



62 CODATA / NEWSLETTER

FEBRUARY 1993

Materials Data for CAE

HIGHLIGHTS

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The Workshop—a joint endeavor of the European Economic Community (CEC) and CODATA—was held Feb. 1-3, 1993, at the facilities of the Dechema Institute, Frankfurt am Main, Germany. Both CODATA and the CEC have long-standing interests in the development of materials data. Two prior CODATA workshops had emphasized the identification of problems affecting the development of the field and means for stimulating international cooperation in their solution. This most recent workshop focussed more narrowly on exploration of the actions needed for a more effective integration of computerized materials databases and information with computer-aided-engineering (CAE) systems in the spheres of both design and manufacturing.

This international workshop developed three principal recommendations. The 34 participants from 8 different countries called for:

- Increased dialogue between the CAE and materials database communities, in particular with regard to close involvement with STEP, the developing ISO standard for the exchange of data for technical products.
- Extension of the application of materials data beyond design and manufacture to the full life cycle of products, including potential environmental impacts and recycling.
- Increased recognition of the implications of present-day industrial trends: concurrent engineering, infinite customization, constant change, and joint ventures between all kinds of institutions.

The underlying assumption is that the potential and capability of computerized engineering systems can only be fully exploited when digitized information for design, production, and materials property can be totally integrated.

A formal proceedings is planned as well as derivative articles for inclusion in various professional journals.

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 ICSU WORLD DATA CENTER SYSTEM

The ICSU World Data Center (WDC) system was established in 1957 under the auspices of the International Council of Scientific Unions (ICSU). It was created as a scientific mechanism to assure the safe collection, archival, and efficient dissemination of data and information collected during the International Geophysical Year (IGY 1957-58). Countries were invited to establish World Data Centers, to be operated under national funding, for the IGY geophysical disciplines, and assure that the data collections would be archived for the long term. The USA and the (then) USSR volunteered to establish complex data center systems (WDC-A and WDC-B, respectively), i.e., covering all of the IGY disciplines. Several countries in Europe, Japan, Australia volunteered to establish various discipline centers and the World Meteorological Organization, a technical agency in the UN system, volunteered to be a WDC for meteorology; these separate discipline centers were called, collectively, WDC-C. The IGY WDC System was supervised by ICSU's Special Committee for the IGY.

After the IGY ended, a series of ICSU resolutions extended the lifetime of the WDC system, so that it has become a permanent part of the international conduct of global geophysical and related solar and environmental programs, under the general guidance and supervision of ICSU's Panel on World Data Centres, which was established in 1968. Several centers active in IGY were discontinued, but the holdings were transferred to centers remaining active. Some geomagnetic, ionospheric, solar activity, and cosmic-ray data centers were combined into Solar-Terrestrial Data Centers. Similarly, Solid Earth Data Centers evolved by combining seismic, gravity, and many other kinds of earth data. As a result of new ICSU international programs, several new centers were added covering disciplines not part of the IGY. Lately, as a response to the ICSU IGBP-Global Change Program, China developed a complex set of centers, and several new Centers were added to WDC-A and WDC-C. Additional centers, specializing in space-based data, are under discussion.

The IGY Data Centers were seen as passive but long-term archives, with primary responsibility to collect and store data, and were enjoined not to do any further processing or quality control - those tasks were to be left to the scientific users. The main tasks then of the ICSU WDCs were (i) to exchange data among related centers to assure that important data are stored in more than one archive, (ii) accepting data from data-gathering or monitoring programs in accordance with guidelines published by ICSU after they have been developed by the ICSU scientific organizations which together comprise the international bodies for each discipline; (iii) providing copies of data to any user, at no more than the direct cost of copying, (iv) providing for working visits to the center, access to all of the data held in that center, along with access to analysis facilities at the center; (v) publishing catalogs of data holdings; (vi) and providing, insofar as is feasible, assistance to users to locate and obtain related data not held in the WDC System.

