

# 44 CODATA / NEWSLETTER

**APRIL 1988**

## **CODATA COMMISSION ON INDUSTRIAL DATA**

### **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.

The Commission met in Zurich, Switzerland, February 1 and 2 with its full membership present.

The CODATA Materials Database Management Task Group work was reviewed. Its two-page quarterly newsletter now appears in English in the CODATA Newsletter (No. 3 in this issue) and should appear soon in Technische Rundschau. A Directory of Database Managers is being prepared.



*Participants in Zurich meeting of CODATA Commission on Industrial Data. (1 to r) seated: Westbrook, Abir, Kuznetsov; standing: Eckermann, Naylor, Schonholzer, Reynard, and Hiraishi.*

In a careful review of the Schluchsee CODATA Workshop (1985) recommendations it was noted that little activity had taken place on many of them, and means to publicize these matters more widely was sought. The outlook for the presentation of industrially important data considerations at the 11th CODATA International Conference (Karlsruhe, September 1988) were reviewed and that for the subsequent Conference

(continued on p. 10)



# VADIM MEDVEDEV

1924 - 1988

Professor Vadim Medvedev, member of the CODATA Task Group on Chemical Thermodynamic Tables, died in Moscow on 24 February 1988 at the age of 63 of a lung embolism. He was an expert of the highest rank in the data field. His erudition and intuition won him an indisputable reputation in scientific community of thermochemists.

Prof. Medvedev was born November 25, 1924 in Gorke, a small city in Byelorussia where his father was a professor at a well known Agricultural University. The family was forced to leave Gorke during the war, when Vadim was 16, and spent the war years in Sverdlovsk.

He entered Moscow State University in 1944 and graduated in 1949 in Radiochemistry. From 1949 until 1952 he was a post graduate student at the Institute of Combustible Minerals of the U.S.S.R. Academy of Science. At that time he studied the enthalpy of formation of several radicals, including OH, using explosion techniques in the spherical bomb. He presented his thesis in 1955 at Moscow State University. Since 1954 he has been involved in the evaluation of thermochemical data, later to be published in a "Reference Book: Thermodynamic Properties of Individual Substances."

Since 1963 he has been Assistant Chief Editor of "Thermal Constants of Substances," another important reference book, published by VINITI from 1963 until 1982. It was a large project in which more than 80 Soviet scientists participated. Medvedev was not only editor, but coordinated the whole project, and in 1984 was awarded the State Prize for this work.

In parallel with his work of data evaluation, Medvedev was doing experimental measurements in the field of fluorine calorimetry and solution calorimetry, and authored, with Leonidov, the first book on fluorine calorimetry. In 1969 he spent three months in Prof. Stig Sunner's laboratory in Lund, Sweden, working on solution calorimetry. Using both fluorine and solution calorimetry, Medvedev and his co-workers obtained the enthalpy of formation of many key substances including NO<sub>2</sub>, WF<sub>6</sub>, and SF<sub>6</sub>.

Since 1968, V.A. Medvedev has taken an active part in CODATA activities. He was a member of the Task Group on Key Values for Thermodynamics and later of the Task Group on Chemical Thermodynamic Tables. It is impossible to overestimate his input into the work of these groups and the resulting recommended key values for thermodynamics. He is

one of the editors of the book "CODATA Recommended Key Values for Thermodynamics" which is currently in press. In addition he was a consultant to the CODATA Task Group on Geothermodynamic Data. He participated in the work of IUPAC and was a titular member of the Commission on Thermodynamics.



At the time of his death, he was Head of the Thermochemical Laboratory of the Chemical Thermodynamic Department at the Institute of High Temperatures in Moscow where he had been working since its opening in 1963, first as Senior Scientist, then as organizer of the Thermochemical Laboratory, and later as head. He was a member of the Editorial Board of the Journal of Chemical Thermodynamics and participated in numerous international and All-Union Conferences, including CODATA Conferences from 1968 until the present. His paper submitted to the 11th CODATA Conference at Karlsruhe will be presented posthumously.

Medvedev was a humble man who enjoyed many different dimensions of life. He was happy collecting stamps, listening to music, enjoying the arts, spending his vacations fishing, camping, and canoeing in different regions of the Soviet Union--the rivers of Siberia, the lakes of Byelorussia, and the river systems of the Volga.

Imposing in size and in mind, V.A. Medvedev will be remembered by his many colleagues at CODATA with great affection. Medvedev is survived by his wife, Vera Shmeleva, and two sons, Grigori, 28, and Andrei, 20.

--by Professor Lev Gurvich

## Reminder!

The 11th International CODATA Conference, "Scientific and Technical Data in a New Era" will be organized by DECHEMA (Deutsche Gesellschaft für Chemisches Apparatewesen, Chemische Technik, und Biotechnologie). It will be held from 26-29 September 1988 at the Karlsruhe Congress and Exhibition Centre, Karlsruhe, Federal Republic of Germany. The aim of the Conference is to discuss the requirements for and the sources, applications, and handling of data in the field of science and technology, especially those aspects which are of importance in a changing modern world.

# **PROGRAM -- TITLES**

## **11th INTERNATIONAL CODATA CONFERENCE**

**KARLSRUHE, F. R. G.**

**September 26 - 29, 1988**

### **OPENING SESSION**

Opening of the 11th International CODATA Conference, H. Behrens, Karlsruhe

Welcoming Addresses by representatives of the State Ministry of Baden-Wittenberg, and the City of Karlsruhe

Keynote Lecture by the Vice President of the Deutsche Forschungsgemeinschaft, Bonn

Keynote Lecture, The Linear Code of DNA and Its Deciphering, E.L. Winnacker, Munich, F.R.G.

