

52 CODATA / NEWSLETTER

MAY 1990

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CODATA REFERRAL DATABASE

The *CODATA Referral Database (CRD)* provides an automated compilation of records describing international numerical data sources in science and technology. It combines the information contained in the CODATA/Unesco Inventory of Data Referral Sources in Science and Technology (to be published by Hemisphere Publishing Corporation) which contains entries collected through 1987 and in several of the CODATA Directories of Data Sources. The database presently contains approximately 1200 records and comes with simple retrieval software and a User Manual.

The *CODATA Referral Database* is designed to permit a rapid search for data centers or other institutions which can provide numerical data or other factual information in many specified fields of science and technology. The result of such a search is the name and location of each relevant institution, along with a description of its scope of coverage, holdings, outputs, and dissemination policies. No actual numerical data are provided. The objective of the *CRD* is to cover all scientific disciplines and related fields of technology. The present version will be continually updated and expanded. Version 2 is expected to be available in March 1991. Purchasers of Version 1 may obtain it for a nominal fee.

The *CODATA Referral Database* and associated retrieval software are provided on several types of diskettes. A minimum of 256 kbytes of RAM and 4.6 Mbytes of free space on the hard disk is required to load the present system; as the database grows, this may expand to 10-12 Mbytes.

(continued on p.3)

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.

**12th Int'l CODATA Conference
Columbus, Ohio, 15-19 July 1990**

URGENT REMINDER

Preregistration is required for all CODATA '90 attendees. Please submit your registration immediately so that arrangements for the social and cultural events for the Conference can be finalized. Likewise, your hotel reservation must be made by June 6. For information, contact: Emmett Crawley at (614) 447-3614.

Biological Macromolecules CODATA TG Meets

The CODATA Task Group on Biological Macromolecules met from 16-19 March 1990 in Menton, France. Representatives of data banks on protein sequences, DNA sequences, complex carbohydrates, protein structures, 2-D gel, NMR data, and enzyme properties reported on current developments and problems. The meeting was a continuation of the Task Group's efforts to act as a platform for discussion between data banks, for information exchange, and to encourage emerging projects in the field. The group was concerned by the danger of restrictions to accessing data freely within the academic world resulting from growing national and commercial interests.



From left to right: J.-M. Claverie, R. Simpson, B. Seavey, D. George, K. Loening, J.L. Markley, T. Kunisawa, E.E. Selkov, F. Pfeiffer, T.F. Koetzle, W. Barker, A. Lesk, B. Keil, J.U. Thomsen, A.S. Kolaskar, W. Mewes, A. Tsugita, J. Rodgers.

The Task Group members felt that the experience and success of the Task Group in coordinating international endeavors strongly warrant its continuation by the 17th CODATA General Assembly especially in the light of the current major projects on elucidation of genetic information on organisms like *E. coli*, yeast, rice, and humans, as well as the development of mapping and sequencing techniques. Prof. A. Tsugita (Science University of Tokyo), a member of the CODATA Executive Committee and Secretary of the Task Group has been proposed as Chairman to replace Prof. B. Keil who recently retired from active scientific work at the Institut Pasteur (Paris). The members expressed their deep gratitude to him for leadership and representation of the Task Group since its creation in 1984 in gentle, generous, ingenuous, and ingenious ways. Prof. Keil will continue to support the Task Group with both sound knowledge and humor in the future.

Scientific and Technical Information Board

The U.S. "Numerical Data Advisory Board" (NDAB)--which works in close partnership with the U.S. National Committee for CODATA--has expanded its scope and changed its name to "Scientific and Technical Information Board" (STI). Its concerns will be to emphasize the users' needs and emphasize the role of information technology in facilitating access to data.

The board consists of an interdisciplinary group of scientists who use information technology and scientific data for research and development. It is charged with overseeing and advising on the utilization of scientific data and information technology by the research and development community. It fosters improvement in the availability, utility, accessibility, quality, reliability, and management of scientific data. It fosters utilization of, and improvement in, the information technologies that can deliver reliable data to the R&D community.