However, times do change: scientific needs change, and technology advances. The WDC System does its best to follow new trends and take advantage of new technologies. For example, powerful personal computers make data-processing

and quality-control procedures very practical to implement. Many WDCs now process received data and, with guidance from the ICSU scientific bodies, produce indices of activity or summary data sets, appropriate to the geophysics of the discipline. Several of the WDCs search out and obtain data related to the international data sets stipulated by ICSU programs. Some of the WDCs work closely with scientists who supply data and also use data, to implement some basic quality-control procedures, and ensure that the documentation of the data sets are such that any user not familiar with the data taking process can, nevertheless, use the data with confidence. WDCs in a discipline often join forces to produce joint catalogs of data holdings, and provide easy access to data listed in these catalogs but not necessarily held in the center to which a user applies for data. STP and SEG data centers produce multidisciplinary databases, with excellent software for display, sort and browse capabilities. Many data centers also have on-line catalogs, and data sets for browsing, accessible to users who have the modern telecommunications facilities needed for such access.

The development in the past decade of convenient and very low cost mass storage as CD-ROMs and other optical/magnetic storage devices, along with new compact high-capacity tape cassette systems, has enabled some WDCs to publish "popular" data sets on CD-ROMs, and to produce one-of-a-kind large data sets for a few users on individual CD-ROMs or on tape cassettes. The WDCs keep abreast of new technology and are prepared to transfer data holdings to any newer and feasible technology which develops. The WDCs are moving towards the goal of producing most of their widely-used data sets on modern high-capacity, random-access media so that the user has very economical access to large multidisciplinary databases, thus enhancing the multivariate analyses needed for the modern era of Earth System Science.

Since modern Earth System Science and Global Change research requires long-term data using as much as possible of the historical data sets, many WDCs are involved in massive and expensive data rescue missions to protect older analog handwritten or even published data in danger of deterioration or being lost as results of institutional changes. A task of great significance is to "rescue" older tabular data by entering them into computer databases so that the resulting data are in computer-compatible form, and can be "published" on CD-ROMs for wide and inexpensive use. This procedure is resulting in the creation of computer-readable long-time series of many geophysical quantities.

However, there are still millions of feet of analog images on film and data-filled rooms of paper records which are also preserved in the WDC system and paper publications of summary data are still appreciated around the world.

The WDC system at this writing consists of 44 discipline centers distributed worldwide as follows:

WDC-A, USA

- Atmospheric Trace Gases, Carbon Dioxide Data and Analysis Center, Oak Ridge, Tennessee,
- Glaciology - University of Colorado, Boulder, Colorado

- Marine Geology and Geophysics, NOAA/National Geophysical Data Center, Boulder, Colorado
- Meteorology, NOAA/National Climatic Data Center, Asheville, North Carolina
- Oceanography, NOAA/National Oceanographic Data Center, Washington, DC
- Remotely-sensed Land Data, USGS/EROS Data Center, Sioux Falls, South Dakota
- Paleoclimate, NOAA/National Geophysical Data Center, Boulder, Colorado
- Rockets and Satellites, NASA/National Space Science Data Center, Greenbelt, Maryland
- Rotation of the Earth, US Naval Observatory, Washington, DC
- Seismology, USGS/National Earthquake Information Center, Golden, Colorado
- Solar-Terrestrial Physics, NOAA/National Geophysical Data Center, Boulder, Colorado
- Solid Earth Geophysics, NOAA/National Geophysical Data Center, Boulder, CO
- WDC-A Coordination Office, National Academy of Sciences, Washington, DC

WDC-B, Russia (Former Soviet Union)

- Solar-Terrestrial Physics, Moscow
- Solid Earth Physics, Moscow Center for IGBP
- Oceanography, Obninsk (near Moscow)
- Meteorology, Obninsk (near Moscow)

