



36 CODATA / NEWSLETTER

APRIL 1986

10th INTERNATIONAL

CODATA CONFERENCE

Ottawa, Canada, 14-17 July 1986

HIGHLIGHTS

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W. Klemm 11

This issue of the newsletter lists the titles of all invited as well as contributed papers on pages 3 through 10. Every indication suggests that this Conference will be highly successful in providing not only an interesting, beautiful, and historical milieu, a generous array of scientific sessions and poster presentations, and opportunities encouraging free and informal discussion, but also incorporates features new to CODATA Conferences, such as displays of relevant products and services. Moreover, we are celebrating CODATA's 20th Anniversary!

New Feature. In addition to the presentation of posters, workshops with an appointed chairman will be organized for several of the poster subject groups. Participants should plan to join in these profitable opportunities for discussion.

Registration. Prospective participants are reminded that to qualify for the reduced registration fee, the remittance must be received by May 15, 1986.

Accommodation. Room reservations at the Westin Hotel or the University of Ottawa should be completed early and in any event before June 15, 1986.

For "new" readers. For more detailed information, please contact the Conference Secretariat:

CODATA '86
Huguette Lacoste, Executive Secretary
National Research Council Canada
Ottawa, CANADA K1A 0R6
Telephone: (613) 993-9009 Telex: 053-3145

Notes. For planning purposes and to facilitate participants' return travel, sessions scheduled for Thursday, July 17 will terminate at 3:30 p.m.

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.

CODATA Calendar

1986

April

- 28-29 Task Group on Phase Equilibrium (partial) meeting, Warsaw, Poland.

May

- 12-14 Task Group on Phase Equilibrium Data, Lyngby, Denmark.
18-23 Workshop on Directions for Internationally Compatible Environmental Data, Montreal, Canada.

June

- 21-23 Task Group on Geothermodynamic Data meeting at Moscow or Irkutsk, U.S.S.R. (tentative).
22 Task Group on Fundamental Constants, Gaithersburg, U.S.A.

July

- 14-17 10th International CODATA Conference, Ottawa, Canada.
18-19 15th General Assembly, Ottawa, Canada.
17-20 Task Group on Chemical Thermodynamic Tables, Ottawa, Canada.
20-23 Task Group on Geothermodynamic Tables, Ottawa, Canada.

September

- 13-14 Task Group on Microbiological Strain Data Network, Manchester, England.

Hydrocarbon Thermodynamics

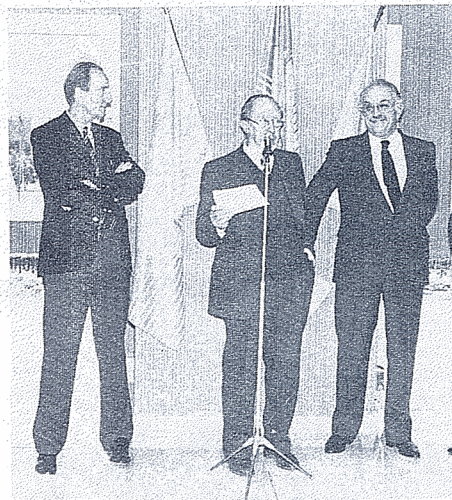
A superb two-volume critically evaluated compilation of data values for three experimentally determined properties (vapor pressures, saturated liquid densities, and second virial coefficients) and two calculated thermodynamic properties (saturated vapor volume and enthalpy of vaporization) plus compound constants (triple, melting, and boiling points, critical temperature, pressure, volume, compressibility factor, acentric factor, dipole moment, and radius of gyration) has been achieved. The first volume covers C_1 through C_9 hydrocarbons and ketones of all carbon numbers; the second provides coverage for alcohols of all carbon numbers but only C_1 and C_2 halogenated hydrocarbon compound, plus only a few C_3 's. Correlation equations are used to produce short tabulations of the experimental property values. By assuming an equation of state, the authors provide the derived property values.

A Master Reference List (MRL) related the literature document with the correlations employed. A variety of correlation relations and equations of state were utilized. Approximately 28,000 documents were retrieved and their citations listed in the MRL. The authors consider that they have examined 95% of the existing relevant documents and over 98% of the useable data on each compound covered extant to a cutoff date indicated (between 1976 and 1984). Procedures used for correlation and for data evaluation have been detailed and an explanatory sample chart is provided. The book represents essentially a computer print out of a pure compound databank designed to permit mixture evaluation and correlation programs.

The typography and presentation are excellent in all respects and though expensive, the more than 1600 data pages provide an excellent access to the data on the compounds covered. This two volume set provides evaluated thermodynamic data of great utility to scientists and technologists involved in hydrocarbon—and related—chemistry.

Inauguration of European Node of Hybridoma Data Bank in Nice, France

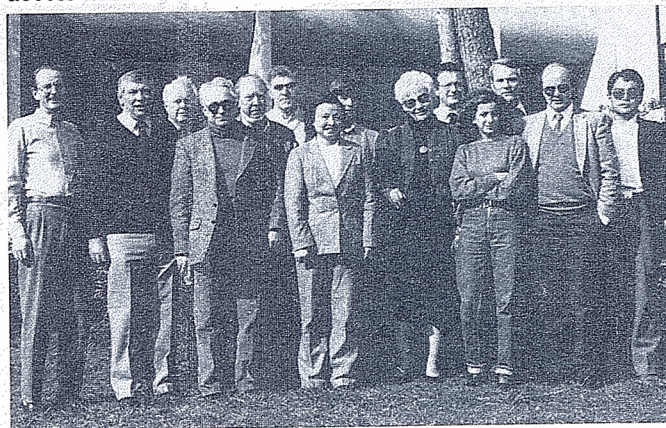
The European node of the Hybridoma Data Bank (HDB) was officially inaugurated on March 3, 1986 during a reception offered by the mayor of Nice, Mr. Jacques Medecin. He expressed his delight at having the center of immunology located on the Côte d'Azur where enormous efforts are being made to encourage biotechnological industries.



(from left to right): R. Masseyeff (HDB Europe), A. Bussard (Chairman CODATA HDB Task Group), Jacques Medecin (Mayor of Nice).

This is the third node of the CODATA/IUIS HDB which already maintains banks in Washington at the American Type Culture Collection offices and in Japan at RIKEN. The European node is being jointly sponsored by the Regional Council of the Alpes-Maritime and the Commission of the European Communities.

Following the inauguration ceremonies (which were shown on French television) the CODATA Task Group met for three days to discuss future plans for the HDB, including access online via ITT DIALCOM.



(from left to right): R. Masseyeff, B. Janicki, R. Stevenson, M. Krichevsky, A. Bussard, P. Reiniger, Dai Shunzi, L. Blaine, P. Glaeser, H. Bazin, D. Amsellem, T. Staehelin, J.C. Roder, H. Sugawara.

(Further information on Thermodynamic Data for Pure Compounds Parts A & B by Buford D. Smith and Rakesh Srivastava of the Thermodynamics Research Laboratory, Chemical Engineering Department, Washington University, St. Louis, Missouri is contained on page 11 of this Newsletter.)

PROGRAM

10th INTERNATIONAL CODATA CONFERENCE

Ottawa, Canada, 14 - 17 July 1986

MONDAY, July 14 - A.M.

SESSION I-A - DATA VALIDATION

- I.A.0 **M. Fournier**, *Telelobe Canada, Montreal, PQ, Canada*. **Keynote Address:** INFORMATION TRANSFER - A LOOK INTO THE FUTURE
- I.A.01 **D.G. Watts**, *Queen's University, Dept. of Mathematics and Statistics, Kingston, ON, Canada*. BENEFITTING FROM MULTIRESPONSE DATA
- I.A.02 **J. Tukey**, *Princeton University, Dept. of Mathematics, Princeton, NJ, USA*. USING PROBABILITY CALCULATIONS FOR GREATER SECURITY, NOT LESS

MONDAY, July 14 - P.M.

