

HIGHLIGHTS

1. 1. CODATA (Tsukuba) Conference Key Lectures and Highlights
2. 2. Other Conference Events
3. 3. CODATA Calendar

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**15th International CODATA Conference**

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Scientific Data in the Age of Networking 29 September - 3 October 1996, Tsukuba, Japan

This pre-Conference Newsletter contains the final scientific program of the 15th International CODATA Conference whose theme is "Scientific Data in the Age of Networking: Their Use for Global Prosperity and Better Human Life." It is not too late to register. From Vice-President of Kyoto University Y. Nishijima's Keynote Lecture through the stimulating Plenary Lectures and the host of Invited Presentations, the Sessions-both presentation and poster, the Workshops and the four Satellite Meetings, the Exhibitions, the Technical Tours, the Database Demonstrations are a world of information revelation. In addition, snatches of sushi and sashimi, a soupcon of saki, not to mention the Welcome Buffet and the Conference Banquet and the corridor conversation with multidisciplinary and world trotting fellow data and information experts makes this an opportunity not to be missed.

CODATA Celebrates Its 30th Anniversary Scientific Program, 15th International CODATA Conference Tsukuba, Japan, 30 September - 3 October 1996 SCIENTIFIC DATA IN THE AGE OF NETWORKING

**Monday, 30 September 1996 (\*=Invited Speaker)**

**Keynote Speaker: Y. Nishijima,\* Japan ;**

Plenary 1: Y. Arskii\* et al., Russia VINITI Coordinates Interstate Exchange of Ecological Sci-tech Information: a System of Interstate Exchange of Ecological Sci-tech Information of CIS Countries Is Considered

Plenary 2: Paul Uhler,\* U.S.A. Summary of Results from the USNC/CODATA -Bits of Power+ Study

Plenary 3: J. Hiraishi,\* Japan Trends and Perspectives of Research and Development Information

**SESSION N: Novel Theory and Application of Data/Knowledge**

Chair: H. Bestougeff and Y. Fujiwara

- o T. Nelson,\* Borderless Transfer of Valuable Information (tentative)
- o H. Bestougeff,\* Intelligent Browsing and Dynamic Decision-making
- o Y. Fujiwara and J. An, Semantic Structures of Chemical Data for Problem Solving Systems
- o H. Dai and F. J. Smith, A Method of Rapid Searching for Technical Data
- o K. Kato, \* An Advanced Full-text Search Engine for Large Japanese Text Bases
- o Z. Pawlak,\* Application of Rough Set Theory for Problem Solving
- o Z. Kierzkowski, The Main Factors for the Synthesis of Virtual Activities+ Organization and New Information Systems
- o F. J. Smith\* et al., The Application of Artificial Intelligence to Data on Science and Technology
- o J.-P. Caliste, Data Measurement and Uncertainty, an Approach for Quality Insurance

**SESSION I: Information/Data Issues in Networking**

Chair: J. Rumble, Jr. and K. Naemura

- J. Rumble, Jr. and D. Blakeslee, Database Quality - How to Achieve it and How Internet Affects it
- K. Naemura,\* Intellectual Property Issues in Global Networks (tentative)
- J. R. Thieman et al., Netscience on the World Wide Web
- H. Kremers, Metainformation: Formalizing Knowledge on Complex Information Systems
- S. R. Heller,\* A Proposal for Publishing on the Internet
- N. D. Gershon et al., Visualizing World Wide Web Resources
- S. Rossouw, African Information Highway: Potential Prospects and Problems .
- A. Gaye, New Communications Technology for the Developing World: an African Point of View

### **SESSION A: Advanced Domain Specific Information**

Chair: J.-L. Delcroix and K. N. Marsh

- A. Itai,\* Innovative Integrated Drug Design (tentative)
- W.-D. Ihlenfeldt, Search and Salvage of Chemical Structure-oriented Information on the Internet
- K. Oshima and K. Horimoto, The Online Database Retrieval Scheme for Editing Systems
- M. Carabedian,\* Strategic Knowledge Notions: Application in CAD Structural Elucidation
- E. Fluck,\* The Quality of Scientific Databases
- S. Fujiwara,\* Fundamentals of Information: Specificity and Generality and Three Modes of Presentation
- J.-L. Delcroix,\* Quality of Data in Physics, Chemistry and Astronomy
- V. S. Iorish and G. V. Belov, The IVTANTHERMO-PC for Windows: an Updated and Expanded Thermodynamic Database and a New Software System