WDC-C

- Earth Tides, Observatoire Royal de Belgique, Brussels, Belgium
- Geomagnetism, Copenhagen, Denmark
- Geomagnetism, British Geological Survey, Edinburgh, UK
- Glaciology, Scott Polar Research Institute, Cambridge, UK
- Recent Crustal Movements, Zdiaby (Prague), Czechoslovakia
- Soil Geography and Classification, ISRIC, Wageningen, The Netherlands
- Solar Activity, Observatoire de Paris, Meudon, France
- Solar Terrestrial Physics, Rutherford Appleton Laboratory, Chilton, UK
- Sunspot Index, Observatoire Royal de Belgique, Brussels, Belgium
- Airglow, Tokyo Astronomical Observatory, Tokyo, Japan
- Aurora, National Institute of Polar Research, Tokyo, Japan
- Cosmic Rays, Nagoya University, Toyokawa, Japan
- Geomagnetism, Kyoto University, Kyoto, Japan
- Ionosphere, Radio Research Laboratories, Tokyo, Japan
- Nuclear Radiation, Japan Meteorological Agency, Tokyo, Japan
- Solar Radio Emission, Nagoya University, Toyokawa, Japan

CODATA Calendar

1993

March

- 10-13 Biological Macromolecules Task Group. Ringberg, Germany
- 10-13 Commission on Standardized Terminology for Access to Biological Data Banks. Ringberg, Germany

April

- 6-7 Task Group on Data for Safety, Environment, Design. Paris, France

October

- 8-9 Materials Database Management Task Group. Gaithersburg, Maryland, USA

1994

September

- 18-22 International CODATA Conference. Chambéry, France
- 23-24 CODATA General Assembly. Chambéry, France

- Solar-Terrestrial Activity, Institute of Space & Astronautical Sciences, Tokyo, Japan
- Geomagnetism, India Institute of Geomagnetism, Bombay, India

WDC-D, China:

- Astronomy (Solar Activity), Beijing Astronomical Observatory, CAS, Beijing
- Geology, Chinese Academy of Geological Sciences, Beijing
- Geophysics, Institute of Geophysics, CAS, Beijing Ministry of Geology and Mineralogy, Beijing
- Glaciology (Snow and Ice) and Geocryology, Lanzhou Inst. of Glaciology and Geocryology, Lanzhou
- Oceanography, NODIC, State Oceanic Administration, Tianjin
- Meteorology, National Meteorological Center, State Meteorological Administration, Beijing
- Renewable Resources and Environment, Commission for Integrated Survey of Natural Resources, CAS, Beijing
- Seismology, Dep't of Science Programming & Earthquake Monitoring, State Seismological Bureau, Beijing
- WDC-D Coordination Office, Chinese Academy of Sciences., Beijing

**--Stan Ruttenberg, Chairman
ICSU Panel on World Data Centers
UCAR, Boulder, CO, USA**

CODATA's Leadership for the Biennium 1992-1994

Officers

Prof. D. Abir, Israel, *President* (1990-1994)
Prof. L. V. Gurvich, Russia, *Vice-President* (1988-1996)
Prof. A. Tsugita, Japan, *Vice-President* (1992-1996)
Dr. G. H. Wood, Canada, *Secretary General* (1990-1994)
Mr. J. Crease, IUGG, *Treasurer* (1988-1996)

Executive Committee

Dr. A. J. Barrett, U.K. (1992-1994)
Dr. M. A. Chinnery, U.S.A. (1992-1994)
Prof. J.-L. Delcroix, France (1992-1994)
Dr. R. Eckermann, Germany (1990-1994)
Academician F. A. Kuznetsov, Russia (1990-1994)
Prof. R. J. Simpson, Australia (1988-1994)
Prof. R. Sinding-Larsen, Norway (1988-1994)
Dr. J. H. Westbrook, U.S.A. (1990-1994)

Task Groups and Commissions 1992-1994

Artificial Intelligence and Computer Graphics, AIGRA

Prof. J.-E. Dubois, ITODYS, 1 rue Guy de la Brosse, 75005, Paris, France

Biological Macromolecules

Prof. Akira Tsugita, Research Institute for Biosciences, Science University of Tokyo, 2669 Yamazaki, Noda, Chiba, 278 Japan

Property Data for Safety, Environment and Design

Dr. Kenneth N. Marsh, Thermodynamics Research Center, Texas A&M Univ. System, College Station, TX 77843-3111, U.S.A.