SESSION I-B - DATA FOR BIOTECHNOLOGY INDUSTRIES

- I.B.01 **R.R. Colwell**, *University of Maryland, Dept. of Microbiology, College Park, MD, USA*. DATA NEEDS FOR BIOTECHNOLOGY INDUSTRY AND INDUSTRY/UNIVERSITY COOPERATION IN THE UNITED STATES
- I.B.02 **E.S. Lennox**, *Celltech Limited, Slough, UK*. DATABASES IN BIOTECHNOLOGY
- I.B.03 **H. Sugawara**, *Y. Tateno, Y. Ugawa, RIKEN, Life Science Research Information Section, Saitama, Japan*. DATA ACTIVITIES FOR LIFE SCIENCE AND BIOTECHNOLOGY IN JAPAN
- I.B.04 **S. Ramachandran**, *Department of Science & Technology, National Biotechnology Board, New Delhi, India*; **A.S. Kolaskar**, *Centre for Cellular and Molecular Biology, Hyderabad, India*. BIOINFORMATION SYSTEM IN INDIA

SESSION I-C - MAPPING IN GEOPHYSICS

- I.C.01 **C. Bardinet**, *J.M. Monget, Ecole des Mines de Paris-CTAMN, Valbonne, France*; **G. Gabert**, *B.G.R., Hannover, FRG*. MULTISATELLITE THEMATIC MAPPING ON TANZANIA: TIROS N, METEOSAT, LANDSAT
- I.C.02 **P.H. Smith**, *M.J. Goldberg, NASA/GSFC, National Space Science Data Center, Greenbelt, MD, USA*. PROBLEMS IN MERGING EARTH SENSING SATELLITE DATA SETS
- I.C.03 **E.E. Davis**, *Pacific Geoscience Centre, Sidney, BC, Canada*. THE APPLICATION OF SWATH BATHYMETRIC AND ACOUSTIC IMAGE MAPPING TO CONTEMPORARY PROBLEMS IN MARINE GEOSCIENCE
- I.C.04 **E. Kilényi**, *Z. Szabó, P. Draskovits, K. Kakas, J. Rimpler, Eötvös Loránd Geophysical Institute of Hungary, Budapest, Hungary*. REGIONAL AND TASK-ORIENTED GEOPHYSICAL MAPPING IN HUNGARY

SESSION I-D - EVALUATION OF MATERIALS PROPERTIES

- I.D.01 **S.K. Foss**, *Deere & Company Technical Center, Moline, IL, USA*. EVALUATION CONSIDERATIONS AND PROCEDURE FOR RAW FATIGUE DATA
- I.D.02 **M.M. Hall**, *D.C. Wright, Rapra Technology Limited, Shawbury, UK*. PROPERTY AND KNOWLEDGE BASES FOR POLYMER ENGINEERS
- I.D.03 **G.M. Ugiansky**, *D.E. Clausen, National Bureau of Standards, NACE-NBS Corrosion Data Center, Gaithersburg, MD, USA*. THE NACE-NBS CORROSION DATA PROGRAM
- I.D.04 **I. Yasui**, *University of Tokyo, Institute of Industrial Science, Tokyo, Japan*. DATA ACTIVITIES IN CERAMIC SCIENCE IN JAPAN

SESSION I-E - GEOSCIENCES DATA

- I.E.01 **J.M. Zarzycki**, *Energy, Mines and Resources Canada, Surveys and Mapping Branch, Ottawa, ON, Canada*. CANADA'S APPROACH TO A NATIONAL DIGITAL TOPOGRAPHIC DATABASE
- I.E.02 **F. Faucher**, *R. Mazaachi, F. Young, Energy, Mines and Resources Canada, Surveys and Mapping Branch, Ottawa, ON, Canada*. ANALYSIS OF LEVELLING DATA IN CANADA
- I.E.03 **R. Gareau**, *M. Bérubé, B. Bresee, Energy, Mines and Resources, Surveys and Mapping Branch, Ottawa, ON, Canada*. GEODETIC OBSERVATIONS TO DETECT CRUSTAL MOTION IN CANADA

- I.E.04 **A. Lakanen**, M.C. Pinch, *Energy, Mines and Resources, Surveys and Mapping Branch, Ottawa, ON, Canada*. GEODETIC DATA MANAGEMENT
- I.E.05 **J.D. Boal**, R.R. Steeves, *Energy, Mines and Resources, Surveys and Mapping Branch, Ottawa, ON, Canada*. ONLINE GEODETIC NETWORKS
- I.E.06 **E.M. Siekierska**, S. Palko, *Energy, Mines and Resources, Geographical Services Division, Ottawa, ON, Canada*. DEVELOPMENT OF THE ELECTRONIC ATLAS OF CANADA
- I.E.07 **A.V. Okulitch**, K.N. Nairn, *Geological Survey of Canada, Calgary, AB, Canada*. A MINI-COMPUTER SYSTEM FOR THE GEOLOGICAL ATLAS OF CANADA
- I.E.08 **R.K. McConnell**, R.A.F. Grieve, *Energy, Mines and Resources, Earth Physics Branch, Ottawa, ON, Canada*. THE CANADIAN GRAVITY DATABASE
- I.E.09 **K.S. Murty**, *University Dept. of Geology, Nagpur, India*. PROCESSING AND DISSEMINATION OF GEOSCIENCE DATA: INDIA
- I.E.10 **R. Siwecki**, *Polish Academy of Sciences, Institute of Oceanology, Sopot, Poland*. OCEANOGRAPHICAL DATABASE IN INSTITUTE OF OCEANOLOGY P.A.S.
- I.E.11 **G.A. Wilkins**, *Royal Greenwich Observatory, East Sussex, UK*; C.D. Boucher, *Institut Géographique National, Saint-Mandé, France*; M. Feissel, *Bureau International de l'Heure, Paris, France*. THE MERIT/COTES DATABASE ON THE ROTATION OF THE EARTH AND TERRESTRIAL REFERENCE SYSTEMS
- I.E.12 **D. Vitorović**, P.A Pfendt, S.R. Niketić, V.D. Krsmanović, *Institute of Chemistry, University of Belgrade, Belgrade, Yugoslavia and Institute of Chemistry, Technology and Metallurgy, Belgrade, Yugoslavia*. CORRELATION OF SOME PORPHYRIN METALS WITH GEOCHEMICAL PARAMETERS OF ALEKSINAC (YUGOSLAVIA) OIL SHALE
- I.E.13 **M. Carapezza**, P.M. Nuccio, M. Valenza, *Istituto di Mineralogia, Petrografia e Geochemica, Palermo, Italy*. GEOCHEMICAL OBSERVATIONS IN THE PHLEGRAEAN FIELDS (ITALY) IN RESPONSE TO THE BRADYSEISMIC ACTIVITY
- I.E.14 **J.J. Royer**, *Centre de Recherches Pétrographiques et Géochimiques, Vandoeuvre-lès-Nancy, France*. COLLECTE, TRAITEMENT ET VALIDATION DES DONNÉES EN GEOSCIENCE: L'IMPRECIS ET LE CERTAIN
- I.E.15 **B. Namysłowska-Wilczyńska**, *Technical University of Wrocław, Institute of Geotechnics, Wrocław, Poland*. AN APPLICATION OF THE GEOSTATISTICAL MODEL TO THE EVALUATION OF COPPER ORE DEPOSIT

SESSION I-F - DATABASE MANAGEMENT AND DATA HANDLING

- I.F.01 **K.-J. Farn**, *Industrial Technology Research Institute, Hsinchu, China*. RELATIONAL DATABASE DESIGN FOR SCIENCE/TECHNOLOGY DATA MANAGEMENT
- I.F.02 **J.M. Hushon**, T.J. Conry, *BBN Laboratories Incorporated, Arlington, VA, USA*. DEVELOPMENT OF MICROCOMPUTER GATEWAY TECHNOLOGY TO ACCESS COMMERCIAL DATABASES
- I.F.03 **E.J. Otoo**, *Carleton University, School of Computer Science, Ottawa, ON, Canada*. MULTIKEY TRIE HASHING FOR SCIENTIFIC AND STATISTICAL DATABASES
- I.F.04 **E.M. Pearson**, *University of Guelph Library, Guelph, ON, Canada*. COMPUTER CONFERENCING AND RESEARCH COMMUNICATION - POTENTIALS FOR THE SCIENTIFIC COMMUNITY
- I.F.05 **O. Thierry**, C. Rolland, *CRIN, Vandoeuvre-les-Nancy, France*. PLUSIEURS EXPÉRIENCES DE GESTION DE DONNÉES EN INFORMATIQUE DE GESTION
- I.F.06 **I. Mistrik**, *GID, Heidelberg, FRG*; G. Kerschhacker, E. Bertha, *IMD, Graz, Austria*. AN INTEGRATED SOFTWARE FOR FLEXIBLE INFORMATION MANAGEMENT
- I.F.07 **J. Rumble, Jr.**, *National Bureau of Standards, Office of Standard Reference Data, Gaithersburg, MD, USA*. DATABASES IN THE SCIENTIFIC AND TECHNICAL DATA CYCLE
- I.F.08 **J.H. Westbrook**, W. Grattidge, *Sci-Tech Knowledge Systems, Scotia, NY, USA*; W. Novinger, *Data Management Associates, Albany, NY, USA*. A VERSATILE DATA CAPTURE SYSTEM FOR ARCHIVAL GRAPHICS AND TEXT
- I.F.09 **E.L. Curry**, *Texas Woman's University, School of Library and Information Studies, Denton, TX, USA*. INTERFACE STANDARDS OF ONLINE BIBLIOGRAPHIC RETRIEVAL SYSTEMS
- I.F.10 **C. Frasson**, *Université de Montréal, Dép. Informatique et Recherche Opérationnelle, Montréal, PQ, Canada*. EVOLUTION DE LA MANIPULATION DANS LES BASES DE DONNEES
- I.F.11 **F. Mie**, *Gesellschaft für Information und Dokumentation (GID), Sektion für Systementwicklung, Heidelberg, FRG*. THE USER INTERFACE FOR FACT RETRIEVAL IN CHEMICAL AND MATERIAL DATA BANKS
- I.F.12 **Z. Kierzkowski**, *Technical University of Poznan, Regional Computer Science Center, Poznan, Poland*. SCIENTIFIC AND TECHNICAL DATABASES IN THE CREATION OF COMPUTER AIDING SYSTEMS
- I.F.13 **J. Christian**, *Memorial University of Newfoundland, Faculty of Engineering and Applied Science, St. John's, NF, Canada*. THE DEVELOPMENT OF THE USE OF MICROCOMPUTERS IN THE CONSTRUCTION INDUSTRY
- I.F.14 **A.S. Kertes**, E. Grushka, Y. Wolman, *The Hebrew University, Institute of Chemistry, Jerusalem, Israel*. THE EXPERT'S ROLE IN BUILDING AN EXPERT SYSTEM. THE CASE OF SEPARATION CHEMISTRY AND TECHNOLOGY
- I.F.15 **C. Michelsen**, D. Shafer, *Los Alamos National Laboratory, Administrative Data Processing Division, Los Alamos, NM, USA*. LOGICAL AND PHYSICAL DATABASE DESIGN WITHIN A FULL-TEXT ENVIRONMENT