### **Posters/Demonstrations: Session A**

- Y. Morikawa, Local Oscillation Properties of Soft Materials Extracted from Free Damped Oscillation Data
- M. Fujita, Some Trials on WWW Servers in the "Data Freeway"
- H. Hayashi, A Database of Fuel Performance of Light Water Reactor
- H. Odaka, Database Created from Calculated Data in the Process of Materials Design
- C. Paoli et al., Use of Textual Information Sources on Internet by Linguistic Methods: the Establishment of Semantic Diction-aries in the Aeronautics
- Domain I. Stokov, A Possibility of a Virtual Book Architecture on the Basis of WYSIWYG TEX
- V. S. Tuninsky, On the Generalization of Systematic Uncertainty
- R. R. Nazyrova et al., The "Thermodynamics of Reacting Systems" Knowledge Base
- B. Messabih et al., Database Remodeling for Communication Eurolab Database Application on the Web: a Case Study
- T. V. Golashvili et al., The State of Radionuclide Contamination at Enterprises Affiliated to the Ministry of the Russian Federation for Atomic Energy and Ways of Decreasing Contaminants
- M. Ghoranneviss et al., The Data Acquisition System in IR-TI Tokamak
- I. A. Sokolova, A Computerized Library of the Transport Properties of Gases and Plasma Mixtures
- K. Tanabe, Constructing a Special Database on CD-ROM V.
- P. Solov+ev et al., Solvent Effects on Crown Ether Complexations
- K. Tanabe and H. Uesaka, A Neural Network System for the Identification of Infrared Spectra
- Y. Feibai et al., A New Computer Representation for Generic Structures and an Experimental Search System for Dye Patent Structures
- X. Li et al., ChIN's WWW Server: a Chance to Promote ChIN Activities
- A. Yamasaki, The Construction of the Hetero-atom NMR Database: Co-59, Nb-93, Rh-103 and Pt-195 for Personal Computers
- K. Zhang, On the Critical Temperature and Molecular Structure of Pure Compounds
- S. G. Yuan et al., Automorphism in Molecular Structure: Automatic Identification of Topological Equivalence Blocks

- R. To , The Enumeration of Symmetric Polyhex Hydrocarbons
- S. Obara et al., The Quantum Chemistry Literature Database (QCLDB)
- D. Maulovi, Generating Polyhex Hydrocarbons: A Parallel Algorithm
- T. Uchimaru and K. Tanabe, CASINO: a Computer-aided Organic Synthesis Design System
- R. V. Galiulin, An Algorithm for the Construction of Data Banks of Crystal Structures with the Given Chemical Formulas

### **Demonstrations**

- R. Nakajima, An Interatomic Potential Database for Material Science
- K. N. Marsh, TRC Databases for Chemistry and Engineering
- H.V. Kehiaian, Bibliographical and Numerical Databases on Physico-chemical Properties and the Electronic Journal Produced by ELDATA
- K. Tanabe
- H. Yokoka
- S. Obarawa

### **Tuesday, 1 October 1996**

Plenary 4: K. W. Neves\*, U.S.A., Design-built Support from a Computer Science Perspective - Application to the Construction Sector

Plenary 5: A. F. Cutting-Decelle\*, A. M. Dubois, France, Standardization of Industrial Data: the ISO Approach Through the Product Data Technology Based Standards: STEP, P-lib and Mandate

