

SCIENTIFIC AND TECHNICAL DATA IN A NEW ERA

Edited by

Phyllis S. Glaeser

Executive Secretary, Committee on Data
for Science and Technology (CODATA), Paris

● **Hemisphere Publishing Corporation**

A member of the Taylor & Francis Group

New York Washington Philadelphia London

TABLE OF CONTENTS

Preface	xvii
Editor's Note	xviii
Acknowledgements	xix
International Scientific Program Committee	xx
List of Participants	xxi

BIOSCIENCES AND BIOTECHNOLOGY

A DATA EXPLOSION IN MOLECULAR BIOLOGY

Ernst-Ludwig Winnacker Zentrum für Gentechnologie Martinsreid, Federal Republic of Germany	1
--------------------------------------------------------------------------------------------------	---

OBTAINING AND STORING KNOWLEDGE: SCIENTIFIC DATA BANKS

A.E. Bussard CERDIC Nice, France	6
----------------------------------------	---

HYBRIDOMA DATA BANK: PURPOSE, ORGANIZATION AND OPERATION

Bernard W. Janicki Dana-Farber Cancer Institute Boston, Massachusetts, U.S.A.	10
-------------------------------------------------------------------------------------	----

EXPLOSION OF SEQUENCE DATA IN MOLECULAR BIOLOGY

B. Keil Institut Pasteur Paris, France	13
----------------------------------------------	----

THE BERLIN RNA DATA BANK: AN EXAMPLE OF A DATA BANK MAINTAINED BY A USER

Thomas Specht, Jörn Wolters and Volker A. Erdmann Institut für Biochemie, Freie Universität Berlin Berlin, Federal Republic of Germany	18
----------------------------------------------------------------------------------------------------------------------------------------------	----

DATA AND KNOWLEDGE BANK ON ENZYMES AND METABOLIC PATHWAYS

E.E. Sel'kov, I.I. Goryanin, N.P. Kaimachnikov, E.L. Shevelev, and Y.A. Yunus Institute of Biological Physics of the U.S.S.R. Academy of Sciences Pushchino, U.S.S.R.	22
-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------	----

BIOLOGICAL DATA BANKS: A PRELIMINARY SURVEY

Gaston Fredj and Michel Meinard Université de Nice, Laboratoire d'Océanographie Biologique Nice, France	28
---------------------------------------------------------------------------------------------------------------	----

CODATA COMMISSION ON THE TERMINOLOGY & NOMENCLATURE OF BIOLOGY HISTORY AND FUTURE GOALS

Lois Blaine American Type Culture Collection Bethesda, Maryland, U.S.A.	37
-------------------------------------------------------------------------------	----

INDUSTRY and ENVIRONMENTAL PROTECTION

DATA FOR INDUSTRIAL HAZARD ANALYSIS AND HUMAN RISK ASSESSMENT

D.A. Jones Major Hazards Assessment Unit Health & Safety Executive Bootle, U.K.	45
---------------------------------------------------------------------------------------	----

ENERGY DATABASES

M.A. Styrikovich U.S.S.R. Academy of Sciences Moscow, U.S.S.R.	48
----------------------------------------------------------------------	----

THE NATIONAL MATERIALS PROPERTY DATA NETWORK - DEALING WITH THE ISSUES IN ONLINE ACCESS TO NUMERIC PERFORMANCE DATA

J. G. Kaufman MPD Network Columbus, Ohio	52
------------------------------------------------	----

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.

Keith W. Reynard Wilkinson Consultancy Services Newdigate, Surrey, United Kingdom	56
-----------------------------------------------------------------------------------------	----

ADVANCED MATERIALS DATA SYSTEMS FOR ENGINEERING

H. Kröckel Commission of the European Communities Joint Research Centre Petten, the Netherlands	61
-------------------------------------------------------------------------------------------------------	----

DATABASES FOR PROPERTIES OF ELECTRONIC MATERIALS

F.A. Kuznetsov, V.A. Titov, S.V. Borisov, V.N. Vertoprakhov Institute of Inorganic Chemistry, Academy of Sciences, Siberian Branch, Novosibirsk, U.S.S.R.	73
-----------------------------------------------------------------------------------------------------------------------------------------------------------------	----

MATERIALS DATA AND CAD/CAM

H.E. Hellwig and J. Kunhenn

Institut für Apparatebau und Anlagentechnik, Technical University of Clausthal
Clausthal, Federal Republic of Germany

76

CONFUSION BETWEEN PHENOMENOLOGICAL CORRELATION AND PHYSICO-BASED CAUSALITY IN HANDLING MATERIALS DATA

Shiori Ishino

Dept. of Nuclear Engineering, Faculty of Engineering, University of Tokyo
Tokyo, Japan