SESSION I-G - NATIONAL AND INTERNATIONAL DATA PROGRAMS

- I.G.01 **B. Marx**, *Ministère de l'éducation nationale, Direction des bibliothèques, des musées et de l'information scientifique et technique, Paris, France*. BANQUES DE DONNÉES DE LA RECHERCHE SCIENTIFIQUE ET TECHNIQUE EN FRANCE
- I.G.02 **K.L. Loening**, *Chemical Abstracts Service, Columbus, OH, USA*; **E.F. Westrum Jr.**, *University of Michigan, Ann Arbor, MI, USA*; **D.R. Lide Jr.**, *US National Bureau of Standards, Gaithersburg, MD, USA*. CURRENT IUPAC DATA COMPILATION PROJECTS AND RECOMMENDED IUPAC SYMBOLS AND UNITS
- I.G.03 **F.J. Smith**, *University of Connecticut, Dept. of Computer Science, Storrs, CT, USA*. A SIMPLE RETRIEVAL SYSTEM FOR THE CODATA REFERRAL DATABASE
- I.G.04 **B.B. Molino**, *National Bureau of Standards, Office of Standard Reference Data, Gaithersburg, MD, USA*. NATIONAL STANDARD REFERENCE DATABASE SERIES
- I.G.05 **B.B. Molino**, *National Bureau of Standards, Office of Standard Reference Data, Gaithersburg, MD, USA*. CODATA REFERRAL DATABASE
- I.G.06 **E. Sutter**, *Association Française de Normalisation, Paris la Defence, France*. LES DONNÉES EXTRAITES DES NORMES: DES DONNÉES VALIDÉES POUR L'INDUSTRIE
- I.G.07 **X. Zhang**, *Academia Sinica, Scientific Databases, Beijing, China*. SOME CONSIDERATIONS IN DESIGNS FOR ESTABLISHING CHINA'S SCIENTIFIC INFORMATION SYSTEMS

SESSION I-H - MATERIALS DATABASES

- I.H.01 **R. Krefeld**, *Joint Research Center Petten Establishment, Petten, The Netherlands*; **G. Fattori**, *Joint Research Center Ispra Establishment, Ispra, Italy*. CONCEPT OF A USER INTERFACE FOR A HIGH TEMPERATURE MATERIAL DATA BANK AND ITS APPLICATION IN A MATERIAL SCIENCE ENVIRONMENT
- I.H.02 **M. Yamazaki**, *Electrotechnical Laboratory, Ibaraki, Japan*. A DESIGN AID EXPERT SYSTEM FOR SEMICONDUCTOR HETERO STRUCTURES
- I.H.03 **J.-P. Caliste**, *Laboratoire National D'Essais, Paris, France*. REFDATA - BANQUE DE DONNÉES NUMÉRIQUE SUR LES MATÉRIAUX DE RÉFÉRENCE

TUESDAY, July 15 - A.M.

SESSION II-A - DATA STRUCTURE AND ACCESS

- II.A.01 **J.L. McCarthy**, *Lawrence Berkeley Laboratory, Computer Science Research Department, Berkeley, CA, USA*. THE STRUCTURE OF SCIENTIFIC DATA: IMPLICATIONS FOR MANAGEMENT AND EXCHANGE OF TECHNICAL INFORMATION
- II.A.02 **H. Bestougeff**, *Université Paris VII, Paris, France*. APPLICATIONS OF DATABASE AND KNOWLEDGE-BASED SYSTEMS TO SCIENTIFIC DATA
- II.A.03 **Y. Fujiwara**, *University of Tsukuba, Institute of Electronics and Information Sciences, Ibaraki, Japan*. DATABASES AND KNOWLEDGE BASES AS SCIENTIFIC RESEARCH TOOLS
- II.A.04 **R. Luckenbach**, *Beilstein Institute, Frankfurt, FRG*. CHEMICAL HANDBOOKS ONLINE: STATUS QUO AND PERSPECTIVES

TUESDAY, July 15 - P.M.

SESSION II-B - DATA FOR NATURAL RESOURCES INDUSTRIES

- II.B.01 **G. Hacklin**, *Brooke, Hunt & Associates Ltd., Surrey, UK*. TITLE NOT AVAILABLE
- II.B.02 **R.O. Lindseth**, *Teknica Resource Development Ltd., Calgary, AB, Canada*. SEISMIC SURVEYING FOR PETROLEUM - THE FIRST 50 YEARS
- II.B.03 **H. Langer**, *Dechema, Frankfurt, FRG*. COALDATA - A COLLECTION OF NUMERICAL DATA ON COAL, COAL LIQUIDS AND COAL CHEMICALS
- II.B.04 **S. Jucha**, *Academy of Mining & Metallurgy, Krakow, Poland*. COMPUTER EVALUATION OF PETROLEUM RESOURCES BASED ON DRILLING, SEISMIC AND LABORATORY EXPERIMENTAL DATA: A NOVEL APPROACH

SESSION II-C - BIOSCIENCES DATA

- II.C.01 **V.A. Erdmann**, **J. Wolters**, **T. Pieler**, **M. Digweed**, **S. Lorenz**, **N. Ulbrich**, *Freie Universität Berlin, Institut für Biochemie, Berlin, FRG*. COMPUTER ANALYSIS OF RIBOSOMAL 5S RNA SEQUENCES AND THEIR CORRELATION WITH BIOCHEMICAL STRUCTURAL DATA
- II.C.02 **B. Keil**, *Institut Pasteur, Paris, France*. PROTEIN DATABASE NETWORK - AN INDISPENSABLE ELEMENT OF FUNDAMENTAL INFORMATION IN BIOLOGY

- II.C.03 **G.R. Howe**, *University of Toronto, National Cancer Institute of Canada Epidemiology Unit, Toronto, ON, Canada*. THE USE OF DATABASES AND COMPUTERIZED RECORD LINKAGE IN EPIDEMIOLOGY
- II.C.04 **J.P. Doucet**, *Institut de Topologie et de Dynamique des Systèmes, Paris, France*. IMAGERIE MOLECULAIRE ET SIMULATION DE DONNÉES THEORIQUES

