- Prof. V.S. Urusov (Moscow State University, Moscow, U.S.S.R.)
- Prof. B.J. Wood (Northwestern University, Evanston, IL, U.S.A.)

**Consultants include:**

- Prof. D.G. Fraser (Oxford University, Oxford, England)
- Prof. N. Kishima (Okayama University, Misawa, Japan)
- Prof. V.A. Medvedev (Institute for High Temperatures, Moscow, U.S.S.R.)
- Prof. E.F. Westrum, Jr. (University of Michigan, Ann Arbor, MI, U.S.A.)

Other consultants may be added later.

The first meeting of the Task Group was held at Hamilton, Ontario, Canada, in August 1984, the second in Suzdal, U.S.S.R., as described elsewhere in this issue.

## IAGC Working Group on Thermodynamics of Natural Processes

The International Association of Geochemistry and Cosmochemistry (IAGC) has created a working group to deal with the thermodynamics of natural processes. It is composed of:

**Officers** - Prof. R.M. Garrels, Honorary Chairman (U.S.A.), Prof. I.L. Khodakovsky, Chairman (U.S.S.R.), Dr. B. Hemingway, Vice Chairman (U.S.A.), Dr. V. Dorofeeva, Secretary (U.S.S.R.),

**Subgroup Chairmen** - Dr. B. Fegley (U.S.A.), Dr. B. Fritz (France), Dr. B. Hemingway (U.S.A.), Dr. I.D. Ryabchikov (U.S.S.R.), Dr. B.R. Staples (U.S.A.), Prof. Y. Tardy (France), Prof. V.S. Urusov (U.S.S.R.), Prof. V.N. Zharkov (U.S.S.R.),

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## First All-Union Symposium on "Thermodynamics in Geology"

In a modern tourist complex in the historical town of Suzdal, about 205 scientists concerned about thermodynamics, planetary- or terrestrial-geoscience, or some combination of the above met to discuss the state of their science. Poster and plenary sessions dealt with:

- thermophysics and thermochemistry of minerals
- thermodynamics in magmatic systems
- thermodynamics of mineral equilibrium
- thermodynamics of hydrothermal systems
- thermodynamics of processes of formation of planetary substance and the pre-planetary nebulae
- thermodynamic bases for models of ore-forming processes.

Although most of the lecture and fast-paced poster sessions were presented by Soviet scientists, approximately twenty foreign scientists from the German Democratic Republic, Bulgaria, Rumania, France, Norway, and Japan and three from the United States participated. The very lively discussions following most presentations attested to the developing interest in the application of thermodynamics to natural processes.

In his opening address Prof. Khodakovsky gave due consideration to the prospects of future trends and development and emphasized--as did many other speakers--the need for reliable critically evaluated data on mineralogical and petrological systems.

The Honorary Chairman was Academician D.S. Korzinsky. Prof. I.L. Khodakovsky and Vice Chairmen V.A. Zharikov and I.D. Ryabchikov (both Corresponding Members of the Academy of Sciences) were assisted by three Scientific Secretaries and a distinguished organizing committee.



Suzdal Symposium logo.

## IMA Commission on Mineral Thermodynamics

Under the chairmanship of Professor L.L. Perchuk of the Institute of Experimental Mineralogy, U.S.S.R. Academy of Sciences, Chernoglovka, an International Mineralogical Association on Thermodynamics of Minerals has been established. It is composed of seven additional members: Prof. Sh. Banno (Japan), Prof. N.D. Chatterjee (F.R.G.), Prof. J. Ganguly (U.S.A.), Prof. D.H. Lindsley (U.S.A.), Prof. Y. Matsui (Japan), Prof. A.B. Thompson (Switzerland), Dr. B.J. Wood (U.S.A.). This group also has goals not unrelated to those of the two groups mentioned above.

## Task Group on Protein Sequence Data Banks

The annual meeting of the Task Group on Coordination of Protein Sequence Data Banks was held at the CODATA Secretariat in Paris on 4-5 March 1985. The first major activity of this group is the preparation of an Index of Databases of Protein Sequences and Related Information. Most of the information has now been gathered and the final document will be drafted shortly. The Task Group plans to update the Index two years after initial publication.