### **SESSION PC1: Physics & Chemistry**

Chair: Y. Itikawa

- R. J. Hanisch,\* Data Management for the Hubble Space Telescope
- A. Li-Scholz\* and W. Scholz, The Dissemination of Atomic and Nuclear Data: Past, Present and Future
- H. Tawara,\* Data Activities Relevant to Fusion Plasma Research at the Data and Planning Center, NIFS
- S. J. Kim, An Ultraviolet and Visible Spectroscopic Database for Atoms and Molecules in Celestial Objects
- Otani et al., Solar Energy Mapping for Designing Solar Power Systems

### **SESSION E: Engineering**

Chair: G. Ostberg and M. Obara

- H. Mizuta,\* Perspectives on Engineering Data Management in the Evolving Information Society
- O. Juvanon, Knowhow, Management and Feedback: An Industrial Experience
- B. R. Allenby\* and T.J. Gilmartin, The Data Requirements of Industrial Ecology
- A. Murata et al., The Development of an Energy and Environment Technology Database GATES under New Sunshine Project
- K. Sato, Virtual Engineering as Strategic Engineering Tools for Complex Systems
- G. F. Voronin, Modern Applications of Chemical Thermodynamic Data in Material Science and Technology

### **SESSION G: Genome Research**

Chair: S. R. Heller and T. Kunisawa

- E. Kutter\* et al., Homologies and Internal Repeats in the ORFS of Bacteriophage T4

- M. Sharma and A. S. Kolaskar, Semi-automated Construction of Physical Maps for *Bacillus subtilis* and *Pseudomonas aeruginosa*
- S. Tabata\* et al., Gene Organization of the Cyanobacterial Genome
- T. Sasaki\* et al., Genome Research Makes Rice a Treasure House of Discovery
- D. Bigwood and S. R. Heller, The USDA Plant Genome Information System
- N. Huang and G. S. Khush, Rice Genome Research at IRRI

## **SATELLITE SESSION: Electronic Publishing**

**Wednesday, 2 October 1996**

Plenary 6: Ferris Webster,\* U.S.A., Geophysical and Environmental Data: Possible Roles for CODATA

### **SESSION GE: Geoscience and the Environment**

Chair: M. A. Chinnery and M. Sugiura

- J.-J. Royer\* et al., Virtual Tools for Investigating Real Complex 3D Objects in Geoscience
- M. A. Chinnery,\* The Dissemination of Environmental Data Through Computer Networks
- D. J. Kerridge,\* Intermagnet: Providing Worldwide Magnetic Observatory Data in Near Real-time
- G. Gabert, Networks for Geoscience Information Systems in Africa and Southeast Asia
- B. Rudolf, Conclusions from Data Acquisition for a Global Climate Research Project (GEWEX-GPCP)
- B. Namysowska-Wilczynska and A. Wilczynski, Geostatistical Evaluation of Environment Pollution in Upper Silesia (S. Poland)
- Y.-N. Huang et al., Ionosphere and Geomagnetism Databases in Taiwan
- G. Wen et al., Management of Global Data and Information to Promote Global Change Studies

### **SESSION PC2: Physics & Chemistry**

Chair: A.J. Hopfinger

- Y. Wolman,\* Numerical Data on the Internet: Collection, Publication and Dissemination and Retrieval
- M. Aoyagi et al., The Development of a Distributed Computational Environment for Molecular Design on the World Wide Web
- H. Boegel, Structural Chemistry: An Educational Project Using Multimedia on the World Wide Web
- P. Mohr
- H. V. Kehiaian, ELDATA: the Development of the Integrated Information System on Physico-chemical Data

### **SESSION S: Species Diversity**

Chair: F. A. Bisby, J. L. Wu and H. Sugawara

- F. A. Bisby\* and R. Froese, The ILDIS World Database of Legumes and Fishbase: the Role of Global Species Databases in the Species 2000 Program
- A. D. Chapman,\* Networking Species Diversity Data in the Clearing House Mechanism under the Convention of Biological Diversity
- K. Iwatsuki,\* Biodiversity and Biology in the 21st Century
- K. Wilson,\* The IOPI Global Plant Checklist: Producing a Global Species Database
- S. Miyazaki et al., A Polyphasic Approach to Microbial Systematics in the Age of Biodiversity
- K. Moriwaki,\* A Genetic Survey of Geographical Isolates in House Mice and Their Implications in Biomedical Sciences