SESSION II-D - SCIENTIFIC AND TECHNICAL DATABASES

- II.D.01 **D. Hammer**, *Institut für Informatik und Rechentechnik der AdW der DDR, Berlin, DDR*. RESEARCH DATABASES IN THE ACADEMY OF SCIENCES OF THE GDR
- II.D.02 **G. Effenberg**, G. Petzow, E.Th. Henig, *Max-Planck-Institut für Metallorschung, Institut für Werkstoffwissenschaften, Stuttgart, FRG*. EVALUATION AND DATABASE STORAGE OF TERNARY ALLOY PHASE DIAGRAMS
- II.D.03 **I. Ansara**, *Domaine Universitaire, Laboratoire de Thermodynamique et Physico-Chimie Métallurgiques-E.N.S.E.E.G., Saint Martin d'Heres, France*. THE SCIENTIFIC GROUP THERMODATA EUROPE - A COOPERATIVE PROJECT IN THERMODYNAMIC DATA BASES
- II.D.04 **C.Y. Ho**, H.H. Li, *Purdue University, CINDAS, West Lafayette, IN, USA*. COMPREHENSIVE, ONLINE, EXPERT NUMERICAL DATA SYSTEM ON MATERIALS PROPERTIES ESTABLISHED AND OPERATIONAL AT CINDAS/PURDUE UNIVERSITY

SESSION II-E - THERMODYNAMIC AND PHASE EQUILIBRIUM DATA

- II.E.01 **D.T. Jamieson**, *National Engineering Laboratory, Glasgow, UK*. PPDS ELECTRONIC DATA MODULE
- II.E.02 **R.A. Alberty**, T.M. Bloomstein, *Massachusetts Institute of Technology, Dept. of Chemistry, Cambridge, MA, USA*. CHEMICAL THERMODYNAMIC DATA FOR GASEOUS ORGANIC SUBSTANCES
- II.E.03 **Z. Xu**, L. Wang, Q. Qi, *Academia Sinica, Institute of Chemical Metallurgy, Beijing, China*; N. Chen, J. Zhu, H. Xu, B. Jiang, *Academia Sinica, Shanghai Institute of Metallurgy, Beijing, China*; B. Chen, *Xian Metallurgy and Architecture College, Beijing, China*. THE PREDICTION OF HIGH TEMPERATURE ENTROPY FOR BINARY OXIDES IN INORGANIC THERMOCHEMISTRY DATA BASE (ITDB)
- II.E.04 **P.D. Desai**, *Purdue University, Center for Information and Numerical Data Analysis and Synthesis, West Lafayette, IN, USA*. HEAT CAPACITY OF SOME KEY ELEMENTS
- II.E.05 **R.C. Wilhoit**, K.N. Marsh, *Texas A&M University, Thermodynamics Research Center, College Station, TX, USA*. DESIGN AND MAINTENANCE OF A LARGE DATABASE OF THERMODYNAMIC DATA FOR PURE COMPOUNDS
- II.E.06 **P. Wang**, L. Wang, Z. Xu, *Academia Sinica, Institute of Chemical Metallurgy, Beijing, China*. INTRODUCTION TO THE AQUEOUS SOLUTIONS THERMODYNAMIC DATA BASE
- II.E.07 **R. Sambasiva Rao**, A. Satyanarayana, *Andhra University, School of Chemistry, Waltair, India*. A KNOWLEDGE BASE FOR STUDY OF COMPLEX EQUILIBRIA IN SOLUTION PHASE
- II.E.08 **G.N. Rao**, P. Vijayalakshmi, K.V. Ramana, R. Sambasiva Rao, *Andhra University, Waltair, India*. A COMPUTER AUGMENTED STUDY OF SOLUTE SOLVENT INTERACTIONS IN AQUODIME-THYL FORMAMIDE MEDIA
- II.E.09 **H. Yokokawa**, *National Chemical Laboratory for Industry, Division of Energy Chemistry, Ibaraki, Japan*. CTC: CHEMICAL THERMODYNAMIC COMPUTATION SYSTEM WITH DATABASE OF INORGANIC COMPOUNDS
- II.E.10 **H. Yokokawa**, *National Chemical Laboratory for Industry, Division of Energy Chemistry, Ibaraki, Japan*; S. Yamauchi, *University of Tokyo, Dept. of Applied Chemistry, Tokyo, Japan*; S. Fujieda, *Ochanomizu University, Dept. of Chemistry, Tokyo, Japan*. MALT: MATERIALS-ORIENTED LITTLE THERMODYNAMIC DATABASE FOR PERSONAL COMPUTERS
- II.E.11 **R. Langhorst**, S. Zeck, H. Knapp, *Technical University of Berlin, Institute of Thermodynamics and Plant Design, Berlin, FRG*. BDBT - BERLIN DATABANK THERMODYNAMICS
- II.E.12 **J. Sangster**, A.D. Pelton, *École Polytechnique de Montréal, Centre de Recherche en Calcul Thermochimique, Montréal, PQ, Canada*. A DATABASE FOR THE CALCULATION OF MOLTEN SALT PHASE DIAGRAMS
- II.E.13 **P.K. Talley**, J. Sangster, A.D. Pelton, C.W. Bale, *École Polytechnique de Montréal, Centre de Recherche en Calcul Thermochimique, Montréal, PQ, Canada*. AN ONLINE COMPUTING SYSTEM FOR ORGANIC MIXTURES
- II.E.14 **C. Frame**, A. San Martin, D. Khatamian, F.D. Manchester, *University of Toronto, Dept. of Metallurgy & Materials Science, Toronto, ON, Canada*; G.C. Weatherly, *University of Toronto, Dept. of Physics, Toronto, ON, Canada*. COMPILATION OF PHASE DIAGRAMS FOR HYDROGEN IN METAL SYSTEMS
- II.E.15 **G. Drăgan**, *ICECHIM-CCF, Bucharest, Romania*. SOLUBILITY DATA BANKS BASED ON TOPOENERGETIC PRINCIPLES
- II.E.16 **D. Garvin**, V.B. Parker, *National Bureau of Standards, Center for Chemical Physics, Gaithersburg, MD, USA*. CODATA CHEMICAL THERMODYNAMIC DATABASES FOR SCIENCE AND TECHNOLOGY
- II.E.17 **C.F. Spencer**, M.W. Kellogg, *CODATA Task Group on Data for the Chemical Industry, Houston, TX, USA*. DATA FOR THE CHEMICAL INDUSTRY - AN OVERVIEW OF INTERNATIONAL DATA PROJECTS AND QUALITY CONTROL OF COMPUTERIZED THERMOPHYSICAL PROPERTY DATABASES
- II.E.18 **R. Pohorecki**, A. Dlugosz, *Warsaw Technical University, Dept. of Chemical Engineering, Warsaw, Poland*. USE OF THERMODYNAMIC DATA FOR THE FEASIBILITY STUDY OF METAL OXIDE SYSTEMS AS DESULFURANTS AT HIGH TEMPERATURES
- II.E.19 **V.Yu. Mindin**, *Academy of Sciences of GSSR, Geological Institute, Tbilisi, USSR*. SYSTEM OF PROGRAMMES FOR MIÑICOMPUTERS, INCLUDING THE BASE OF THERMODYNAMIC DATA - THE EXPERIENCE OF THE WORKING OUT, AND USING FOR CALCULATIONS MULTICOMPONENT EQUILIBRIA IN CHEMISTRY, METALLURGY, GEOLOGY

- III.B.02 **G. Östberg**, *University of Lund, Engineering Materials, Lund, Sweden*. OVERVIEW OF THE CODATA MATERIALS WORKSHOP AT SCHLUCHSEE IN SEPTEMBER 1985
- III.B.03 **J.W. Hastie**, *National Bureau of Standards, Ceramic Division, Gaithersburg, MD, USA*. THE NBS-ACeS CERAMIC PHASE DIAGRAM DATA PROGRAM
- III.B.04 **L.B. Sibley**, *Tribology Consultants Inc., Paoli, PA, USA*; **M.B. Peterson**, *Wear Sciences Corporation, Arnold, MD, USA*; **T. Levinson**, *DOE Headquarters, Washington, DC, USA*. DEVELOPMENT OF THE DOE/ECUT AND NBS COMPUTERIZED TRIBOLOGY DATABASES AND INFORMATION SERVICE

SESSION III-C - MODELLING IN THE GEOSCIENCES

- III.C.01 **I.L. Khodakovsky**, **V.I. Vernadsky**, *USSR Academy of Sciences, Institute of Geochemistry and Analytical Chemistry, Moscow, USSR*. FEEDBACK OF ALGORITHMS OF THERMODYNAMIC DATA CORRELATION AND COMPUTER SIMULATION IN GEOLOGICAL SYSTEMS
- III.C.02 **K. Wadatsumi**, *Osaka City University, Dept. of Geosciences, Osaka, Japan*. DEVELOPMENT AND USAGE OF ACCUMULATIVE FILE SYSTEM IN GEOSCIENCE
- III.C.03 **R.V. Moore**, *Natural Environment Research Council, Institute of Hydrology, Wallingford, UK*. DIGITAL MAPPING IN HYDROLOGY
- III.C.04 **M.I. Petaev**, **G.I. Ruzajkin**, **Yu.A. Shukolyukov**, **A.A. Yavnel**, *USSR Academy of Sciences, V.I. Vernadsky Institute of Geochemistry and Analytical Chemistry, Moscow, USSR*. METEORITE DATABANK: GENERAL PRINCIPLES OF ORGANIZATION