## ***Plenary and Invited Lectures***

### **BIOSCIENCES AND BIOTECHNOLOGY**

Chairman: B. Keil, Institut Pasteur, Paris, France

Plenary Lecture: Exponential Growth of Biological Data, A.E. Bussard, Nice, France

Chairman: A.E. Bussard, Nice, France

Protein and Nucleic Acid Sequences, B. Keil, Paris France

Hybridoma Data Bank: Purpose, Organizational Operation, B. Janicki, Boston, MA, U.S.A.

Data and Knowledge Banks on Enzyme, Enzymatic Reactions and Metabolic Pathways, E.E. Sel'kov, I.I. Goryanin, N.P. Kaimatchnikov, I. Shevelev, I.A. Yunus, Puschino, U.S.S.R.

The Microbial Strain Data Network: Combining Traditional Laboratory Notebooks and Personal Networking with Modern Telecommunications, M.I. Krichevsky, Bethesda, MD, U.S.A.

Chairman: M.I. Krichevsky, Bethesda, MD, U.S.A.

Biological Data Banks: A Survey, G. Fredj, Nice, France

Databases in Fermentation Technology, T. Ohta, Tokyo, Japan

### **WORKSHOP ON THE VOCABULARY AND NOMENCLATURE OF BIOLOGY**

Organizer: L. Blaine, Rockville, Maryland

After the workshop different working groups will summarize the conclusions for interested participants..

### **INDUSTRY AND TECHNOLOGY**

Chairman: H. Behrens, Karlsruhe, F.R.G.

Plenary Lecture: Rationalization and Access of Diverse Databases to Solve Specific Industrial Problems, N.G. Rambidi, Moscow, U.S.S.R.

Chairman: H. Knapp, Berlin, F.R.G.

Prediction of Phase Equilibrium Data, A. Bylicki, Warsaw, Poland

Prediction of Thermodynamic Properties in Complex Multicomponent Systems, M.T. Rätzsch, H. Kehlen, Merseburg, G.D.R.

Chairman: A.J. Barrett, Chalfont St. Giles, U.K.

Kinetic Data for Industrial Application, J. Warnatz, Heidelberg, F.R.G.



Data Needs for Computer Design and Simulation Advanced Materials Systems for Engineering, H. Kröckel, Petten, Netherlands

Databases for Properties of Electronic Materials, F.A. Kuznetsov, V.A. Titov, S.V. Borisov, Y.N. Vertoprachov, Novosibirsk, U.S.S.R.

Chairman: D. Abir, Ramat Aviv, Israel

Impact of the PC on Mechanical Design, K.A. Waters, London, U.K.

Materials Data and CAE, H.E. Hellwig, Goslar, F.R.G.

Chairman: H. Kroeckel, Petten, The Netherlands

Requirements of Spectral Databases, E. Pretsch, Zurich, Switzerland

Associative Database Techniques to Search for Materials with Unique Properties, S. Murakimi, Osaka, Japan

Energy Databases, M.A. Styrikovich, Moscow, U.S.S.R.

## SAFETY AND ENVIRONMENTAL PROTECTION

Chairman: H. Behrens, Karlsruhe, F.R.G.

Plenary Lecture: Data for Industrial Hazard Analysis and Human Risk Assessment, D.A. Jones, Bootle, U.K.

Chairman: L.V. Gurvich, Moscow, U.S.S.R.

Data Needs for Writing Rational Regulations in Genetic Engineering, M. Cantley, Brussels, Belgium

Knowledge and Data on Acute and Chronic Exposure to Combustion Products, U. Taitelman, Haifa, Israel

Chairman: G.C. Carter, Washington, D.C., U.S.A.

Environmental Data Needs in a New Era, F. Schmidt-Bleek, Neuherberg, F.R.G.

The Agricultural Research Service (ARS) Pesticide Properties Database, S. Heller, Beltsville, MD, U.S.A.

Databases for Atmospheric Chemistry, R.F. Hampson, Gaithersburg, MD, U.S.A.

## GEO- AND SPACE SCIENCES

Chairman: E.F. Westrum, Jr., Ann Arbor, MI, U.S.A.

Plenary Lecture: General Problems of Earth Observation Satellite Data Handling, L. Marelli, Frascati, Italy

Chairman: D.R. Lide, Gaithersburg, MD, U.S.A.

Recovery and Use of Historical Data: Dendrochronology, F.H. Schweingruber, Birmensdorf, Switzerland

Compilation of over 500 Years of Historical Documents on Climate Changes in China, Shao-Wu Wang, Beijing, China

Chairman: G. Westerhout, Washington, D.C., U.S.A.

International Astronomical Data Networks, P. Benvenuti, Garching, F.R.G.

Recovery and Use of Historical Data: Astronomy, C. Jaschek, Strasbourg, France

Organization of Databases in Astronomy, Especially Space Astronomy, J.M. Mead, Greenbelt, MD, U.S.A.

Atomic and Molecular Data Needed for Astronomy and Astrophysics, J.W. Gallagher, Boulder, CO, U.S.A.

Chairman: B.B. Molino, Bethesda, MD, U.S.A.