## Poster/Demonstrations: Session B

- A. Barth, Existing GIS-applications and a Vision of a GIS Management for Environmental and Geological Data (Saxony, Germany)
- H. Ishibashi, Space Environment Distributed Database Using WWW (World Wide Web)
- C. Le Carlier et al., Use of Archeometallurgical Slags as Natural Analogues for Municipal/Nuclear/Industrial Slagged Wastes: from Database to Applications
- M. Kamo et al., Protein Map Image-text Type Databases of Two-dimensional Electrophoresis for Two Plant Proteins, Rice and Arabidopsis
- K. Horimoto et al., Improvement of the Protein Superfamily Database (PROSUP): Detection of the Similarity of a Short Amino Acid Peptide
- S. Kanaya and Y. Kudo, A Multivariate Method of Estimating Species-Specific Diversity of Codon Usage Among Genes
- Y. Kudo and S. Kanaya, The Induction of Consensus Genic Sequences of tRNA Genes from Bacteria
- H. Suzuki et al., TOPIQUS, a Multi Database Retrieval System
- N. Manning
- T. F. Koetzle
- H. Tomita et al., Monte Carlo Simulation of DNA Strand-break Induction in Supercoiled Plasmid DNA from Low LET Radiation
- T. Morimasa, Patient's Database on the Network System
- K. Horiguchi, A Medicinal Plant Database for Papua New Guinea
- T. Igarashi, CDNDB as a Viewer for Biological Data on the Internet
- K. Nakata, An Integrated Receptor Database
- Y. Nadaoka, An Integrated Search Interface for Distributed Databases in the Internet Environment
- K. Akabane, The Concept of the Food Composition Database System and its Prototype
- K. T. Shao, Applying the WWW and GIS (GRASS) to the Fish Distributional Database of Taiwan
- C. S. Vishwas, Documenting Indian Marine Biodiversity: Strategy and Structure for a Database
- A.S. Kolaskar, A Software on the WWW Server for Probabilistic Identification of Viruses and Bacteria
- O. Vedina, The Impact of Agriculture on the Environment and Human Health

## Demonstrations

- R. Shen et al., 2-DE Electrophoresis Database
- Y. Maruoka, TOPIQUS
- K. Miyazaki, T4 Phage Database
- Y. Ugawa, Japanese Ants Color Image Database
- K. Watanabe and A. Hayashi, Lipid Database
- F. A. Bisby, Species 2000 Common Access System
- F. A. Bisby, World Database of Legumes
- J. R. Shimura, CHRONBACT: A List of Bacterial Names
- P. H. Schalk, ETI World Biodiversity Database CD-ROM Series. Integrated Species Identification Tools and Information Retrieval Systems on a Series of Compact Disks
- K. L. Wilson, Global Plant Checklist
- R. Froese, FishBase: A Database with Key Information on Coral Reef Fishes
- L. Blaine, The ICTVdB: A World Virus Database

## SESSION M: Materials

Chair: J.H. Westbrook and N. Onodera

- M. T. Michalewicz,\* Strategic Applications of HPC for Science and Technology;
- T. M. King and Y. Monma, Promoting Knowledge of Materials and Chemical Property Databases
- J.-Z. Yu et al., The Construction and Application of KIND, a Materials Database

- M. Obara et al., Development of New Alloy Database System in JICST
- A. Truyol, Structural Modelisation of the Pre-rupture of Materials: Systemic and Experimental Approach
- Z. Qu et al., A Database System for Natural Environmental Corrosion
- H. Tanaka et al., The Characterization of Micro Structures of Stainless Steels for Evaluation of Long-term Creep Properties
- P. C. Lacaze,\* Protection of Metals Against Corrosion: Promising New Electrochemical Route to the Formation of Protective Organic Layers via Interacting Multilayers
- M. V. Alfimov et al., The Factual Database in Macrocyclic Chemistry
- P. Villars\* et al., The Linus PAULING File (LPF): A Basic Database for Alloys, Intermetallics and Inorganics