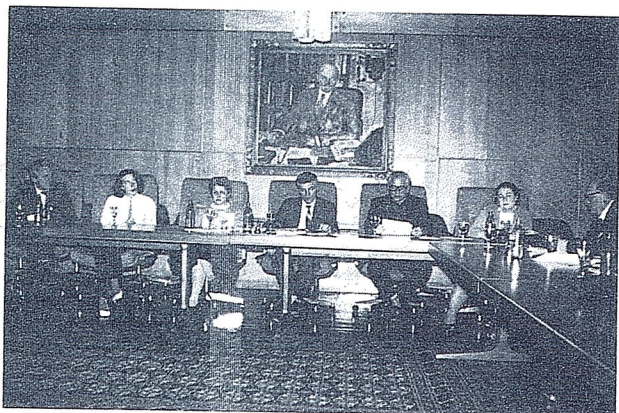
One of the interests of the Task Group is to foster awareness of Protein Data Banks and of the opportunities for cooperation. To this end, the Task Group will be organizing scientific programs in various locations. The first such program was presented at the Institute Pasteur in Paris on 4 March 1985; the speakers were A. Tsugita, J.-M. Claverie, W.C. Barker, B. Keil, A.M. Lesk, and Masao Kotani. In June, members of the Task Group will join with other guests and Japanese colleagues to participate in a Lecture Meeting in Tokyo followed by a symposium and workshop in Osaka and in Kyoto.

The Task Group will also in the next year continue its efforts to devise an exchange format for protein sequence data, and will undertake additional projects to foster training of scientists in the use of protein databases and associated software.

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and **National Representatives** - Dr. S. Arnorsson (Iceland), Dr. H. Bilinski (Yugoslavia), Dr. J. Cadek (Czechoslovakia), Dr. B. Hemingway (U.S.A.), Dr. J.T. Iiyama (Japan), Prof. I.L. Khodakovsky (U.S.S.R.), Dr. G.K. Kirov (Bulgaria), Dr. T.M. Seward (New Zealand), Dr. P. Tremaine (Canada), Dr. P. Vieillard (France), Prof. R.F. Wollast (Belgium).





The "head" table at tripartite geothermo data meeting (l to r): Prof. V.S. Urusov, Irena Platonova, Irena Drozdevskaya, Prof. I.L. Khodakovsky (Chairman of CODATA & IAGC groups), L.L. Perchuk (Chairman, IMA Commission), Dr. V. Dorofeeva (Secretary, IMA Commission), and Prof. V.A. Medvedev.

### Tripartite Group on Geothermodynamic Data

Amid Suzdal's (U.S.S.R.) wintry splendor and religious architectural monuments, members of CODATA's Task Group on Geothermodynamics (1) met with representatives of the Working Group on Thermodynamics of Natural Processes of the International Association of Geochemistry and Cosmochemistry (IAGC) (2) and the Commission on Thermodynamics of Minerals of the International Mineralogical Association (IMA) (3). The ensuing discussions were focused on the plan for preparation of international tables of thermodynamic properties of minerals and mineral-forming substances.

Among initiatory activities are the development of

- key values for iron and manganese oxides and related aqueous systems
- procedures for treatment of solid solutions, melts, and vitreous phases
- treatment of data on order/disorder in solid solutions, in vitreous phases, and in pure mineral compositions (especially on synthetic samples)
- procedures for extrapolation of thermodynamic properties to terminal-member compositions and to other desired compositions
- Debye-Hückel slopes for consistent treatment of data for aqueous systems over wide ranges of pressure and temperature
- reconciliation of calorimetric and equilibrium data on solid solutions and melts.

In many respects the developments made by the CODATA Task Group on Thermodynamic Tables--and the former CODATA Task Group on Key Values--provide an essential base, framework, and procedures which can be supplemented and enlarged upon for geothermodynamic tables. However, in some of the areas mentioned above, problems of prime concern to mineralogical and petrological applications require new developments.

Meetings begun in Suzdal on March 14 were followed by several days of working sessions in Moscow.

Organization of the sessions was primarily provided by Dr. Igor L. Khodakovsky who chaired the sessions. Participants (affiliation indicated) in the tripartite meeting included: Dr. V. Dorofeeva (2), Prof. D.G. Fraser (1), Prof. I.L. Khodakovsky (1, 2), Dr. G.K. Kirov (2), Prof. N. Kishima (1), Prof. V.A. Medvedev (1), Dr. C. Monnin (1), Prof. L.L. Perchuk (3), Dr. B.R. Staples (1, 2), Prof. V.S. Urusov (1,2), Dr. P. Vieillard (2), Prof. E.F. Westrum, Jr. (1).