87

EMPIRICALLY BASED CONCEPTS FOR MATERIALS INFORMATION SYSTEMS

K.I. Ammersbach, N. Fuhr, G.E. Knorz

GMD F4 (IPSI), TH Darmstadt, FH Darmstadt
Darmstadt, Federal Republic of Germany

92

OPERATION OF THE HIGH TEMPERATURE MATERIALS DATA BANK OF THE CEC AS AN EXPERT SYSTEM FOR MATERIAL DATA EVALUATION

G. Fattori, H. Kröckel, H.H. Over and P. Vannson

Commission of the European Communities, Joint Research Centre
Ispra, Italy

97

MATERIALS DATA HANDLING. INTERFACES BETWEEN AN EXPERT KNOWLEDGE SYSTEM AND USER ORIENTED PROBLEM SOLVING

U. Bengtson and D. Parsmo

Department of Engineering Metals, Chalmers University of Technology
Göteborg, Sweden

102

MATERIALS DATABASES FOR STRUCTURAL INTEGRITY ASSESSMENT AND ESTIMATION OF REMAINING LIFE OF POWER PLANT COMPONENTS

D. D'Angelo, A. Garzillo, S. Ragazzoni, and V. Regis

ENEL - Thermal and Nuclear Research Center
Milan, Italy

107

DESIGN AND REALIZATION OF A DATABASE CONCEPT FOR ENGINEERING APPLICATIONS

Manfred Tischendorf

Institut für Kernenergetik und Energiesysteme
Stuttgart, Federal Republic of Germany

112

DATA NEEDS FOR COMPUTER DESIGN AND SIMULATION OF CHEMICAL PLANTS

E. Futterer

TUHH
Hamburg, Federal Republic of Germany

116

A KNOWLEDGE BASE FOR THE PROPERTIES OF MATERIALS

J.G. Hughes, F.J. Smith and S.R. Tripathy

Department of Computer Science, The Queen's University
Belfast, N. Ireland

..... 122

ASSOCIATIVE DATABASE TECHNIQUES TO SEARCH FOR MATERIALS WITH UNIQUE PROPERTIES

Shigezo Murakami

Sumitomo Electric Industries Ltd.

Osaka, Japan.

..... 127

MATERIALS DATA BANKS IN FRANCE

Bernard Marx

DBMIST/MENJS

Paris, France

..... 132

DATA VALIDATION: CONCERNING A PROBLEM OF APPRAISING THE UNCERTAINTIES OF THERMOCHEMICAL VALUES

V. A. Medvedev and V. S. Yungman

Institute of High Temperatures of the Academy of Sciences

Moscow, U.S.S.R.

..... 138

DATA ON THERMODYNAMIC PROPERTIES OF SUBSTANCES AND ERRORS IN PROCESS PARAMETER CALCULATIONS

V.E. Alemasov and A.F. Dregalin

Physical and Technical Institute

Kazan, U.S.S.R.

..... 143

PREDICTION OF THERMODYNAMIC PROPERTIES IN COMPLEX MULTICOMPONENT SYSTEMS

Margit T. Rätzsch and Horst Kehlen

Chemistry Department, "Carl Schorlemmer" Technical University

Merseburg, German Democratic Republic

..... 147

PREDICTION OF PHASE EQUILIBRIA IN MULTICOMPONENT MIXTURES.

Andrzej Bylicki and Pawel Gierycz

Institute of Physical Chemistry, Polish Academy of Sciences

Warsaw, Poland

..... 151

ADVANCED USES OF THERMODYNAMIC DATA BANKS IN TEACHING STUDENTS SPECIALIZING IN PHYSICAL CHEMISTRY

V.S. Iorish and G.F. Voronin*

Institute for High Temperatures

Moscow, U.S.S.R.

*Department of Chemistry, University of Moscow

Moscow, U.S.S.R.

158

HOLOTRANSFORMATION: A NEW TECHNIQUE FOR EVALUATION OF A FORCED CONVECTION EQUATION FROM EXPERIMENTAL DATA

Edip Buyukkoca

Chemical Engineering Department, Engineering Faculty of Yildiz University,

Sisli-Istanbul, Turkey

162

PROGRESS IN THE DEVELOPMENT OF A CHEMICAL KINETIC DATABASE FOR COMBUSTION CHEMISTRY

Wing Tsang, W.G. Mallard and John R. Herron

Chemical Kinetics Division, National Institute of Standards and Technology

Gaithersburg, Maryland, U.S.A.