Fundamental Constants

Dr. Barry N. Taylor, National Institute of Standards and Technology, Bldg. 221, Room B160, Gaithersburg, MD 20899, U.S.A.

Geothermodynamic Data

Prof. S. K. Saxena, University of Uppsala, Geochemistry Program, Dept. of Mineralogy & Petrology, Box 555, S-75122 Uppsala, Sweden

Materials Database Management

Mr. J. G. Kaufman, National Materials Property Data Network, Inc., 2540 Olentangy River Road, P. O. Box 02224, Columbus, OH 43202, U.S.A.

CODATA Referral Database

Mr. Keith Reynard, Wilkinson Consultancy Services, Stable Cottage, Broad Lane, Newdigate, Dorking, Surrey RH5 5AT, U.K.

Data Sources in Asian-Oceanic Countries

Prof. M. Tasumi, Faculty of Science, University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113, Japan

Databases for Experimental Data and Electronic Publishing

Prof. E. Fluck, Gmelin Institut, Postfach 90 04 67, D-6000 Frankfurt (Main) 90, Germany

Commission on Industrial Data

Dr. J. H. Westbrook, Brookline Technologies, 5 Brookline Rd., Ballston Spa, NY 12302, U.S.A.

Commission on Standardized Terminology for Access to Biological Data Banks

Ms. Lois Blaine, Hybridoma Data Bank, American Type Culture Collection, 12301 Parklawn Drive, Rockville, MD 20850-1776, U.S.A.

Data for Global Change Commission

Dr. Michael A. Chinnery, NOAA E/GC, 325 Broadway, Boulder, CO 80303

Data for Discovery — Proceedings of the 12th CODATA Conference

Phyllis Sloane Glaeser, Editor

Focus: Presenting the data requirements for the rapidly expanding studies of human impact on the biosphere and geosphere

- discussion on generic aspects of data handling, including expert systems, storage and retrieval strategies, and knowledge tools. New developments in information that may have applications in various types of scientific data management are addressed.

- plans and programs for quality control, storage, generation, dissemination, and use of the data involved in major aspects of global change.

- database developments in specific scientific fields, particularly in materials science, chemistry, and chemical engineering, and molecular biology. Finally, there are several papers reviewing CODATA's role in international data management programs.

Cat. No.: BB0002, December 1992, 528 pp., ISBN 1-56700-002-0. U.S. \$95 / Outside U.S. \$114. Add \$7.50 per volume for shipping and handling charge on U.S. and Canadian orders. Sales tax will be charged where applicable. Mail order to CRC Press, Inc., 2000 Corporate Blvd., N.W., Boca Raton, FL 33431, U.S.A. or call toll free 1-800-272-7737 Monday through Friday.

CODATA Publications

Materials Database Management—Global Trends, Standards, and Issues, CODATA Bulletin 24-1. (a,b)

Scientific Program and Abstracts, Thirteenth International CODATA Conference, October 1992, Beijing, China, edited by P. Glaeser and Y. Hu, *CODATA Bulletin*, 24-2. (c,b)

Physico-Chemical Data Centers, edited by Kenneth Marsh, *CODATA Bulletin*, 24-3. (d,b)

Selected Proceedings of the 13th CODATA Conference, October 1992, Beijing, China, edited by P. S. Glaeser, *CODATA Bulletin* 24-4. (e,b)

Data for Discovery, Proceedings of the 12th CODATA Conference, October 1990, Columbus, Ohio, USA, edited by P. S. Glaeser. (f)

Other Books

Thermodynamic Properties of Individual Substances, Vol. 1, Parts 1 and 2 (4th ed.), edited by L. V. Gurvich, I. V. Veyts, C. B. Alcock, and V. S. Iorish. (g,h)

Other Books (cont'd)

Thermodynamic Properties of Individual Substances, Vol. 2, Parts 1 and 2 (4th ed.), edited by L. V. Gurvich, I. V. Veyts, C. B. Alcock, and V. S. Iorish. (i,h)