Satellite Data for Inclusion in Weather Forecasting and Climatic Models, H. Böttger, Reading, U.K.

Observation and Numerical Simulation of Turbulent Transport and Chemical Transformation of Air Pollutants over Complex Terrain, F. Fielder, Karlsruhe, F.R.G.



Chairman: J. Crease, Wormley, U.K.

ICSU International Global Change Program, S.I. Rasool, Washington, D.C., U.S.A.

Earthquake Data Auto-Processing System for Earthquake Prediction, M. Mizoue, Tokyo, Japan

Chinese Mapping Projects Using Satellites, C. Bardinet, Y. Chen, G. Gabert, Z.-M. Wan, S.-R. Yang, Valbonne, France

## SCIENTIFIC ASPECTS OF COLLECTING AND DISTRIBUTING DATA

Chairman: B. Keil, Paris, France

Plenary Lecture: Standardizing Exchange Formats, J.J. Schmidt, Vienna, Austria

Chairman: A.S. Kertes, Jerusalem, Israel

Computer Evaluation of Crystallographic Data, J.R. Rodgers, Ottawa, Canada

Reliability of Data Banks, V.G. Alemasov, Kazan, U.S.S.R.

Chairman: G.H. Wood, Ottawa, Canada

Data Validation, V.A. Medvedev, V.F. Yungman, Moscow, U.S.S.R.

Confusion Between Phenomenological Correlation and Physico-based Causality in Handling Materials Data, S. Ishino, Tokyo, Japan

## LEGAL AND SOCIAL ASPECTS OF DATA

Public Discussion on: Copyright Issues Affecting Scientific Numerical Databases with an introductory Keynote entitled Necessary Legal Steps to Protect Ideas before Disseminating Data by: D.R. Lide, Gaithersburg, MD, U.S.A.

Chairman: R. Abbel, Frankfurt am Main, F.R.G.

Intellectual Property Protection, L. Cargill, Birmingham, MI, U.S.A.

Transborder Data Flow, Schulte-Hillen, Köln, F.R.G.

Chairman: J.E. Dubois, Paris, France

Privacy Considerations and Scientific Research, E.K. Scheuch, Köln, F.R.G.

Social Status of Data and the Persons Involved, L. Rechaussat, Paris, France

Social Implications of Data Quality, A.J. Barrett, Chalfont St. Giles, U.K.

## INNOVATIONS IN DATA HANDLING

Chairman: E.F. Westrum, Jr., Ann Arbor, MI, U.S.A.

Plenary Lecture: Proper Use of Expert Systems, S. Ohsuga, Tokyo, Japan

Chairman: J.H. Westbrook, Scotia, NY, U.S.A.

True Automated Data Thesaurus: A New Tool for Scientific Information, J.L. McCarthy, Berkeley, CA, U.S.A.

Multi Media System, T. Sakai and Y. Ariki, Kyoto, Japan

Chairman: D.G. Watson, Cambridge, U.K.

Critical Review of Data Storage and Distribution, J.C. Gale, Alexandria, VA, U.S.A.

Criteria for Use of CD-ROM, T.C. Bagg, Gaithersburg, MD, U.S.A.

Chairman: N.G. Rambidi, Moscow, U.S.S.R.

Spatial "Data Graveyards" Versus Dynamic Planning of Environmental Problems - A Misconceptual Practice Reevaluated, A. Degani, Tel Aviv, Israel

Practical Experience with a Large Database, N.A. Farmer, Columbus, OH, U.S.A.

Chairman: S. Iwata, Tokyo, Japan

Advanced Uses of Thermodynamic Data Banks in Teaching Students Specializing in Physical Chemistry, V.S. Iorish, G.F. Voronin, Moscow, U.S.S.R.

Human Factors in User Interfaces, L.F. Normore, Columbus, OH, U.S.A.

## ***Contributed Lectures***

### **SESSION 1: INDUSTRY AND TECHNOLOGY**

Chairman: G. Dathe, Düsseldorf, F.R.G.

Progress in the Development of a Chemical Kinetic Database for Combustion Chemistry, Wing Tsang, Gary Mallard, and John T. Herron, Gaithersburg, MD, U.S.A.

The National Materials Property Data Network - Dealing with the Issues in Online Access to Numeric Performance Data, J. Gibert Kaufman, Columbus, OH, U.S.A.

A Knowledge Base for the Properties of Materials, F.J. Smith and J.G. Hughes, Belfast, Ireland

Data Collection, Data Evaluation, Data Estimation, and Databases in the Field of Chemical Technology of China, Ma Dexian, Beijing, China

Data Flow in Value Added Process of Materials Information, S. Iwata, T. Ashino, S. Ishino, Tokyo, Japan

Standards for the Presentation and Use of Materials Data. A Review of the Activities of ASTM, CEC, CODATA, and VAMAS with Proposals for the Future. K.W. Reynard, South Croydon, U.K.

### **SESSION 2 - SCIENTIFIC, LEGAL AND SOCIAL ASPECTS OF DATA**

Chairman: G. Steven, Luxembourg

The Berlin RNA Data Bank, V. Erdmann, J. Wolters, Berlin, F.R.G.

A Data Capture System for Printed Tabular Data, W. Grattidge, J.H. Westbrook, Scotia, U.S.A.

An Electronic Journal for Sharing Data on Crop Growth, B. Acock, S.R. Heller, S.L. Rawlins, Beltsville, U.S.A.