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## CODATA PROFILE

**Igor L'vovich Khodakovsky**, a rapidly developing young specialist in the thermodynamics of terrestrial and extraterrestrial geochemical processes, is becoming increasingly prominent in CODATA affairs. Already Professor Khodakovsky has authored--or co-authored--more than 170 experimental and scientific papers. No stranger to the critical evaluation of thermodynamic data, he has long been involved with Professors Lev Gurvich and Vadim A. Medvedev and a distinguished group of other evaluators as editor and co-author in the production of the ten-volume series of important thermodynamic tables--the Soviet Thermal Constants of Substances. Igor co-authored the Russian Handbook of Thermodynamic Data (for Geologists) with G.B. Naumov and V.N. Ryzhenko in 1971. It was translated into English in the U.S.A. in 1974. He is co-author of an IAEA monograph (in preparation) on actinide compounds in solution, a member of the Chemical Thermodynamics Council of the Academy of Science Presidium and of other national compilation and estimation endeavors.



His studies in the physical chemistry of the Venusian planetary surface rock-atmosphere interaction are recognized internationally, and he is a frequent visitor to America and elsewhere to present reports on recent progress in some aspects of his wide-ranging program. He is the principal creator of the renowned online database DIANIK which parallels the Soviet chemical-thermodynamic database IVTAN-THERMO in providing--through the Vernadsky Institute--thermophysical and thermochemical data on geochemical substances, systems, solid solutions, magmatic solids, etc.

Igor has been designated Chairman of the CODATA Working Group on Geothermodynamic Data by CODATA President W.W. Hutchison.

He was born in 1941, graduated from Moscow's Lomonosov State University in 1963, and was admitted to the Vernadsky Institute. In 1969 he obtained a master's degree and in 1975 a doctorate in chemical science. Igor did his doctoral research under the inspired leadership of Academician A.P. Vinogradov of the Vernadsky Institute on the subject of experimental and theoretical investigation of hydrothermal systems in 1975.

For the past eight years he has been Chief of the Laboratory of the Thermodynamics of Natural Processes at the U.S.S.R.'s Academy of Sciences Institute of Geochemistry and Analytical Chemistry, named in honor of V.I. Vernadsky. This laboratory is engaged in experimental studies on the thermodynamic properties of minerals and of components of aqueous electrolyte solutions as well as the physicochemical parameters of rock and ore-forming processes by using computer modelling of formation of meteoric matter, of atmosphere formation on terrestrial planets, of the interaction between (for example, on Venus) such atmospheres and surface rocks, and of hydrothermal processes in ore deposits. He is assisted in these endeavors by twenty co-workers with specialization in various fields.

His charm as a personable human being is exceeded only by that of his wife Tatiana and his six-year-old daughter Julia (who distributed "certificates" to foreign conferees at the recent Suzdal "Thermodynamics in Geology" conference organized by her father). He also has a son, Gleb. Although devoted to his family, Professor Khodakovsky's interests are predominantly and enthusiastically scientific.



# International Meetings on Phase Equilibrium and Related Property Data



Organized by the Institut de Topologie et de Dynamique des Systèmes (ITODYS), Université Paris VII - CNRS - under the sponsorship of the International Union of Pure and Applied Chemistry (IUPAC) and four Task Groups of the Committee on Data for Science and Technology (CODATA), these meetings represent a scientific event of such magnitude that they have--not inappropriately--been described as a "thermodynamics festival." The endeavors of the International Advisory and Scientific Program Committees headed by Prof. J.E. Dubois and Dr. H.V. Kehiaian, respectively, and an Organizing Committee chaired by Dr. Kehiaian have resulted in an extensive program over three consecutive meetings. The third circular--now being circulated--contains full general information and details for participation. Today's users of phase equilibrium and related property data expect the data to be available from computerized, evaluated databases without their having to retrieve and assess them from dispersed primary literature sources. Hence, challenges regarding the reliability of phase equilibrium data stored in databases, the necessity for establishing the best possible data correlation and prediction methodologies, and the homogenization of phase equilibrium and related property database contents must be met if data gaps are to be spanned and if further development in design work and theory is to be achieved.