Thermodynamic Properties of Individual Substances, Vol. 3, Parts 1 and 2 (4th ed.), edited by L. V. Gurvich, I. V. Veyts, C. B. Alcock, and V. S. Iorish. (j,h)

Computerization and Networking of Materials Databases, 2nd Volume, J. G. Kaufman and Glazman. (k,l)

Computerization and Networking of Materials Databases, 3rd Volume, edited by T. I. Barry and K. W. Reynard. (m,l)

Thermochemical Data of Pure Substances (2nd rev. edition), authored by Ihsan Barin. (n)

Macmillan's Chemical and Physical Data, A. M. Janes and M. P. Lord. (o)

Chemical Thermodynamics of Uranium, authored by I. Grenthe, J. Fuger, R. J. Lemire, A. B. Müller, C. Nguyen-Trung Cregu, and H. Wanner, edited by H. Wanner and I. Forest. (p)

(a) 1992. Begell House Inc., v + 97 pp., \$40, ISSN 0366-757X.

(b) Begell House Inc., Suite 1106, 79 Madison Avenue, New York, NY 10016-7892, USA

(c) 1992. Begell House Inc., xxxix + 190 pp, \$40, ISSN 0366-757X.

(d) 1992. Begell House Inc. v + 50 pp., \$40, ISSN -0366-757X.

(e) 1992. Begell House Inc., \$40, ISSN -0366-757X.

(f) 1992. (Begell House Inc.) 528 pp. (See advertisement on page 4 of this *Newsletter* for details.)

(g) Containing elements O, H(D,T), F, Cl, Br, I, He, Ne, Ar, Kr, Xe, Rn, S, N, P and their compounds. 1992. \$225 in USA, \$270.00 outside USA, ISBN 0-8911-6760-9. Cat. No. BB6760HYT.

(h) Each of the three Volumes has both (in separate hard bound books) a Methods and Computation part and a Tables part. This is a five-volume revised and augmented English translation of the Third Russian Edition. This important reference provides scientists and engineers with reliable data on the thermodynamic properties of 56 elements and more than 1,700 of their compounds in solid, liquid, and gaseous states at standard pressure over a wide range of temperatures. Radicals, positive and negative ions in gaseous state, as well as metastable and vitreous solids are included in the list of substances. There is an extensive bibliography. Uncertainties are provided for selected constants and recommended properties. Thermodynamic properties were calculated using the fundamental constants, key thermodynamic values, and atomic masses recommended by CODATA-ICSU and IUPAC. CRC Press, Inc., 2000 Corporate Blvd.,

N.W., Boca Raton, FL 33431, USA (407-994-0555).

(i) Containing elements C, Si, Ge, Sn, Pb, and their compounds. 1992. \$265 in USA, \$315 outside USA, ISBN 0-8911-6533-9. Cat. No. BB6533HYT.

(j) Containing elements B, Al, Ga, In, Tl, Sr, Be, Ba, Mg, Ca, and their compounds. Due January 1993. \$524 in USA, \$625 outside USA, 688 pp, 242 tables, ISBN 0-8493-9927-0. Cat. No. BB9926HYT.

(k) 21 peer-reviewed papers (12 from outside of the United States) focus on the international nature of this effort; the progress being made in standardization and the definition of guidelines to aid newcomers to the activity; and the application of such databases to different aspects of the materials business. For materials scientists and engineers starting to pan and build new computerized materials databases, and to those well underway who wish to keep their work current. 1991. ASTM, 285 pp., hard cover, \$84, ISBN 0-8031-1411-7. PCN: 04-011060-63.

(l) ASTM Publications Division, 1916 Race Street, Philadelphia, PA 19103-1187

(m) Materials information is a commercial resource comparable with the finance, plant and the workforce, and it needs management to be used efficiently. The nomenclature and data required to characterize materials and their properties are complex, which makes the need for standards for the exchange and use of data particularly pressing. With these points in mind, STP 1140 reflects a shift in emphasis from producers to users of materials data. 32 peer-reviewed papers discuss: Standards and Data Representation, Integration of Materials Information,

Expert Systems and Materials Databases, Data Issues for Engineering Materials. 1992. ASTM, 504 pp, \$77, ISBN 0-8031-1473-0. PCN: 04-011400-63.