Evolving Databases and Copyright of Experts, I.L. Khodakovsky, Moscow, U.S.S.R.

STN Numeric Data Service, A. Barth, P. Luksch, Karlsruhe, F.R.G., J. Mockus, Columbus, Ohio

Data Reliability and Active Environment: Chemical Shift Models, J.E. Dubois, J.P. Doucet, A. Panaye, Paris, France

### **SESSION 3 - INNOVATIONS IN DATA HANDLING**

Chairman: N.A. Farmer, Columbus, U.S.A.

Empirically Based Concepts for Materials Information Systems, K.I. Ammersbach, N. Fuhr, G.E. Knorz, Darmstadt, F.R.G.

Impact of CD-ROM on the Dissemination of Scientific Data, M.A. Chinnery, Boulder, U.S.A.

Operation of the High Temperature Materials Data Bank of the CEC as an Expert System for Material Data Evaluation, G. Fattori, Ispra, Italy, H. Kröckel, H. Over, P. Vannon, Petten, The Netherlands

Materials Data Handling. Interfaces Between an Expert Knowledge System and User Orientated Problem Solving, U. Bengtson, Gotteborg, Sweden

Is Sequence Data Enough for Protein Engineering?, A. Tsugita, Noda, Japan

The Integration of Multimedia Data, P. Kanciruk, Oak Ridge, U.S.A.

## ***Poster Papers***

### **TOPIC 1 - BIOSCIENCES AND BIOTECHNOLOGY**

Medical Data Bank, New Principles of Collection, Presentation and Utilization of Numerical Medical Data, K.P. Ivanov, Leningrad, U.S.S.R.



- Data Bank Activity on Viruses, Cell Lines and Organ Cultures, A.S. Kolaskar, Poona, India
- Creating Chinese Medicinal Plant Database, Senliang Li, Nianhua Xiao, Beijing, P.R.C.
- Formats for Data Banks on Metabolic Pathways and Enzymes, E.E. Selkov, Pustchino, U.S.S.R.
- Network Access to the "Directory of Protein Sequences and Nucleic Acid Sequence Data", J.R. Rodgers, G.H. Wood, Ottawa, Canada
- Development of WFCC World Data Center on Microorganisms, Hideaki Sugawara, Yoshihiro Ugawa, Kazuo Komagata, Saitama, Japan
- A Two-Step Heat Treatment Process for Milk Stabilization, S. Pierucci, E. Pagliani, C. Peri, Milan, Italy

## TOPIC 2 - INDUSTRY AND TECHNOLOGY

- Standard Technological Data in Industry, A. Moore, Bristol, England
- Design and Realisation of a Database Concept for Engineering Applications, G. Bleher, M. Tischendorf, Stuttgart, F.R.G.
- Study and Improvement of Rihani-Doraiswamy Estimation Method of Cpx with Computer Program, Dong Qian, Yan Xinjian, Xu Zhihong, Beijing, P.R.C.
- Estimation of Cp of Intermetallic Compounds, Huang Guosheng, Xu Zhihong, Beijing, P.R.C.
- Computer Aided Comparison of Different Parameter Estimation Methods for Phase Equilibrium Data Models, D.A. Lempe, W. Lüneburg, Merseburg, G.D.R.
- Computation System for Thermophysical Properties COMDAT - Design and Application in Research and Development, H. Freydank, K.Bähr, H. Lehmann, W.Wettengel, Luna, G.D.R.
- Evaluation of Thermophysical Data by Means of Thersyst, R. Brandt, G. Jaroma-Weiland, G. Neuer, G. Pflugfelder, Stuttgart, F.R.G.
- Physical Property Data of Mixtures: Estimation with DETHERM-PC, R. Sass, R. Eckermann, Frankfurt am Main, F.R.G.
- The Sensitivity of Process Design to the Accuracy of Thermodynamic Data Correlational Models, W.B. Whiting, Morgantown, WV, U.S.A.
- Transfer of Physico-Chemical Property Data in a Computerized Database System - An Experience Report, R. Erb, H. Hey, S. Müller, Frankfurt am Main, Höchst, F.R.G.
- Mobile "IVTANTERMO" Data Bank Software with Relational DBMS "DIOD" and the Flexible Dialogue Monitor, V.S. Iorish, A.D. Goldstein, Moscow, U.S.S.R., A.V. Ivanosov, V.K. Polyschuk, A. Yu. Proskurnev, T.Z. Chekovskoi, Moscow, U.S.S.R.
- Collection and Evaluation of Low Pressure Vapor-Liquid Equilibrium Data Published in China, Jin Zhang Li, Jiang Chu Sheng, Beijing, P.R.C.
- PPEC & JANAF Online System, Wang Leshan, Zhou Weibiao, Beijing, P.R.C.
- On-Line Retrieval System of the NBS Inorganic Crystal Data, Jianju Zhou, Ying Zhang, Zhihong Xu, Heng Fu, Beijing, P.R.C.
- COALDATA - A Factual Data Bank on Coal and its Liquefaction Products, H. Langer, L. Hildebrandt, R. Eckermann, Frankfurt am Main, F.R.G.
- The Analysis of Electrolyte Data with the Help of the ELDAR Data and Method Bank, J. Barthel, H. Hopp, G. Schmeer, Regensburg, F.R.G.
- A New Spectroscopic Information System, P. Luksch, Eggenstein-Leopoldshafen, F.R.G.
- On-Line ESCA Database on VAX 11/780 Computer, Jiaju Zhou, Qingsheng Wen, Lingxiao Cao, Hong Wang, Beijing, China
- EC Demonstration Programme on Materials Databanks, G. Steven, G. Heine, Luxembourg
- Utilization and Production of Materials Data Banks in France, B. Marx, Paris, France
- Critical Metadata Issues in Materials Property Databases, J.H. Westbrook, W. Grattidge, Scotia, U.S.A.
- SPAO Computer Assisted Selection of Polymers, J.P. Caliste, Paris, France
- The ACerS-NBS Ceramic Phase Diagram Program, C.R. Hubbard, Gaithersburg, MD, U.S.A.
- Surface Analysis Data about Rare Earth Intermetallic Compounds, Jin Kang, Beijing, P.R.C.
- The Data Bank on Coatings and High Temperature Corrosion; an example of Materials Data Bank, R. Streiff, Marseille, France
- A New Technique (Holotransformation) for the Evaluation of a Forced Convection Equation from Experimental Data, E. Büyükcoca, Istanbul, Turkey