Three consecutive meetings are scheduled:

● (1) THE SECOND INTERNATIONAL IUPAC WORKSHOP ON VAPOR-LIQUID EQUILIBRIA IN 1-ALKANOL + n-ALKANE MIXTURES, 5-7 September 1985;

● (2) THE FIRST CODATA SYMPOSIUM ON CHEMICAL THERMODYNAMIC AND THERMOPHYSICAL PROPERTIES DATABASES, 9-10 September 1985;

● (3) THE SECOND CODATA SYMPOSIUM ON CRITICAL EVALUATION AND PREDICTION OF PHASE EQUILIBRIA IN MULTICOMPONENT SYSTEMS, 11-13, September 1985.

All three meetings will be held at the Maison Internationale (International House), which is one of the many buildings of the Cité Internationale Universitaire de Paris in southern Paris. The official languages are French and English.

Prospective presenters and database demonstrators are requested to

submit a short abstract to Dr. H.V. Kehiaian as soon as possible so that a camera-ready extended version in appropriate format will reach Paris by 1 June 1985. Dr. Kehiaian may be contacted at:

Dr. Henry V. Kehiaian  
Université Paris VII-CNRS  
Institut de Topologie et de  
Dynamique des Systèmes  
1, rue Guy de la Brosse  
75005 Paris, France  
Telephone: +33 1 7071165 or  
3362525, ext. 6053  
Telex: 630553 F  
Cable: ICSU PARIS 016

A terse summary of communications already received for the three meetings is:

## Meeting 1

For pure components: Single- and Multiproperty Compilations, Correlations and Predictive Methods

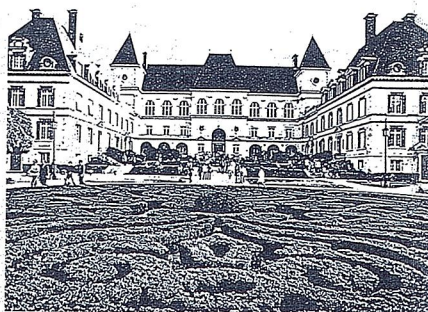
For mixtures: VLE, LLE, LSE, CPE, PVT; Single- and Multiproperty Correlations, etc; Theoretical Models and Predictive Methods.

## Meeting 2

Multiproperty Organic/Inorganic Databases; Multiproperty Nonelectrolyte/Organic Databases; Multiproperty Inorganic Databases; Single Property Nonelectrolyte/Organic Databases; Review and Correlations; six discussion sections.

## Meeting 3

General/Phase Equilibria and Related Properties; General/Thermodynamics of Multicomponent Systems; Experimental Techniques; PVT/LVE/Solubility of Gases in Liquids; SLE/Solubility of Solids in Liquids; Multiproperty Correlations; SLE/LLE; General/Theoretical Models; PVT/High Pressure VLE; Low Pressure VLE/Gas Solubilities; Critical Reviews/Recommendations.



*Maison Internationale--the site of the three international meetings on phase equilibrium and related property data.*

## Ottawa Conference...

(continued from page one)

Abstracts will be required by December 15, 1985. Authors will be notified before February 1, 1986 about the acceptance of their contribution and will receive instructions on providing the full text at that time.

## Database Demonstrations and Exhibitions

Facilities for scientific and technical source database producers to give demonstrations during the afternoon of each day of the conference will include use of a terminal and data networks for access to a host mainframe computer or, for microcomputer databases, table space and power. Those who wish to participate in such online demonstrations or provide commercial displays of relevant equipment and would like to receive further information should so indicate to the Conference Secretary.

## Intent to Attend the Conference

Persons who wish to receive the second circular and/or additional information are requested to contact:

Mrs. Lois Baignée, Executive  
Secretary CODATA '86  
Conference Services  
National Research Council of  
Canada, Montreal Road  
Ottawa, Canada K1A 0R6

## Conference Hosts

The Conference will be hosted by The National Research Council of Canada (NRC) with the collaboration of The Royal Society of Canada, and the Ministry of Industry and Trade of the Government of Ontario.

The Scientific Program Committee is chaired by Prof. C.B. Alcock of Toronto, Canada, who is also the Chairman of the Canadian National Committee for CODATA. Dr. G.H. Wood of NRC (Ottawa) chairs the local organizing committee.