### **SESSION PC3: Physics & Chemistry**

Chair: J.-E. Dubois

- J. Gasteiger\* et al., A Novel Code for the 3D Structure of Molecules and Its Application to Infrared Spectra Simulation
- A. J. Hopfinger\* et al., A Partnership of Tensor Representation, Partial Least Squares and Factor Analysis to Solve Highly-Oversubscribed Correlation Problems in Molecular Design
- C. Maeda et al., Conversion of the Data in the JICST Chemical Dictionary Database into Molfile
- A. Cosse-Barbi, Molecular Shape Similarity Analysis by Computer: Three-dimensional Pattern Recognition and Chirality Measure

### **SESSION PC4: Physics & Chemistry**

Chair: Y. Wolman

- K. Funatsu,\* AIPHOS: Recent Advances in the Organic Synthesis Design System
- J.-E. Dubois\* and P. Mezey, A Functional Group Database: a Charge Density DARC Approach
- M. Nakakubo and K. Maeda, Structural Analysis of Chemical Compounds Using the String-handling Method
- H. Yokokawa\* et al., Utilizing the Thermodynamic Database MALT 2 in Materials Chemistry

### **SESSION BM: Biological Macromolecules**

Chair: A.M. Lesk, W.C. Barker and Y. Tateno

- A. S. Kolaskar\* and D. Choudhury, Online Nucleic Acid Structural Database and Management System
- R. J. Simpson,\* Protein Structure and the Human Genome Project
- W. C. Barker\* et al., A Study of Terminology Usage in Macromolecular Sequence Databases: Keywords and Features
- Y. Tateno,\* The International DNA Data Banks for Molecular Evolutionary Study
- T. Sakai,\* Amphiphilic Amino Acid Residues at the Peripheral Rim or Channel Mouth of Membrane Proteins
- M. G \* and K. Yura, Module and Architecture of DNA-binding Proteins
- A. M. Lesk,\* Computational Investigations of Biological Macromolecules
- E. Abola,\* PDB: Protein Structure Database K. Satake, Biological Activity Databases

### **Thursday, 3 October 1996**

Plenary 7: M. I. Krichevsky,\* U.S.A., CODATA Educational Initiatives: a Cross-disciplinary Perspective

Plenary 8: V. P. Bhatkar,\* India, Advanced Education and Re-search Through Simulation: A Case for Developing Countries

Plenary 9: Yoshio Fukao,\* Japan, How and Why Do Earthquakes Occur?

### **SESSION MB: Medical Biology**

Chair: H. Vliegthart and A. Tsugita

- o H. Vliegthart,\* CARBBANK: A Database for Carbohydrate Structures
- o A. Hayashi\* and K. Watanabe, The Preparation and Application of Lipid Databases
- o M. Caffrey\* et al., LIPIDAT: a Database of Lipid Phase Transition Types, Temperatures and Enthalpy Changes: an Update
- o S. Fucharoen\* et al., A Database for Thalassemia
- o K. Imai,\* Mutant Hemoglobin Databases
- o M. B. Konnur, Untapped Sources and Problems in Medicinal Herbs Databases
- o A. Gaye, Film (synopsis): Evaluation of Medicinal Plants and Traditional Medicine
- o T. Kaminuma et al., A Global Information Network for Chemical Safety

### **SESSION PC5: Physics & Chemistry**

Chair: K. Funatsu

- o J.-P. Doucet\* and A. Panaye, Topology, Fragments and Neural Networks in Property Prediction and Structural Elucidation
- o P. C. Jurs,\* The Prediction of Chemical Properties of Organic Compounds from Molecular Structure
- o K. Varmuza,\* Cluster Analysis and the Selection of Chemical Structural Data
- o S. Ohe, The Neural Network System for Predicting and Processing Thermodynamic Properties

### **SESSION UA: User Aspects of Materials;**

Chair: M.T. Michalewicz and Y. Monma

- o G. Oestberg, Enhancing the Development of Materials Information Systems by Applying the Concept of Value Creation;
- o J. H. Westbrook,\* Activities of ASTM in Data Standards, Data Access and Metadata
- o K. Hoshimoto et al., Construction and Exploration of Information Space in Metallurgy
- o F. A. Kuznetsov,\* Russian Materials Oriented Databases
- o T. Ashino et al., Tools for Utilization of Basic Information for Materials Design

### **SESSION K: Kotani Memorial**

Chair: E.F. Westrum, Jr.