Data Collection and Prediction for a New Vitamin Synthesis Technology, V.V. Beregovykh, G. Kuleshov, L.L. Gurarij, Minsk, U.S.S.R.

Materials Databases for Structural Integrity Assessment and Restlife Estimation of Power Plant Components, D. D'Angelo, A. Garzillo, S. Ragazzoni, V. Regis, Milan, Italy

Failure and Accident Expert Bases and Their Maintenance Through Fuzzy Mathematics, P. Vaija, Espoo, Finland M. Dohnal, Brno, C.S.S.R.

The Viscosity of Industrial Hydrocarbons. An Experimental Research and Development of Reference Data Tables, B.A. Grigorious, A. S. Kramidi, Y. L. Rastorguyez, S. I. Rodchenko, Gorsny, U.S.S.R.

Data Sources for Materials Scientists & Engineers, H. Wawrousek, J.H. Westbrook, W. Grattidge, Scotia, U.S.A.

### TOPIC 3 - SAFETY AND ENVIRONMENTAL PROTECTION

Safety and Hazard Data for Fire and Explosion Protection with CHEMSAFE, K. Januschewski, R. Eckermann, Frankfurt am Main, F.R.G.

Database on Radioactive Materials Released from United States Nuclear Power Plants, J.L. Tichler, Upton, NY, U.S.A.

The Hazardous Substances Data Bank (HSDB), G.J. Cosmides, Bethesda, MD, U.S.A.

### TOPIC 4 - GEO- AND SPACE SCIENCE

Mineral Exploration Using Multiple Remote Sensing Data in Western China, Guo Huadong, Beijing, P.R.C.

Cartographic Information Systems in Open Communication Networks, H. Kremers, Stuttgart, F.R.G.

Regional Databases and Structural Phenomena, A.T. Solecki, Wroclaw, Poland

Preparation of Complex Regional Databases of Simultaneous Ground-Based and Satellite-Borne Measurements, C.U. Wagner, G. Lenners, W. Singer, Berlin, G.D.R.

Geo- and Space Science Data Growth Rate Problems, G.K. Hartmann, Katlenburg-Lindau, F.R.G.

Applied Astrophysics from a Number of Databases, J. Spicker, Bochum, F.R.G.

Geological-Engineering Database System for Flotation Deposits Tank, B. Namyslowska-Wilczyńska, M. Kaminska, R. Sibiliski, Wroclaw, Poland.

### TOPIC 5 - SCIENCE ASPECTS OF COLLECTING AND DISTRIBUTING DATA

CAN/SND - An International Online Source of Scientific Numeric Data, G.H. Wood, J.R. Rodgers, S.R. Gough, Ottawa, Canada

Creating Scientific Databases System in Academia Sinica - Self-Creating Numerical Databases, Li Senliang, Xiao Nianhua, Beijing, P.R.C.

Representing Database Contents, S. Weitz-Ingber, Jerusalem, Israel

The Microcomputer as a Tool for Information Retrieval in Nuclear Physics, J.W. Tepel, Eggenstein-Leopoldshafen, F.R.G.

The ICSTI Directory of Numeric Machine Readable Databases, B.B. Molino, Gaithersburg, U.S.A.; P.S. Wilson, Coiumbus, U.S.A.

Ivtantermo-87 - Expanded and Updated Data Bank on Thermodynamic Properties of Individual Substances, L.V. Gurvich, Moscow, U.S.S.R.

A New Approach to the Creation of an International Thermodynamic Database, I.L. Khodakovsky, Moscow, U.S.S.R.

Parameter Evaluation Based on Direct and Indirect Measurements with General Correlations, D.W. Muir, Los Alamos, NM, U.S.A.

Vapor Pressure and Acentric Factor of Organic Coumpounds Part 1 Halogenated Hydrocarbons, Ma Peisheng, Xu Ming, Tianjin, P.R.C.

Vapor Pressure and Acentric Factor of Organic Coumpounds Part 2 Alcohols and Phenols, Ma Peisheng, Xu Ming, Tianjin, P.R.C.

Critical Assessment of Critical Properties on Organic Compounds, Ma Peisheng, Tianjin, P.R.C.

Revised Van der Waals Radius for Hydrogen Using Cambridge Structural Data, R. Srinivasan, M. Hariharan, J. Vijayalakshmi, Madras, India

Computerized Collection of Dietary Intake Data, D. Feskanich, Cambridge, MA, U.S.A.