SESSION III-D - PHYSICAL AND CHEMICAL DATA FOR ADVANCED TECHNOLOGIES

- III.D.01 **F.P. Okamura**, *National Institute for Research in Inorganic Materials, Ibaraki, Japan*. APPLICATION OF DATABASES TO CAD OF INORGANIC MATERIALS
- III.D.02 **A.D. Pelton**, *École Polytechnique de Montréal, Centre de Recherche en Calcul Thermochimique, Montréal, PQ, Canada*. NUMERICAL DATABASES AND THERMODYNAMIC COMPUTATIONS IN METALLURGY AND MATERIALS SCIENCE
- III.D.03 **K.B. McAfee, Jr.**, *AT&T Bell Laboratories, Murray Hill, NJ, USA*. MODELLING ELECTRONIC MATERIALS PREPARATIONS AND PROCESSES - OPTICAL COMMUNICATIONS FIBRES AND III-V SEMICONDUCTORS
- III.D.04 **L.V. Gurvich**, *Academy of Sciences USSR, Institute for High Temperatures, Moscow, USSR*. DATA BANK ON THERMODYNAMIC PROPERTIES AS EXAMPLE OF SOME PROBLEMS IN CREATION OF CHEMICAL DATABASES

SESSION III-E - ENVIRONMENTAL AND AGRICULTURAL DATA

- III.E.01 **S.R. Heller**, **S.L. Rawlins**, *Agricultural Research Service, US Department of Agriculture, Beltsville, MD, USA*. THE AGRICULTURAL RESEARCH SERVICE SYSTEMS RESEARCH ACTIVITIES
- III.E.02 **J.C. Hock**, *National Oceanic and Atmospheric Administration, Washington, DC, USA*. GLOBAL ENVIRONMENTAL MONITORING OF RENEWABLE RESOURCES
- III.E.03 **R.H. Kummier**, **S.O. Salley**, *Wayne State University, Dept. of Chemical Engineering and Urban Science Applications Inc., Detroit, MI, USA*. A DATA MANAGEMENT SYSTEM FOR THE DETROIT INDUSTRIAL PRETREATMENT PROGRAM
- III.E.04 **C.M. Benkovitz**, *Brookhaven National Laboratory, Dept. of Applied Science, Upton, NY, USA*. IMPLEMENTATION OF A DATABASE IN SUPPORT OF A LARGE SCALE SCIENTIFIC EXPERIMENT
- III.E.05 **J.L. Tichler**, *Brookhaven National Laboratory, Atmospheric Sciences Division, Upton, NY, USA*. DATA MANAGEMENT OF A MULTILABORATORY FIELD PROGRAM USING DISTRIBUTED PROCESSING
- III.E.06 **M.J. Leach**, **H.J. Bernstein**, **J.L. Tichler**, **R.J. Moran**, **L.L. Lawrence**, **D.W. Niebuhr**, **P.A. Kessler**, *Brookhaven National Laboratory, Dept. of Applied Science, Upton, NY, USA*. THE ACQUISITION, USE, AND ARCHIVING OF REAL-TIME WEATHER DATA
- III.E.07 **D.G. Swartz**, **D. Jacobs**, **R.R. Colwell**, *University of Maryland, Sea Grant College, College Park, MD, USA*. DEVELOPMENT OF SPECIALIZED MAPPING PROGRAMS TO REPRESENT ENVIRONMENTAL DATA
- III.E.08 **C.T. Cushwa**, **F.A. Servello**, *Virginia Polytechnic Institute and State University, Dept. of Fisheries and Wildlife Sciences, Blacksburg, VA, USA*. STATUS, DEVELOPMENT, IMPLEMENTATION AND APPLICATIONS OF COMPUTERIZED FISH AND WILDLIFE INFORMATION SYSTEMS
- III.E.09 **J.R. Thieman**, **J.H. King**, *NASA Goddard Space Flight Center, National Space Science Data Center, Greenbelt, MD, USA*. NASA/NSSDC CENTRAL ONLINE DATA DIRECTORY (Codd)
- III.E.10 **B.E. Lowrey**, *NASA Goddard Space Flight Center, National Space Science Data Center, Greenbelt, MD, USA*. A PLAN FOR DISSEMINATING AND COORDINATING THE DATA FROM THE DIVERSE EXPERIMENTS OF THE DYNAMICS EXPLORER SATELLITE SYSTEM
- III.E.11 **D.M. Sawyer, Jr.**, *NASA Goddard Space Flight Center, National Space Science Center, Greenbelt, MD, USA*. SPACE DATA CATALOGS: CONCEPTUAL MODEL FOR REPRESENTATION AND AUTOMATED UPDATE
- III.E.12 **D. Zhang**, **P. Yang**, **Z. Sun**, *Nanjing University, Computer Science Dept., Nanjing, China*. SN-2: A DATA ACQUISITION AND PROCESSING SYSTEM

- II.E.20 **D.F. Redmiles**, J.S. Sims, C.L. Qualey, J.L. Murray, *National Bureau of Standards, Metallurgy Division, Gaithersburg, MD, USA*. NUMERICAL AND GRAPHICAL DATABASE FOR ALLOY PHASE DIAGRAMS
- II.E.21 **Yu.V. Semenov**, A.I. Shapkin, I.L. Khodakovskiy, *USSR Academy of Sciences, Vernadsky Institute of Geochemistry and Analytical Chemistry, Moscow, USSR*. THE PROBLEMS OF CLASSIFICATION AND STORAGE OF THERMODYNAMIC DATA IN COMPUTER SYSTEMS
- II.E.22 **B.A. Grigoryev**, S.A. Plotnikov, *Groznsky Petroleum Institute, Grosny, USSR*. INDUSTRIAL HYDROCARBONS. TABLES OF THERMOPHYSICAL PROPERTIES
- II.E.23 **T.B. Selover**, *Shaker Heights, OH, USA*; E. Buck, *Union Carbide Corporation, Charleston, WV, USA*. A STATUS REPORT OF DIPPR IN ITS SEVENTH YEAR
- II.E.24 **J.R. Dennis**, P.J. Schenck, *National Bureau of Standards, Ceramics Division, Gaithersburg, MD, USA*. COMPUTER GRAPHICS FOR CERAMIC PHASE DIAGRAMS
- II.E.25 **J.P. Bros**, M. Gaune-Escard, G. Hatem, N. Mossarello, Y. Fouque, *Université de Provence, S.E.T.T., Marseille, France*. THERMODYNAMIC DATA COMPILATION OF MOLTEN SALT MIXTURES
- II.E.26 **M. Gaune-Escard**, N. Mossarello, *Université de Provence, S.E.T.T., Marseille, France*. THERMODYNAMIC DATA COMPILATION OF MOLTEN SALT MIXTURES. CRITICAL ASSESSMENT OF THE $\text{KNO}_3\text{-NaNO}_3\text{-RbNO}_3$ TERNARY SYSTEM