The Westin Hotel at Ottawa will be the site of the Conference.

## Accommodations

Blocks of rooms have been reserved at the Westin Hotel and the University of Ottawa. Several other hotels are within easy walking distance.

## Volcano Warning Network

A radio-linked network--to provide warning of a change in geochemical parameters of fumarolic gases and to warn of impending volcanic activity--installed in certain Aeolian Islands is described by M. Carapezza, P.M. Nuccio, and M. Valenza of the University of Palermo.

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## New CODATA Publications

- CODATA Brochure (in French).<sup>a</sup>
- CODATA (Name & Address) Directory, 1985 Edition.<sup>a</sup>

## Books for the Bookshelf . . .

The Carbon Dioxide Information Center has now completed eight numeric data packages (NDP) and one computer model package (CMP). The contents of these packages are described briefly below.

● **NDP-001.** Atmospheric CO<sub>2</sub> Concentrations--Mauna Loa Observatory, Hawaii, 1958-1983.

● **NDP-002.** Tree Ring Chronology Indexes and Reconstructions of Precipitation in Central Iowa, USA.

● **NDP-003.** Surface Air Temperature Anomalies for the Northern Hemisphere, 1881-Present.

● **NDP-004.** Transient Tracers in the Oceans (TTO) Hydrographic Data and Carbon Dioxide Systems.

● **NDP-005.** Atmospheric CO<sub>2</sub> Concentrations--The NOAA/GMCC Flask and Continuous Sampling Network.

● **NDP-006.** Production of CO<sub>2</sub> from Fossil Fuel Burning by Fuel Type, 1860-1982.

● **NDP-007.** Atmospheric CO<sub>2</sub> Concentrations--The CSIRO (Australia) Monitoring Program from Aircraft for 1972-1981.

● **NDP-008.** Seasonal Tropospheric and Stratospheric Temperature Anomalies, 1958-1983.

● **CMP-002.** The IEA/ORAU Long-Term Global Energy-CO<sub>2</sub> Model.

● **Metals and Alloys in the Unified Numbering System,** Third Edition.<sup>c</sup>

● **Handbook of Data on Organic Compounds.** R.C. Weast and M.J. Astle, Editors.

● **Data Base Alert.**<sup>e</sup>

● **Awareness of Information Sources.** Theodore B. Selover, Jr. and Max Klein, Editors.<sup>f</sup>

\* Further details on content, identification, price, source, etc. (if available) for above items are referenced below.

a. Available from the CODATA Secretariat.

b. Obtainable from the Carbon Dioxide Information Center, Oak Ridge National Laboratory, P.O. Box X, Oak Ridge, Tennessee 37831-2008, U.S.A.

c. The new and revised, third edition of Metals and Alloys in the Unified Numbering System has been completed and is now available (ASTM Data Series, DS 56B). Listings for over 6500 metals and alloys, as compared to over 3500 entries in the second edition, are included in the handbook as well as descriptions, chemical compositions, and more than 3000 cross-referenced specifications for each entry. Hard cover: US \$75; soft cover: US \$65. Available from ASTM Sales Services. PCN 05-056002-01.

d. Contents: chemical and physical data on 240 000 compounds (e.g., synonym(s), melting point, boiling point, molecular formula, molecular weight, line formula, refractive index, density, color, crystalline form, specific rotation, solubility, structural formulas, empirical formulas, and spectra references (UV, NMR, infrared and mass spectra references are provided to at least one major collection of spectra)). Two volumes. (Due 1985.) 7 1/2" x 10". c. 2000 pp. US \$200 (inside U.S.); US \$230 (outside U.S.). CRC Press, Inc., 2000 Corporate Blvd. NW, Boca Raton, FL 33431. ISBN-0-8493-0400-8.



Undaunted conferees at tripartite geothermodynamic data meeting prepare at Suzdal's tourist/conference complex for the return to Moscow.

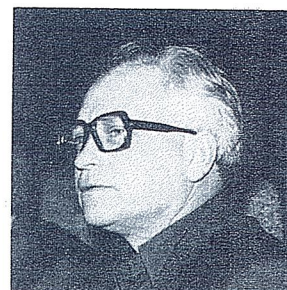
## Geothermodynamics Groups

(continued from page 5)

In addition a number of other conferees were invited to join in the initial deliberations. These included: Prof. Ch. Balarev, Prof. J. Holm, Prof. G. Hovis, Prof. J. Ionescu, Dr. R. Nauman, Dr. V. Seifert, and Dr. D.C. Tuan. At one session the observers swelled the attendance to 32 scientists.