Interchanging and Merging Food Composition Data, W.M. Rand, J.C. Klensin, Cambridge, MA, U.S.A.

Interchange of Water Resources Data, M.J. Goodspeed, Canberra, Australia



## TOPIC 6 - LEGAL AND SOCIAL ASPECTS OF DATA DISSEMINATION

The UNESCO/CODATA Inventory of Data Sources in Science & Technology, J.H. Westbrook, W. Grattidge, Scotia, U.S.A.

## TOPIC 7 - INNOVATIONS IN DATA HANDLING

- An Integrated Data Entry System for Capturing Printed Scientific & Technical Data for Input to Computerized Systems, B. Lund, Graddige, Scotia, N.Y., U.S.A.
- An Evaluators Database for Aqueous Thermodynamic Properties, D.B. Neumann, Gaithersburg, MD, U.S.A.
- Intelligent Interface and Front-End Analyzer for SEAT, J.S. Dreicer, C. Michelson, D. Morgeson, Los Alamos, NM, U.S.A.
- Materials Image: Storage, Analysis and Classification, G. Bonifazi, La Sapienza, Italy
- Integrated DB/KB Systems for Organic Synthesis Design, Y. Fujiwara, N. Ohbo, I. Suzuki, T. Nakayama, Sakurabarak, Japan
- An NMR Spectral Database with Intelligent Search Systems, O. Yamamoto, K. Hayamizu, M. Yanagisawa, Ibaraki, Japan
- Management of An Expert Scientific Database, J.G. Hughes, F.J. Smith, Belfast, Ireland
- A Computerized Tribology Information System (ACTIS), G.E. Reisz, C. Michelsen, Los Alamos, NM, U.S.A.
- Cambridge Crystal Structural Database (in part) on Microcomputers, J. Vijayalakshmi, R. Srinivasan, Madras, India
- RCDC Online: An Integrated System Containing Bibliographic and Numeric Databases, I. Carmichael, W.P. Helman, G.L. Hug,
- Contribution of Factor Analysis and Automatic Classification for Bibliographic Databases Analysis, P. Billard, P. Blanchet, C. Paoli, C. Longbvalle, Paris, France.
- Data Base Handling in Instructional Aids for Wargaming Models, S. Ramgopal, P. Thomas, P. Arulmani, E.S.R. Gopal, Bangalore, India
- A Microcomputer System for the Collection and Coding of Dietary Intake Data, I.M. Buzzard, D. Feskanich, K.R. Chong, Minneapolis, MN, U.S.A.
- Artificial Intelligence Applications to Information Handling in Medecine, E.L. Curry, Denton, U.S.A.
- Method for Predicting Quaternary Structure of Hepatitis B Virus Surface Antigen, K. Nagano, Tokyo, Japan, F. Iinuma, Tokyo, Japan....
- Computer-Aided Modeling of E. coli Ribosome, K. Nagano, Tokyo, Japan

## Books

- Crystallographic Databases.** Editors: F. H. Allen, G. Bergerhoff, and R. Sievers.(a)
- Multivariate Data Analysis.** By F. Murtagh and A. Heck.(b)
- Data Analysis in Astronomy II.** Editors: V. Di Gesu, L. Scarsi, P. Crane, J. H. Friedman, S. Levialdi.(c)
- Guide to the World Data Center Systems. Part 1. The World Data Centers.(d)**
- (a) Available from J. N. King, Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester, UK, CH1 2Hu. US \$20. This book is a publication of the Commission on Crystallographic Data of the International Union of Crystallography. (See review on p. 10 this Newsletter.)
- (b) Kluwer Academic Publishers Group, P. O. Box 989, Spuiboulevard 50, 3300 AH Dordrecht, The Netherlands, or P.O.Box 358, Accord Station, Hingham, MA, 02018-0358 U.S.A., 1987, Dfl. 120/US \$49.50. ISBN 90-277-2425-3. (See review on p. 10 this Newsletter.)
- (c) Proceedings of an International Workshop on Data Analysis in Astronomy in Erice, Italy, 1984. Ettore Majorana International Science Series, Physical Sciences, 27, 399 pp, Plenum Press, 233 Spring Street, New York, NY 10013, U.S.A., 1986. \$69.50. (See review on page 10 this Newsletter.)
- (d) 92 pp. Issued by the Secretariat of the ICSU Panel on World Data Centers. Address: WDC-A, NOAA E/GC2, 325 Broadway, Boulder, CO 80303, U.S.A.

## Data Analysis in Astronomy. II.

The follow-up proceedings of the 1984 Erice workshop provides the reader with the development of advanced techniques for automated reduction, archiving, retrieval, and dissemination of astronomical data, as well as new analysis methodologies and state-of-the-art computational procedures. Such developments involving retrieval and analysis of astronomical systems involving hundreds of thousands of items are described.

The SIMBAD databank in Strasbourg, created by the international network of astronomical data centers, is described briefly as to its data content and accession online through a software system that is user-friendly.

The book is organized into four primary sections covering methodologies for data analysis, data handling and systems for large experiments, parallel computing, and new developments.

As might be expected, the peculiarly astronomical problems of storage and retrieval of data and of astronomical numbers of systems are featured, but the application of the book to more general types of data treatment and statistical analysis should not be overlooked. Indeed, it should be applicable for data analysis in many other fields of scientific endeavor. Further details about the book are to be found on page 9.