SESSION II-F - BIOSCIENCE, NUTRITION AND TOXICOLOGY DATA

- II.F.01 **A.S. Kolaskar**, *Centre for Cellular and Molecular Biology, Hyderabad, India*. ANALYSIS OF BIOMACROMOLECULAR DATA
- II.F.02 **S.C. Skoryna**, *McGill University, Medical Research Unit, Montreal, PQ, Canada*; J.T. Nolan, *Université de Montréal, Dép. de Biologie, Montréal, PQ, Canada*. ANALYSIS OF STOCHASTIC PROCESSES IN THE CAUSATION OF GASTRIC CANCER
- II.F.03 **J.T. Nolan**, R.J. Pivon, J. Perras, G. Cousineau, S.C. Skoryna, *St. Mary's Hospital Center, Medical Research Unit, Montreal, PQ, Canada*. APPLICATION OF DATABASES IN CLINICAL STUDIES OF CHRONIC ALCOHOLICS
- II.F.04 **M. Larue**, M. Baril, G. Lapointe, *Commission de la santé et de la sécurité du travail du Québec, Répertoire toxicologique, Montréal, PQ, Canada*. INFOTOX, BANQUE DE DONNÉES DU RÉPERTOIRE TOXICOLOGIQUE DE LA COMMISSION DE LA SANTÉ ET DE LA SÉCURITÉ DU TRAVAIL DU QUÉBEC
- II.F.05 **D.D. Singer**, *Ministry of Agriculture, Fisheries and Food, London, UK*. THE NEW UK NUTRIENT DATABASE
- II.F.06 **W.M. Rand**, *Massachusetts Institute of Technology, INFOODS, Cambridge, MA, USA*. PROBLEMS AND STATUS OF FOOD COMPOSITION DATA
- II.F.07 **P.Y. Lu**, J.T. Ensminger, S.M. Hubner, *Oak Ridge National Laboratory, Oak Ridge, TN, USA*. GENERATION OF MATERIAL SAFETY DATA SHEETS
- II.F.08 **J.S. Leitzke**, *US Environmental Protection Agency, Office of Toxic Substances, Washington, DC, USA*. CECATS AND THE TRACKING OF ASSESSMENTS BY THE CHEMICAL SCREENING BRANCH
- II.F.09 **W.C. Barker**, S.L. Chen, D.G. George, *National Biomedical Research Foundation, Protein Identification Resource, Washington, DC, USA*. COMPATIBLE FORMATS FOR PROTEIN AND NUCLEIC ACID SEQUENCE DATABASES
- II.F.10 **W.C. Barker**, D.G. George, *National Biomedical Research Foundation, Protein Identification Resource, Washington, DC, USA*. UTILITY OF INDEXES GENERATED FROM PROTEIN AND NUCLEIC ACID SEQUENCE DATABASES
- II.F.11 **R.R. Butrum**, J.A.T. Pennington, *National Institutes of Health, NCI, Division of Cancer Prevention and Control, Bethesda, MD, USA*. TERMINOLOGY SYSTEMS USED FOR FOOD COMPOSITION DATABASES: AN HISTORICAL PERSPECTIVE
- II.F.12 **E. Styczynska-Jurewicz**, Z. Klusek, *Polish Academy of Science, Institute of Oceanology, Sopot, Poland*. MICROCOMPUTER EVALUATION OF ECHOSOUNDING DATA ON KRILL SWARMS

WEDNESDAY, July 16 - A.M.

SESSION III-A - DATA HANDLING AND DISSEMINATION

- III.A.01 **C.C. Gotlieb**, *University of Toronto, Dept. of Computer Science, Toronto, ON, Canada*. OPTIONS FOR DISSEMINATION
- III.A.02 **J. Hilsenrath**, *Silver Spring, MD, USA*. MICRO COMPUTERS FOR DATA CORRELATION. DISSEMINATION AND USE
- III.A.03 **T. Yamamoto**, *University of Library and Information Science, Tsukuba Academic City, Japan*. DATA HANDLING IN THE AGE OF EXPERT SYSTEMS
- III.A.04 **R.J. Feldmann**, *National Institutes of Health, Division of Computer Research and Technology, Bethesda, MD, USA*. MOLECULAR MODELLING: INTERPOLATING BETWEEN STRUCTURE DATA POINTS

WEDNESDAY, July 16 - P.M.

SESSION III-B - ADVANCES IN MATERIALS DATABASES

- III.B.01 **A.D. Kozlov**, *VNIIMS, Moscow, USSR*. INDUSTRIAL MATERIALS DATABANKS. BASIC PRINCIPLES AND PROBLEMS OF ORGANIZATION

- III.E.13 J. Chen, J. Che, X. Zeng, C. Sun, G. Tang, *Fudan University, Dept. of Nuclear Science, Shanghai, China*. ANALYSIS OF ATMOSPHERIC AEROSOL COMPOSITIONS
- III.E.14 P. Kanciruk, L. Hook, R. McCord, *Oak Ridge National Laboratory, Environmental Sciences Division, Oak Ridge, TN, USA*. RESEARCH DATA MANAGEMENT FOR A LARGE ENVIRONMENTAL SURVEY
- III.E.15 L.J. Allison, R.J. Olson, I.L. Munroe, *Martin Marietta Energy Systems Inc., Information Resources Organization, Oak Ridge, TN, USA*. ADDNET: THE ACID DEPOSITION DATA NETWORK
- III.E.16 R.J. Olson, R.C. Durfee, D.L. Wilson, *Oak Ridge National Laboratory, Oak Ridge, TN, USA*. A GEOGRAPHIC INFORMATION SYSTEM USED TO STUDY ACIDIC DEPOSITION
- III.E.17 M.P. Farrell, T.A. Boden, *Oak Ridge National Laboratory, Information Resources Organization, Oak Ridge, TN, USA*. WORLDWIDE DISTRIBUTION OF DATA: CO₂-RELATED NUMERIC DATA PACKAGES

SESSION III-F - CHEMICAL REACTION, STRUCTURE AND KINETICS

- III.F.01 C.D. Wagner, *Surfex Company, Oakland, CA, USA*. THE DATA BANK IN X-RAY PHOTOELECTRON SPECTROSCOPY
- III.F.02 A.B. Ross, W.P. Helman, *University of Notre Dame, Radiation Chemistry Data Center, Notre Dame, IN, USA*. NUMERIC DATABASES FOR RADICAL PROCESSES IN AQUEOUS SOLUTION
- III.F.03 A.B. Ross, I. Carmichael, G.L. Hug, W.P. Helman, *University of Notre Dame, Radiation Chemistry Data Center, Notre Dame, IN, USA*. NUMERIC DATABASES FOR PHOTOCHEMICAL AND PHOTOPHYSICAL PROCESSES IN SOLUTION
- III.F.04 I.D. Brown, U.D. Altermatt, *McMaster University, Institute for Materials Research, Hamilton, ON, Canada*. SOFTWARE FOR THE INORGANIC CRYSTAL STRUCTURE DATABASE
- III.F.05 Z. Qian, *Academia Sinica, Institute of Chemical Metallurgy, Beijing, China*. COMPUTER APPLICATION IN CHARACTERIZING FLUIDIZATION BY THE BED OF COLLAPSING METHOD
- III.F.06 X. Li, *Academia Sinica, Institute of Chemical Metallurgy, Beijing, China*. COMPUTERIZED FLUIDIZATION SYSTEM
- III.F.07 W. Tsang, *National Bureau of Standards, Chemical Kinetics Division, Gaithersburg, MD, USA*. EVALUATED KINETIC DATABASE FOR COMBUSTION CHEMISTRY
- III.F.08 V.L. Himes, A.D. Mighell, *National Bureau of Standards, Reactor Radiation Division, Gaithersburg, MD, USA*. THE NBS CRYSTAL DATA FILE: COMPOUND IDENTIFICATION AND CHARACTERIZATION USING LATTICE-MATCHING TECHNIQUES
- III.F.09 R.W.A. Oliver, *University of Salford, Dept. of Biological Sciences, Salford, UK*; K.R. Davies, *University of Salford, Library, Salford, UK*. A REVIEW OF MASS SPECTRAL DATABASES
- III.F.10 P.E. Tomaszewski, K. Lukaszewicz, *Polish Academy of Sciences, Institute for Low Temperature and Structure Research, Wroclaw, Poland*. DATABASE OF STRUCTURAL PHASE TRANSITIONS IN CRYSTALS
- III.F.11 A. Panaye, J.P. Doucet, P. Peguet, J.E. Dubois, *CNRS, Institut de Topologie et de Dynamique des Systèmes, Paris, France*. SIMULATION DE SPECTRES INFRA-ROUGE PAR APPROCHE TOPOLOGIQUE DARC - SYSTÈME SIRS
- III.F.12 D.G. Cameron, D.J. Hooley, J. Thompson, S. White, E. Armstrong, J.R. Mooney, *The Standard Oil Company (Ohio), Cleveland, OH, USA*. TOWARDS A LABORATORY INFORMATION MANAGEMENT SYSTEM FOR AN ANALYTICAL LABORATORY
- III.F.13 K. Okasi, *Osaka University, Protein Research Institute, Osaka, Japan*; H. Takeda, *University of Tokyo, Mineralogical Institute, Tokyo, Japan*; N. Yasuoka, *Himeji Institute of Technology, Hyogo, Japan*. AN ATTEMPT AT DATA CONVERSION ON CRYSTAL STRUCTURE DATA
- III.F.14 G. Sicouri, P. Chambert, Y. Sobel, J.E. Dubois, *Institute de Topologie et de Dynamique des Systèmes, Paris, France*. CONSTITUTION PAR APPRENTISSAGE D'UNE DE CONNAISSANCES SUR LA FAISABILITÉ DES REACTIONS
- III.F.15 X. Lu, G. Li, S. Wang, K. Zhao, J. Sun, *Academia Sinica, Changchun Institute of Applied Chemistry, Jilin, China*. CARBON-13 NRM SEARCH SYSTEM WITH MICROCOMPUTER FOR STRUCTURE INTERPRETATION OF ORGANIC COMPOUNDS
- III.F.16 J. Zhou, A.D. Mighell, *National Bureau of Standards, Office of Standard Reference Data, Gaithersburg, MD, USA*. THE NBS CRYSTAL DATA FILE: DATA DISSEMINATION AND STATISTICS