167

KINETIC DATA FOR INDUSTRIAL USE

J. Warnatz

Interdisciplinary Center of Scientific Computing, Heidelberg University

Heidelberg, Federal Republic of Germany

172

REQUIREMENTS OF SPECTRAL DATABASES

E. Pretsch, M. Farkas, A. Furst

Department of Organic Chemistry, Swiss Federal Institute of Technology (ETH)

Zurich, Switzerland

176

THE ARS PESTICIDE PROPERTIES DATABASE (PPD)

Stephen R. Heller, Douglas W. Bigwood, Patricia Laster, and Karen Scott

ARS, NRI

Beltsville, Maryland, U.S.A.

180

ARE SEQUENCE DATA ENOUGH FOR PROTEIN ENGINEERING?

Akira Tsugita

Life Science Institute, Science University of Tokyo

Chiba, Japan

184

DATABASES IN FERMENTATION TECHNOLOGY

Takahisa Ohta

Department of Agricultural Chemistry, The University of Tokyo

Tokyo, Japan

188

GLOBAL CHANGE, GEO AND SPACE SCIENCES

THE INTERNATIONAL GEOSPHERE-BIOSPHERE PROGRAM: A STUDY OF GLOBAL CHANGE

F.W.G. Baker
Executive Secretary, ICSU

..... 191

GENERAL PROBLEMS OF EARTH OBSERVATION SATELLITE DATA HANDLING

Livio Marelli
European Space Agency ESA/ESRIN
Frascati, Italy

..... 198

DATABASES FOR ATMOSPHERIC CHEMISTRY

R.F. Hampson and W.G. Mallard
National Institute of Standards and Technology (formerly National Bureau of Standards)
Gaithersburg, Maryland, U.S.A.

..... 205

SATELLITE DATA FOR INCLUSION IN WEATHER FORECASTING AND CLIMATIC MODELS

Horst Böttger
European Centre for Medium-Range Weather Forecasts
Shinfield Park, Reading, United Kingdom

..... 209

CHINESE MAPPING PROJECTS USING SATELLITES

C. Bardinat (1), Chen Yi-yun (2) G. Gabert (3) Wan Zheng-ming (4) and Yang Shi-ren (4)
(1) Ecole Normale Supérieure, Paris, France
(2) Remote Sensing Ground Station (RSGS), Academia Sinica, Beijing, China
(3) Bundesanstalt für Geowissenschaften und Rohstoffe (BGR), Hannover, F.R.G.
(4) Institute of Remote Sensing Application (IRSA), Academia Sinica, National Remote Sensing
Center, Beijing, China

..... 213

EARTHQUAKE DATA AUTO-PROCESSING SYSTEM FOR EARTHQUAKE PREDICTION

Megumi Mizoue
Earthquake Research Institute, The University of Tokyo
Tokyo, Japan

..... 219

ATOMIC AND MOLECULAR DATA NEEDED FOR ASTRONOMY AND ASTROPHYSICS

Jean W. Gallagher
Office of Standard Reference Data, National Institute of Standards and Technology
Gaithersburg, Maryland, U.S.A.

..... 224

THE ORGANIZATION OF DATABASES IN ASTRONOMY, ESPECIALLY SPACE ASTRONOMY

Jaylee M. Mead and Wayne H. Warren Jr.
NASA Goddard Space Flight Center
Greenbelt, Maryland, U.S.A.
..... 228

DATA IN ASTRONOMY: STRUCTURE AND ORGANIZATION

C. Jaschek
Centre de Données de Strasbourg (CDS), Observatoire Astronomique
Strasbourg, France
..... 232

RECOVERY AND USE OF HISTORICAL DATA - DENDROCHRONOLOGY

F.H. Schweingruber
Swiss Federal Institute of Forestry Research
Birmensdorf bei Zurich, Switzerland
..... 236

COMPILATION OF OVER 500 YEARS OF HISTORICAL DOCUMENTS ON CLIMATE CHANGES IN CHINA

Shao Wu Wang
Department of Geophysics, Peking University
Beijing, China
..... 241

DATA STORAGE, RETRIEVAL, ETC.

STANDARDIZING EXCHANGE FORMATS

H.D. Lemmel and J.J. Schmidt
International Atomic Energy Agency, Nuclear Data Section
Vienna, Austria
..... 245

PROPER USE OF EXPERT SYSTEMS

Setsuo Ohsuga
Research Center for Advanced Science and Technology, The University of Tokyo
Tokyo, Japan
..... 256

THE AUTOMATED DATA THESAURUS: A NEW TOOL FOR SCIENTIFIC INFORMATION

John L. McCarthy
Computer Science Research Department, Information and Computing Sciences Division
Lawrence Berkeley Laboratory
Berkeley, California, U.S.A.
..... 260

MULTI-MEDIA SYSTEM - IMES

Toshiyuki Sakai and Yasuo Arika
Department of Information Science, Faculty of Engineering, Kyoto University
Kyoto, Japan
..... 265