(n) Contains thermochemical data on almost 2400 pure substances, including 100 organic compounds. The scope of thermochemical data presented is broad, ranging from heat capacity, entropy, and Gibbs energy to enthalpy and equilibrium constant of formation. 1992. VCH, 1834 pp., 10 figures, 2406 tables, hardcover, £ 272.00, ISBN 3-527-28531-8. VCH, 8 Wellington Court, Cambridge CB1 1HZ, UK or VCH, 220 East 23rd Street, New York, NY 10010-4606, USA.

(o) Provides data on the more important properties of the most widely used compounds in 17 subject areas. Given in SI units and IUPAC nomenclature the data is presented in some 439 tables. Most tables are provided with references for further information and/or additional data. 1992. Macmillan Press, Houndmills, Basingstoke, Hampshire RG21 2XS, U.K. [FAX (0256) 810526]. 608 pp, hard cover, £35, (please add £1.50 per book for postage and packing), ISBN 0-333-51167-0.

(p) This volume provides a comprehensive overview on the chemical thermodynamics of those elements that are of particular importance in the safety assessment of radioactive waste disposal systems. Compiled under the auspices of the OECD Nuclear Agency. 1992. North Holland, xx + 656 pp., \$228.50 / Dfl. 400, ISBN 0-444-89381-4. NH (Elsevier Science Publishers), P. O. Box 103, 1000 AC Amsterdam, The Netherlands or Elsevier Science Publishing Co., Inc., P. O. Box 882, Madison Square Station, New York, NY 10159, USA.

Two-dimensional Gel Protein Databases Workshop

Two-dimensional (2-DE) gel protein databases were the subject of a workshop organized by the CODATA Task Group on Biological Macromolecules on March 9, 1992. Eleven scientists from eight countries representing protein microsequencing methodologies and cellular protein database development explored means of integrating the rapidly expanding body of information on 2-DE resolved proteins from different laboratories.

Dr. Richard J. Simpson reports that a major proposal resulting from the discussion was that a *relational* 2-DE gel protein database be established as an intermediary tool to catalog pertinent information on such proteins—e.g., experimental source, 2-DE loci, biological background information, etc.—as an adjunct tool accessed through extant international protein sequence databases.

The proposed 2-DE protein database would provide an information model accessible to the scientific user community. The data in the *integrated* database would provide information for the identification of protein spots and information on the biological background of the samples from which the sample originated. This *integrated/interlinking* database would also indicate respective "boutique" 2-DE protein data banks where additional highly specialized information might be contained.

Computer Aided Molecular and Material Design

The second CHIN (Chemical Information Network) Seminar in Beijing, China, October 18, 1992, hosted 14 invited speakers (including distinguished CODATA-related scholars, e.g., Xu Zhihong, J.-E. Dubois, John Rumble, Shuichi Iwata, and M. W. Chase). Their presentations focused on computer aided molecular and material design as did a round table discussion on the exchange of information and mutual cooperation between groups involved in these developments. A brochure on the conclusions of the conference is expected.

Moreover, annotated sequence information could be contained in the established international protein and DNA sequence databases. The protein sequence databases (e.g., PIR International databases) provide the "national" environment to handle this relational database information.

The participants proposed that an experimental model of an *integrated* database of identified protein spots be developed by collaboration of interested laboratories with the PIR-International and they established a working committee to implement the *integrated/interlinking* 2-DE protein database.

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Published four times per year (February, May, August, November)

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75016 Paris, France
Telephone: 33 1 45250496 / Telex: 645554 F
FAX: +33 1 42881466 / Cables: ICSU Paris 016

Assistance in dissemination provided by National Committees

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CODATA / NEWSLETTER

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