SESSION III-G - PHYSICS DATA

- III.G.01 M.R. Whalley, *University of Durham, Dept. of Physics, Durham, UK*. DATA COMPILATIONS IN PARTICLE PHYSICS: THE IMPORTANCE OF THE USER AND OF INTERNATIONAL COLLABORATIONS
- III.G.02 J.W. Gallagher, P.L. Ruttenberg, *University of Colorado, Joint Institute for Laboratory Astrophysics, Boulder, CO, USA*. THE ATOMIC COLLISIONS DATABASE
- III.G.03 W.H. Warren Jr., *NASA Goddard Space Flight Center, Astronomical Data Center, Greenbelt, MD, USA*. THE TREATMENT OF CATALOG DATA IN ASTRONOMY AND ASTROPHYSICS
- III.G.04 M. Suffczynski, *Polish Academy of Sciences, Institute of Physics, Warsaw, Poland*. BINDING ENERGY DATA FOR NEGATIVE IONS AND DIMERS OF ELEMENTS
- III.G.05 H. Xu, C. Ren, J. Tang, F. Yang, *Fudan University, Dept. of Nuclear Science, Shanghai, China*. PRECISE DETERMINATION OF PROTON INDUCED K-SHELL IONIZATION CROSS-SECTION

THURSDAY, July 17 - A.M.

SESSION IV-A - INTERNATIONAL COOPERATION

- IV.A.01 **K. Mooson**, Z. Xu, *Academia Sinica, Institute of Chemical Metallurgy, Beijing, China*. OVERVIEW OF CHINA'S SCIENTIFIC DATABASE
- IV.A.02 **A.D. Kozlov**, *VNIIMS, Moscow, USSR*. SYSTEMS OF STANDARDS AND REFERENCE DATA OF COMECON
- IV.A.03 **G. Steven**, H. Krockel, *Commission of the European Communities, Luxembourg*. THE INTEGRATION OF MATERIALS PROPERTIES DATABANKS INTO A COOPERATIVE EUROPEAN DATA SUPPLY SYSTEM
- IV.A.04 **M. Graham**, *Exxon Research & Engineering Company, Florham Park, NJ, USA*. INDUSTRIAL DATA SHARING IN A MULTINATIONAL ORGANIZATION
- IV.A.05 **W.W. Hutchison**, *Energy, Mines and Resources Canada, Earth Sciences Sector, Ottawa, ON, Canada*. CODATA EVOLVES

THURSDAY, July 17 - P.M.

SESSION IV-B - REPORT ON CODATA WORKSHOP - ENVIRONMENTAL DATA

- IV.B.01 **J.H. Hahn**, *Max-Planck-Institut fuer Chemie, Mainz, FRG*. DIRECTIONS FOR INTERNATIONALLY COMPATIBLE DATA ON BACKGROUND ATMOSPHERIC POLLUTION
- IV.B.02 **J. Forslund**, *National Agency of Environmental Protection, Copenhagen, Denmark*. ENVIRONMENTAL MEASUREMENTS IN WATER
- IV.B.03 **B.-O. Fabricius**, *University of Helsinki, Dept. of Microbiology, Helsinki, Finland*. ENVIRONMENTAL MEASUREMENTS IN SOILS/BIOTA
- IV.B.04 **G.C. Carter**, *National Academy of Sciences, Numerical Data Advisory Board, Washington, DC, USA*. ENVIRONMENTAL DATA MANAGEMENT

SESSION IV-C - EXPERT SYSTEMS IN THE PHYSICAL SCIENCES

- IV.C.01 **R. Michelsen**, *Los Alamos National Laboratory, Los Alamos, NM, USA*. EXPLOITING PARALLELISM IN EXPERT SYSTEMS
- IV.C.02 **G. Guiho**, *Compagnie generale d'electricité centre de recherche, Division de l'informatique, Marcoussis, France*. EXPERT SYSTEMS: A CHALLENGE FOR INDUSTRY
- IV.C.03 **W. Wahlster**, *FRG*. ROLE OF NATURAL LANGUAGE IN ADVANCED KNOWLEDGE BASED SYSTEMS
- IV.C.04 **E.W. Hoffmann**, *National Center of Scientific and Technological Information, Tel-Aviv, Israel*. CHARACTERIZATION AND IDENTIFICATION OF EXPERT SYSTEMS

SESSION IV-D - DATA FOR INDUSTRIAL PROCESS CONTROL

- IV.D.01 **D. Robertson**, *Imperial college of Science and Technology, Dept. of Metallurgy and Materials Science, London, UK*. TITLE NOT AVAILABLE
- IV.D.02 **C.B. Alcock**, P.G. Komorowski, *University of Toronto, Toronto, ON, Canada*. REAL TIME DATA ACQUISITION FOR METALLURGICAL PILOT PLANT OPERATION
- IV.D.03 *TO BE NAMED*
- IV.D.04 **B. Westhead**, *Barry Westhead Associates, Rexdale, ON, Canada*. PROCESS DATA MANAGEMENT

Data Treatment through Education

Although a panel of the National Research Council has concluded that the "accuracy and precision of measurement and the handling, evaluation, tabulation, dissemination, and retrieval of data are, in the eyes of much of the research community, subjects that are second-class, unglamorous, and a nuisance," they suggest means for achieving greater success in coping with these problems. Data must be salvaged in such a form that ultimate tabulation and critical evaluation are possible.

If not, time, talent, scientific and technological progress will be less effective. The Education Panel of U.S.A.'s Numerical Data Board recommends short courses, workshops, college lab instruction, and journal articles be used to help scientists and engineers appreciate the importance of good data practices. The panel's report, "Improving the Treatment of Scientific and Engineering Data Through Education," is available on request from the Numerical Data Advisory Board, National Research

Council, 2101 Constitution Ave., N.W., Washington, D.C. 20418. CODATA'S team members with an educational affiliation should find its 36 pages printed in 1986 of great interest.

IUPAC

The next IUPAC General Assembly will be held in Boston, Massachusetts 21-29 August, 1987 with Professor Robert A. Alberty of Massachusetts Institute of Technology as organizer and Boston University for the site.

New CODATA Publications . . . *

Nonbibliographic Data Banks in Science and Technology. Edited by Stephan Schwarz, David Watson, and Olov Alvfeldt.^a

Database Management in Science and Technology. Edited by John R. Rumble, Jr. and Viktor E. Hampel (reprint edition).^b

Thermodynamic Databases. (Selected Papers from the First CODATA Symposium on Chemical Thermodynamic and Thermophysical Properties Databases, Paris, France, September 1985), Bulletin 58 (November 1985).^c

Thermophysical Properties of Some Key Solids. Heat capacity, thermal expansion, electrical resistivity, thermal conductivity, and absolute thermopower of Cu, Fe, Si, Pt, W, and/or Al₂O₃. (A Report of the CODATA Task Group on Thermophysical Properties of Solids). Edited by Guy K. White and Merrill L. Minges, Bulletin 59 (December 1985).^c

CODATA Constitution Statutes and By-Laws.^d

CODATA Membership Directory 1986-1.^d

Books/Microcomputer Programs . . . *

Thermodynamic Data for Pure Compounds. Part A: hydrocarbons and ketones. Part B: halogenated hydrocarbons and alcohols. Buford D. Smith and Rakesh Srivastava.^e

Standard Potentials in Aqueous Solution. Edited by A.J. Bard, R. Parsons and J. Jordan.^f

University Standards Package of Digital Infrared Spectra for the IBM-PC.^g

Full Spectrum FT-IR Search Libraries.^h

Digital Library ¹³C NMR Spectra of Monomers & Polymers.ⁱ

Standard Infrared Vapor Phase Spectra Volume 24.^j

Capillary Gas Chromatography Retention Index Library.^k

Infrared Polymer Search Libraries for Use on the IBM-PC. Sadtler Basic Digital Monomers and Polymers Library Package, Polymer Library Package, Polymer Additives Library Package, Hummel/Sadtler Polymer Library.^l

Improving the Treatment of Scientific and Engineering Data Through Education. Panel on Education, Numerical Data Advisory Board, Commission on Physical Sciences, Mathematics, and Resources, National Research Council.^m

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

^aPapers presented at a CODATA/Unesco/DFI Seminar, Stockholm, October 15-22, 1983. 1985, ICSU Press, 51 Bl. de Montmorency, 75016, Paris, France. Distributed exclusively by UNIPUB, P.O. Box 1222, Ann Arbor, Michigan 48106, U.S.A. viii + 218 pp. ISBN 0-93057-06X. \$39.50. Cat. No. ICSU-100.