## Multivariate Data Analysis

A book entitled *Multivariate Data Analysis* by F. Murtagh (ST-ECF, European Southern Observatory, Garching bei Munchen, F.R.G. and Space Science Dept., ESTEC, Noordwijk, The Netherlands) and A. Heck (C.D.S. Observatoire Astronomique, Strasbourg, France) covers the most useful techniques in multivariate statistics, including data coding; initial treatment of data; principal components, cluster-, discriminant- and other analyses; as well as a case study on IUE low dispersion spectra, and a review of strategies for analysing data.

A wide-ranging annotated set of general and astronomical bibliographic references follows each chapter, providing valuable entry-points for research workers in all astronomical sub-disciplines. Although the applications considered focus on astronomy, the algorithms used can be applied to similar problems in other branches of science. Fortran programs are provided for many of the methods described. Further details will be found on page 9.

## Crystallographic Databases

A new volume entitled *Crystallographic Databases* focusing on information content, software systems, and scientific applications has been edited by F. H. Allen, G. Bergerhoff, and R. Sievers.

It covers database descriptions: Cambridge Structural Database (CSD: organo-carbon compounds), Inorganic Crystal Structure Database (ICSD), Metals Crystallographic Data File, Protein Data Bank, NBS Crystal Data File, JCPDS Powder Diffraction File, Database of Order-Disorder Structures, and NBS Biological Macromolecule Crystallization Database.

The software systems described are: Cambridge (CSD) Systems, ICSD-CRYSTIN, NBS, SEARCH, JCPDS Search/Match Systems, Chemical Databank System (CDS: SERC, UK), Canadian Scientific Numeric Database Service (CAN/SND: NRC Ottawa). Moreover, the book incorporates an overview of crystal structure analysis for non-specialists, survey of printed information sources in crystallography, and a bibliography of scientific applications. Procurement details are indicated on page 9.

## NICRYS Hosts Indian Workshop

NICRYS (National Information Centre for Crystallography), at the Department of Crystallography and Biophysics, University of Madras, hosted a regional (East Asian) workshop focused on modern, computerized databases (particularly the non-bibliographic, hard data variety selected in the area of chemical and molecular biosciences) January 18-23, 1988. About fifteen specialist speakers drawn from U.S.A., U.K., Europe, and India presented lectures, extensive packets of course materials, and demonstrations to 50 fully participating scientists and an equal number of auditors. The delegates were mostly from India and the surrounding countries of Bangladesh, Malaysia, and Thailand.

The Organic Cambridge Structural Data (CSD), Inorganic Crystal Structural DATA (ICSD), Powder Diffraction Data, and NBS-Crystal Data were featured items. Crystallographic data, mass spectroscopic data, Beilstein Chemical Data--all for use on PC's--were covered. In the molecular biosciences area, the protein structural and sequence data, the nucleic acid sequence data (GENBANK) were covered. Molecular graphic displays of both nucleic acids and proteins were demonstrated using the NEXUS 3000 Graphic Workstation. Nucleic acid sequence data analysis using a PC-AT system with a CD-ROM optical disk unit was a noteworthy demonstration.

## CODATA Calendar

1988

### May

- 23 Phase Equilibrium Task Group, Paris, France
- 23-24 Materials Database Management Task Group, London, U.K.
- Multisatellite Thematic Mapping, Beijing, P.R.C.

### June

- 13-14 Mapping Human Genome Workshop, Paris, France

### July

- 23-24 CODATA Task Group on Geothermodynamic Data, Strasbourg, France
- 25-28 First International Symposium on Thermodynamics of Natural Processes, Strasbourg, France

### September

- Multisatellite Thematic Mapping, Karlsruhe, F.R.G.
- 26-29 CODATA Task Group on Materials Database Management, Karlsruhe, F.R.G.
- 26-29 11th International CODATA Conference, Karlsruhe, F.R.G.
- 30- CODATA General Assembly, Karlsruhe, F.R.G.
- Oct. 1 F.R.G.

## Industrial Data

(continued from page 1)

in Columbus, Ohio, U.S.A. in July 1990 was also discussed. Progress on the CODATA Directory Chapter on Mechanical Properties was reviewed and further chapters considered.

The Commission seeks to survey industrial data to ascertain the data needs and to make industry more aware of the activities of CODATA.

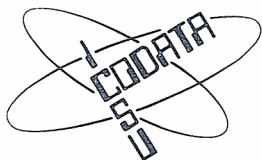
Finally, the Commission reviewed the status of a number of national and international (i.e., regional) databases of industrial relevance.

The Commission is now composed of:

- Drs. J. H. Westbrook, Chairman (Sci-Tech Knowledge Systems) Scotia, NY, U.S.A.;
- Peter Schonholzer (Schweizerisch Aluminum AG) Neuhausen, Switzerland;
- Jiro Hiraishi (National Chemical Laboratory for Industry) Tsukuba, Japan;
- Reiner Eckermann (DECHEMA) Frankfurt/Main, F.R.G.;
- James Naylor (Centre Technique des Industries--CETIM) Senlis, France;
- Fedor A. Kuznetsov (Institute of Inorganic Chemistry, USSR Academy of Science) Novosibirsk, U.S.S.R.;
- Keith W. Reynard (Wilkinson Consultancy Services) South Croydon, U.K.; and
- Prof. David Abir, Executive Committee Liaison (Tel Aviv University) Tel Aviv, Israel.