- o Keith Berrington,\* Northern Ireland, U.K., Calculating Data for Atomic Processes: the International Opacity and Iron Projects;
- o James L. Green,\* U.S.A., Advanced Data Systems in Space Plasma Physics
- o R. S. Chen\* and L. J. Ling, China, From Sequence Data of DNA to 3D Structure of Protein

### **CLOSING SESSION**

J.-E. Dubois, France, President, CODATA

A.S. Kolaskar, India

### **SATELLITE MEETING: Species 2000 (STABD)**

Chair: L. Blaine, F. A. Bisby and H. Sugawara

Open Satellite Meeting of the CODATA STABD Commission on Standardised Terminology for Access to Biological Databanks

This is an open meeting to present and discuss the work of the Commission in its three areas of activity:

- 1) Species 2000: Indexing the World's Known Species. F. A. Bisby, Developing the Species 2000 Project  
J. R. Shimura, The Species 2000 Common Access System (see also demonstrations)
- 2) The ICTV World Virus Database. L. Blaine, Progress Report (see also demonstration)
- 3) Developing Terminologies M. Krichevsky, Report on the Spore Terminology Workshop L. Blaine,  
Planned Work on Protein Terminology

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### *Other Conference Events*

#### **Satellite Meeting Schedule**

TODAI Symposium: "Sharing and Utilization of Scientific and Engineering Data in Asian-Oceanic Countries," organized by S. Iwata and M. Tasumi\* et al.; Friday, 27 Sept.-Saturday, 28 Sept., Sanjo Kaikan, The University of Tokyo, Hongo, Bunkyo-ku, Tokyo

Task Group Meeting, "Biological Macromolecules," organized by T. Kunisawa, Y. Sakaki, Y. Tateno and A. Tsugita, Sanjo Kaikan; Saturday, 28 Sept. (9:00-18:00) - Sunday, 29 Sept. (9:00-12:00), The University of Tokyo, Hongo, Bunkyo-ku, Tokyo

"Electronic Publishing," organized by John R. Rodgers, E. Fluck and S. Iwata; Tuesday, 1 Oct. (1000-1800), The Auditorium of Agency of Industrial Science & Technology, Tsukuba

IUBS-CODATA-IUMS, "Species 2000: Indexing the World's Known Species," organized by Frank A. Bisby and H. Sugawara; Thursday, 3 Oct. (1300-1700), The Auditorium of Agency of Industrial Science & Technology, Tsukuba

\*underlined names are contact persons

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### *Social Events*

Welcome Buffet-Sun. Evening, Sept. 29, Daitchi Hotel Conference Banquet -Tues. Evening, Oct. 1, at Satsui-toi

plus Technical Tours and Database Demonstrations

## **CODATA Calendar 1996**

September

- o 26-29 CODATA Task Group on the Survey of Data Sources in Asian-Oceanic Countries: "Sharing and Utilization of Scientific and Engineering Data in Asian-Oceanic Countries." Tokyo University Sanjo Kaikan, Tokyo, Japan
- o 28-29 CODATA Task Group on Biological Macromolecules. Tokyo University, Sanjo-Kaikan, Tokyo, Japan
- o 29 -Oct 3 International CODATA Conference. Tsukuba, Japan

October



- 1 CODATA Working Group on Electronic Publishing (1000 to 1800), Tsukuba, Japan
- 3 CODATA Commission on Standardized Terminology for Access to Biological Data Banks: "Species 2000: Indexing the World's Known Species." (1300-1700), Tsukuba, Japan
- 4-5 CODATA General Assembly, Tsukuba, Japan Editors

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