^bA CODATA Sourcebook on the Use of Computers in Data Activities. 1984, Elsevier Science Publishers B.V. (North-Holland), P.O. Box 1991, 1000 BZ Amsterdam, The Netherlands; Elsevier Science Publishing Co., Inc., 52 Vanderbilt Avenue, New York, New York 10017, U.S.A. xiv + 263 pp. ISBN 0-444-86865-8.

^cIndividual copies available for US \$15 from Pergamon Press, Ltd., Headington Hill Hall, Oxford, United Kingdom OX3 0BW.

^dAvailable from the CODATA Secretariat.

^e1986. Elsevier Science Publishers B.V., Sara Burgerhartstraat 25, P.O. Box 211, 1000 AE Amsterdam, The Netherlands; Elsevier Science Publishing Co., Inc., 52 Vanderbilt Avenue, New York, New York 10017, U.S.A. x + 883 pp. ISBN 0-444-42576-4 (Vol. 25A), \$166.75; x + 999 pp. ISBN 0-444-42577-2 (Vol. 25B), \$166.75; Set: ISBN 0-444-42579-9, Set Price \$294.50.

^fMarcel Dekker Inc., New York, 1985, xii + 834 pp.; ISBN 0-8247-7291-1.

^gSadtler Research Laboratories has published the Standard University Package of Digital Infrared Spectra for the IBM-PC. This newly published package of 300 digital spectra is designed to be used by colleges and universities on the IBM-PC for instructional purposes. Price: \$275. This library is packaged together with the Sadtler Infrared IBM-PC Search Software. Sadtler Research Laboratories, 3316 Spring Garden Street, Philadelphia, PA 19104.

^hThese FT-IR search libraries now include over 100,000 spectra with 9,200 Vapor Phase IR spectra and 93,000 Condensed Phase IR spectra. Formatted and configured to operate directly with the FT-IR equipment for which they are intended. Sadtler Research Laboratories, 3316 Spring Garden Street, Philadelphia, PA 19104.

ⁱThe continuing collection includes ¹³C NMR spectra of monomers, polymers and resins. The digital library includes the digital spectrum, Peak Position (ppm), Name File and Number File. The search software also includes the capability of searching by name. All spectra are also available in paper format (8 1/2" x 11" loose leaf sheets housed in heavy-duty, three-ring binders) on 16 mm microfilm (magazine or reel) or on microfiche. Sadtler Research Laboratories, 3316 Spring Garden Street, Philadelphia, PA 19104.

^jThis volume contains spectra from a wide range of samples representing pure compounds of many different functional groups. This library is also available in a digital

format for use with the IBM-PC and FT-IR spectrometer systems. Sadtler Research Laboratories, 3316 Spring Garden Street, Philadelphia, PA 19104.

^kThis library is designed for qualitative analysis using capillary GC. The library, which is available in both printed and fully digitized formats, can be used independently or can be used together with GC/Mass Spec or GC/FT-IR. This first release contains 2000 compounds, including a variety of pollutants and a broad range of simple and complex chemicals selected from Sadtler's Infrared Vapor Phase Spectra Collection. The collection is indexed alphabetically, by molecular formula, molecular weight, CAS Registry No. and Sadtler IR Vapor Phase No. Sadtler Research Laboratories, 3316 Spring Garden Street, Philadelphia, PA 19104.

^lInfrared Polymer Search Libraries are now available for use on the IBM-PC and FT-IR spectrometer systems. The spectra included in these libraries have all been selected and reviewed by experts in the field of polymer chemistry. Each of Sadtler's Polymer Reference Libraries include Sadtler's IBM-PC INFRARED SEARCH SOFTWARE. Sadtler Research Laboratories, 3316 Spring Garden Street, Philadelphia, PA 19104.

^mNational Academy Press, Washington, D.C., 1986. ix + 36 pp. Available from Numerical Data Advisory Board, National Research Council, 2101 Constitution Avenue, N.W., Washington, D.C. 20418.

Decease of Wilhelm Klemm

CODATA has lost one of its distinguished founding officers in the October passing of Professor Klemm. He was, together with Professor Boris Vodar, one of CODATA's first vice-presidents (1966-68) and was subsequently elected to serve as Secretary-Treasurer (1968-72). He was much involved in CODATA's establishment of the Central Office in Frankfurt, F.R.G. This office was CODATA's international focal point for several years after the headquarters were moved from Washington, D.C. until the establishment of the Paris Secretariat.

He served also as an IUPAC Bureau member 1955-63, Vice-President Inorganic Chemistry Division 1955-59, Inorganic Chemistry Nomenclature

Commission and Editorial Board 1959-63. Professor Klemm was elected (1965-67) as the first—and to date the only—German President of IUPAC.

With his death, chemistry loses an eminent man of science who made exceptional contributions to the development of chemistry. He helped German chemistry achieve its high repute and world-wide recognition.

He numbered among the founders of the Society of German Chemists after World War II, and as a member of its Board of Directors, and as President in 1952-53, he so greatly influenced the work and development of the Society that it achieved recognition both at home and abroad.

He had been Director of the Institute of Inorganic Chemistry and Rector of the Wilhelms-University,

Münster in Westphalia, as well as an Honorary Trustee of the University of Münster.

He held memberships in various scientific academies and honorary memberships in numerous scientific societies. He was a recipient of the Great Medal of Merit of the Federal Republic of Germany's Order of Merit. He was awarded the "Carl-Duisberg-Plaque" and the "Liebig-Medal" of the Society of German Chemists, and received other scientific distinctions.

In 1982 the Society of German Chemists founded the "Wilhelm-Klemm-Award" for achievement in inorganic chemistry.

Professor Klemm died on 24 October 1985 at the age of 89.

A New Book—

On Data Banks

The development and use of scientific/technological databases is known to lag behind those in the economics/financial areas and their use has been primarily in developed countries. CODATA in 1983 organized a course in Stockholm, Sweden jointly with Unesco and the Swedish Delegation for Scientific and Technological Information to focus on improving the accessibility, transfer, and dissemination of scientific information on the international scale.

The course had the following objectives:

- to service the current and future role of nonbibliographic data services;
- to describe and critically review nonbibliographic data services and services currently available to different users;
- to analyze the particular problems of data production, data service organization, and utilization of nonbibliographic data in science and technology;
- to examine through R&D case studies problems in the application of nonbibliographic data and lessons to be drawn by data producers, by service organizations, and for user education.

Texts of the lectures were collected and printed in this publication to broaden the impact of this information.

In addition to a guide to generic property databases, special types of databases—such as one for thermochemical calculations in which a normal user will never peruse the information actually stored in the bank, but interact only with application programs utilizing the data (e.g. in Gibbs energy minimization and in the calculation of phase diagrams from thermodynamic data).

The planning and design of numeric database systems (by Rumble) and the overview of database management systems (by Neumann) present very practical education and the warning, "Not surprisingly, in many cases, there is a long time between the promise and the working system, and the best rewards from DBM's come from the smaller well defined systems, not the vast all-encompassing ones."

Finally, the highly animated discussions of the problems of developing countries are aired and the consensus views regarding relevance, strategies and promotion for data service development are provided as recommendations from the training course.

"Nonbibliographic Data Banks in Science and Technology," edited by S. Schwarz, D. Watson, and O. Alvfeldt. (See Newsletter, page 11 for details.)

Standard Potentials

The landmark volume "Oxidation Potentials (or the Oxidation States of the Elements and Their Potentials in Aqueous Solutions)" by Wendell M. Latimer, which was first published in 1938 and last revised in 1952, had an almost "gospel" quality to the amphibious chemists concerned with water solutions. Although rumors and attempts at authorship of an updated successor volume have not been rare, none of the efforts seemed to come to fruition.

Finally in 1977 at the IUPAC General Assembly at Warsaw, Allen J. Bard, Roger Parsons, and Joseph Jordan agreed to cooperate in editorial roles and assembled the elect to author the chapters at IUPAC Lenven (1981). Bard's firm conviction was that the anticipated 500-page volume must be available to chemists and students at a price less than 30 US\$! By IUPAC Lyngby (1983) there was still no publisher, but by IUPAC Lyon (1985) Marcel Dekker printed the burgeoning 834 + xii volume "Standard Potentials in Aqueous Solution". The price: 29.95 US\$, despite inflation. After seeing one after another CODATA—and IUPAC—volumes sold at high prices despite sacrifices made by the authors to keep the final price within a decent range for students, this success should not pass unheralded.

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