**INTRODUCTION TO DIGITAL MULTIMEDIA
(CD-I, DVI, CVD, Hyper TV, PC Engine, FM Towns, CD-ROM XA, et al)**

John C. Gale
Information Workstation Group
Alexandria, Virginia
..... 271

CRITERIA FOR USE OF COMPACT DISC-READ ONLY MEMORY (CD-ROM)

Thomas C. Bagg
National Institute of Standards and Technology
Gaithersburg, Maryland, U.S.A.
..... 276

IMPACT OF CD-ROM ON THE DISSEMINATION OF SCIENTIFIC DATA

Michael A. Chinnery, Director
National Geophysical Data Center National Oceanic and Atmospheric Administration
Boulder, Colorado, U.S.A.
..... 283

PRACTICAL EXPERIENCE WITH A LARGE DATABASE

Nick A. Farmer
Chemical Abstracts Service
Columbus, Ohio, U.S.A.
..... 287

**SPATIAL "DATA GRAVEYARDS" VERSUS DYNAMIC PLANNING OF ENVIRONMENTAL
PROBLEMS: A Misconceptual Practice Reevaluated**

Avi Degani
Dept. of Geography, Tel-Aviv University
Tel Aviv, Israel
..... 293

HUMAN FACTORS IN USER INTERFACES

Lorraine F. Normore
Chemical Abstracts Service
Columbus, Ohio, U.S.A.
..... 298

A DATA CAPTURE SYSTEM FOR PRINTED TABULAR DATA

Walter Grattidge, W. Bruce Lund and Jack H. Westbrook
Sci-Tech Knowledge Systems, Inc.
Scotia, New York, U.S.A.
..... 302

AN ELECTRONIC JOURNAL FOR SHARING DATA ON CROP GROWTH

Basil Acock, Stephen R. Heller, and Stephen L. Rawlins
USDA, ARS, Systems Research Laboratory
Beltsville, Maryland, U.S.A.
..... 307

STN NUMERIC DATA SERVICE

- A. Barth, P. Luksch and J. Mockus
Fachinformationszentrum Karlsruhe
Eggenstein-Leopoldshafen, Federal Republic of Germany
..... 312

DATA RELIABILITY AND ACTIVE ENVIRONMENT: CHEMICAL SHIFT MODELS

- J.E. Dubois, J.P. Doucet, A. Panaye
Institut de Topologie et de Dynamique des Systèmes, associé au C.N.R.S.
Paris, France.
..... 316

AN EXPERT DRIVEN DATABASE ON ATOMIC AND MOLECULAR PHYSICS

- F.J. Smith and J.G. Hughes
Department of Computer Science, The Queen's University of Belfast
Belfast, U.K.
..... 321

ONLINE RETRIEVAL SYSTEM OF THE NBS INORGANIC CRYSTAL DATA

- Jiaju Zhou, Ying Zhang, Zhihong Xu, and Heng Fu^{*}
Institute of Chemical Metallurgy, Academia Sinica, Beijing, China
^{*}Institute of Chemistry, Academia Sinica, Beijing, China
..... 327

LEGAL AND SOCIAL ASPECTS

DATA NEEDS FOR WRITING RATIONAL REGULATIONS ON GENETIC ENGINEERING

- Mark F. Cantley
Concertation Unit for Biotechnology in Europe, Commission of the European Communities
Brussels, Belgium
..... 335

SOCIAL IMPLICATIONS OF DATA QUALITY

- Anthony J. Barrett
ESDU International
London, U.K.
..... 339

NECESSARY LEGAL STEPS TO PROTECT IDEAS BEFORE DISSEMINATING DATA

- Lynn E. Cargill
Registered Patent Attorney
Birmingham, Michigan, U.S.A.
..... 343

COPYRIGHT ISSUES AFFECTING SCIENTIFIC NUMERICAL DATABASES

- David R. Lide
National Institute of Standards and Technology
Gaithersburg, Maryland, U.S.A.
..... 346

EVOLVING DATABASES AND COPYRIGHTS OF EXPERTS

I.L. Khodakovsky and A.A. Kosorukov

**Vernadsky Institute of Geochemistry and Analytical Chemistry, U.S.S.R. Academy of Sciences,
Moscow, U.S.S.R.**

..... 349

PRIVACY CONSIDERATIONS AND SCIENTIFIC RESEARCH IN THE SOCIAL SCIENCES

Erwin K. Scheuch

Universität de Köln

Köln, Federal Republic of Germany

..... 353

INFORMATION FLOW RESTRICTIONS IN THE UNITED STATES

Schulte-Hillen

BDU

Köln, Federal Republic of Germany

..... 360

Author Index 365

Subject Index 366

Acronyms 371