Translators/interpreters from the Vernadsky Institute, Irena Brozalevskaya and Irena Platonova, greatly facilitated communication and Prof. Medvedev also provided expert commentary in several languages and, with Prof. Westrum, reviewed relevant CODATA activities. Dr. V. Dorofeeva and Dr. Yu. Semenov provided secretarial service.

Prof. L.L. Perchuk (IMA Commission Chairman) comments at tripartite data conference at Suzdal.



Professor Vadim Medvedev--a "bridge" between chemical and geochemical thermodynamics at Suzdal Conference.

e. News and reference service for database users and providers. Data Base Alert is part of Data Base User Service, a new service providing online access to database information. Monthly. Subscription: US \$48/year. Knowledge Industry Publication, Inc., 701 Westchester Ave., White Plains, N.Y. 10604. Tel: 800-431-1880. ISSN-0737-951X.

f. American Institute of Chemical Engineers Symposium Series, 237, Vol. 80. (1984.) Available from: American Institute of Chemical Engineers, 345 East 47 Street, New York, New York 10017.



## Nuclear Wallet Cards

The 1985 edition of Nuclear Wallet Cards may be requested from the National Nuclear Data Center (NNDC), Brookhaven National Laboratory, Upton, New York 11973, U.S.A. Wallet Cards contain nuclear properties, e.g., half-life, spin and parity, abundance, mass excess, and decay modes for all known nuclides and selected isomers, as well as many useful appendices.

The NNDC is responsible for data compilation, evaluation, and information services for neutron, charged-particle, and nuclear-structure physics. It maintains bibliographic, experimental, and evaluated data files for these three areas of physics and provides data services. The NNDC is responsible for the development, maintenance, promotion, and distribution of the reference nuclear databases, the Evaluated Nuclear Data File (ENDF/B), and the Evaluated Nuclear Structure Data File (ENDSDF).

The NNDC coordinates interlaboratory groups of experts to provide recommended values for nuclear data. In particular, these include the Cross Section Evaluation Working Group (CSEWG), representing over 20 U.S. laboratories and meeting annually to develop an internationally recognized database for nuclear energy applications, and the U.S.

Nuclear Data Network, consisting of low energy nuclear physics information centers, meeting annually to develop an internationally recognized database for nuclear energy research.

Periodically, the Center prepares publications from its computerized databases. The Center also prepares the monthly issues of Nuclear Data Sheet Journal published by Academic Press.

### --In Memoriam--

#### Dr. Ernst Becker

Dr. Ernst Becker, born in Darmstadt, was Professor of Mechanics at the Technical University of Darmstadt. He died on November 14, 1984 after a severe illness. He was an outstanding scientist and a popular lecturer. His passing is a great loss, for the Technical University of Darmstadt where he was active for more than 20 years, and for the whole scientific community.

His research interests involved continuum mechanics, gas dynamics, and rheology. His research led to the publication of five books and more than 60 papers. He had been the Delegate to CODATA from the International Union of Theoretical and Applied Mechanics from 1977 until his death.

(continued from page 6)

Due to the kind of activity as well as to the density of urbanization, there is a high risk of volcanic activity on the Aeolian Islands of Lipari and Vulcano. In recent years, especially on Vulcano, the geochemical surveillance of volcanic activity has been improved. Since 1978 the reducing capacity of fumarolic gases of Vulcano crater has been recorded on a continual basis.

In the last two years a new, computerized system for the remote monitoring of geochemical parameters has been developed. This, the first such network in the world, was realized in the Aeolian Islands. It is governed by a Central Unit--installed in Palermo--which cyclically interrogates, by radio, each of the three remote units (two located on Vulcano and one on Lipari). The system acquires and records the data, compares the values of monitored parameters (actually the temperature and the reducing capacity of fumarolic gases) to those pre-selected by the operator. Temperature is sensed by a platinum resistance thermometer housed in a teflon-coated stainless steel tube. The coulometric sensor for reducing capacity provides an electric signal proportional to the total concentration of oxidizable volcanic gases. Significant deviations from prescribed values can activate an alarm.

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