Corresponding members are being sought from CODATA countries and from organizations throughout the world. The Commission will endeavor to arrange an associate membership in the Alloy Phase Diagram International Commission with liaison provided by Dr. John Rumble.





# Task Group on Materials Database Management

## Materials Database Newsletter

April 1988, Number 3

The purpose of this Newsletter is to provide an overview of national and international developments relating to all aspects of materials property databases, and to promote cooperation with respect to database design, management and use. The Editor welcomes

contributions and comments from database builders, operators and users. There are no restrictions on the reproduction and distribution of the contents of this Newsletter.

### NETWORKS

The **Pilot MPD Network** is now available online to USA and overseas financial sponsors of the **NATIONAL MATERIALS PROPERTY DATA NETWORK, Inc.** Thirty accounts are active in experimental use and evaluation of the pilot system, operating from Stanford University and accessible via Telenet public communications. Upgrading of the pilot MPD Network and the addition of another new database is expected to be complete by late summer 1988. Through its agreement with the American Chemical Society, the MPD Network expects to be operating in a commercial mode on STN International by early 1990. **FURTHER INFORMATION:** J. G. Kaufman, MPD Network, Inc., 2540 Olentangy River Road, P. O. Box 02224, Columbus, OH, U.S.A.

The **European Space Agency-Information Retrieval Service (ESRIN)** has announced the availability of **QUESTNUMERIC**, a new facility for numeric data searching. The facility allows for both single value and range value searching. A floating point representation for numeric data is used internally, thus avoiding character string plurality problems in the data as well as at the user interface. **QUESTNUMERIC** has already been implemented on the **INSPEC** database and will also be available on Materials Information's Metals Datafile. **SOURCE:** ESRIN News and Views, November 1987, Volume 12, No 6, pp 6-7.

The first seminars associated with the **CEC MATERIALS DATABASE DEMONSTRATOR PROGRAMME** were held in February and March 1988 in France, Denmark, and the UK. The series of six seminars will be followed by a full workshop programme beginning in autumn this year. **FURTHER INFORMATION:** Mr. G. Steven, DG XIII/B, Bat. J. Monnet, Plateau du Kirchberg, L-2920 Luxembourg.

### DIRECTORIES

A short User Manual has been published for the **DOMIS** database (**Director of Materials Data Information Sources**). **DOMIS** is an online directory of information sources and services currently available in Europe, and may be used to identify the data sources (databanks and bases, technical centres, scientific and technical laboratories, private and university laboratories, publications, experts, etc.) most likely to be able to provide information on specific properties of particular materials. Materials covered include metals and alloys, ceramics, composite materials, plastics and rubber, and electronic materials; mechanical, physical thermodynamic, electrical, electronic, corrosion and service properties are covered. Copies of the User Manual are available from **ECHO** Customer Service, 177 route d'Esch, L-1471, Luxembourg.

### STANDARDS

Following the publication of the report entitled "The Need for Standards" of the **VAMAS** Technical Working Area 10, Materials Databanks, the **VAMAS Steering Committee** has approved three follow-up activities: (1) the compilation of a **WORLDWIDE INVENTORY OF MATERIALS DESIGNATION SYSTEMS** (further information from: K.W. Reynard, Wilkinson Consultancy Services, 32 Croham Park Avenue, South Croydon, U.K. CR2 7HH); (2) the establishment of a round robin type **COMPARISON OF DATA EVALUATION METHODS** (further information from: Dr. S. Nishijima, NRIM, 2-3-12, Nakameguro, Meguro-ku, Tokyo 153, Japan); and (3) the organization of a **VAMAS WORKSHOP ON STANDARDS FOR FACTUAL MATERIALS DATABANKS** (see Calendar listing).

### CALENDAR

9-13 May 1988: London, United Kingdom

**MATERIALS '88; MATERIALS AND ENGINEERING DESIGN.** Topics include: Materials Databanks and Expert Systems for Use in Computer-Aided Engineering. **CONTACT:** Conference Manager, The Institute of Metals, 1 Carlton House Terrace, London, UK, SW1Y 5DB.

CALENDAR

12-13 May 1988: London, United Kingdom

CODATA TASK GROUP ON MATERIALS DATABASE MANAGEMENT meeting.

26-29 September 1988: Karlsruhe, Federal Republic of Germany

11th International CODATA Conference **SCIENTIFIC AND TECHNICAL DATA IN A NEW ERA**. CONTACT: DECHEMA, Abt. Tagungen, POB 97 01 46, Theodor-Heuss-Allee 25, D-6000, Frankfurt am Main, FRG.

11-14 October 1988: Toronto, Ontario, Canada

ASTM Committee E49 on **COMPUTERIZATION OF MATERIAL PROPERTY DATA** meeting.

15-17 November 1988: Petten, The Netherlands

VAMAS Workshop on **STANDARDS FOR FACTUAL MATERIALS DATABANKS**. Participation will be by invitation only. CONTACT: Dr. J. Rumble, NBS, A323 Physics Building, Gaithersburg, MD 20899, USA; or H. Kroeckel, CEC-JRC, NL-1755 ZG Petten, The Netherlands.

27-29 June 1989: St. Louis, Missouri, USA

ASTM Committee E49 on **COMPUTERIZATION OF MATERIAL PROPERTY DATA** meeting.

5-7 December 1989: Orlando, Florida, USA

ASTM Committee E49 on **COMPUTERIZATION OF MATERIAL PROPERTY DATA** meeting.

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