The board provides a user's forum for:

- Promoting initiatives that lead to improvements in the use of scientific data and information technology.
- Interfacing among the different federal agencies and branches of government to help develop and sustain a national data system that promotes advances in research and development.
- Advising on infrastructure and support policies required for scientific data to be readily available and highly reliable.

The board advises on user needs for:

- Application of information technology and development of new technologies for accessing and assimilating data sets in research.
- Evaluated scientific and technological data and information.
- Documentation of quality contents of computerized data sets.
- Guidelines and standards for the reporting, exchange, integration, and dissemination of data.

The board serves as the National Research Council's coordination center for STI matters and data studies of disciplinary units of the National Research Council (NRC). It also serves as advisory unit for matters related to:

- Standards for basic scientific measurements.
- Data standards for scientific and technical databases, database interfaces, and data exchange.

Coverage

- Physical, astronomical, chemical, biological, clinical, and earth sciences.
- Engineering and technical design.
- Interdisciplinary sciences such as environment and energy.
- Selected topics in social and behavioral sciences.

CODATA Referral Data

(continued from p.1)

The CRD is the creation of the CODATA Referral Database Task Group (TG) under the chairmanship of Dr. David G. Watson. It was initiated under funding from the Unesco General Information Program. Their most recent meeting held at the Unesco headquarters in Paris in March 1990 marks the completion of Version 1 of the database which will be continually updated and expanded in preparation for a larger coverage and scope for the 1991 Version 2.



Participants in the CRD meeting (left to right): J. Crease (ex officio), D.G. Watson, B.B. Lide, P. Crookes, D. Pélissier (Unesco), E.F. Westrum, Jr. Not shown: D.R. Lide, P. Glaeser, J.H. Westbrook. (Other Task Group Members: C.B. Alcock--Liaison, Q. Dong, F.J. Smith)

The TG is providing examination copies for institutions in 12 developing countries to provide feedback reports at an early date. An update of the present database is already underway and additional CODATA Directory chapters will be updated and added during 1990. Moreover, new subject areas will be selected for the extension of the scope of the Referral Database and--where appropriate--for the production of new printed Directories to supplement the 12 already in existence.

Survey of East-Asian Data Sources

In a Task Group (TG) meeting/symposium dedicated to the recently deceased former TG Chairman, Professor Jiro Osugi, on March 1-3 in Kyoto, Japan, the group has undertaken a significant expansion of its scope. The original Directory chapter (CODATA Bulletin 21-3, 1989) embraced only China, Japan, and Korea, but the recent meeting included representation from Australia, India, Indonesia, Malaysia, Pakistan, Philippines, Republic of China, and Thailand.



The participants in the meeting/symposium of the TG at the Kyoto Conference Center.

The Chairman of the Local Organizing Committee, Professor Kazuo Takayanagi, had provided a very detailed program in which the invitees from the countries not previously involved in the survey presented papers on database activities in their own

(continued on p. 6)

To: CODATA SECRETARIAT
51 Bd. de Montmorency
75016 Paris, FRANCE

Please send to (name and address):

ORDER FORM

☐ copies of CODATA REFERRAL DATABASE (CRD) -- Version 1 in format ()

Formats:

(1) 5.25 inch (1.2 Mbytes) (2) 5.25 inch (360 kbytes) (3) 3.5 inch (1.44 Mbytes)

Please send this order form to the Secretariat together with \$175(US) for each copy by check (payable to CODATA) or by Unesco coupons, etc.

Designs for a Global Plant Species Information System

An International Symposium organized by the IUBS Commission for Taxonomic Databases in partnership with the Systematics Association, the Linnean Society and the European Cultural Center of Delphi will be held at the European Cultural Center of Delphi, Greece on 12-16 October 1990. It is sponsored by CODATA and the Commission of the European Communities. The focus is on the exposition of a range of designs for a global species diversity information system for plants--a design which should enable scientists in all countries to access information on the names, classification, and geographical distribution of all of the world's plants. The designs would involve technical aspects both of biological computer information systems and decision-making amongst taxonomists. Assessments of the type of demand from conservation, agroforestry, natural products research, and other research applications will be set in scenarios for implementing such a system.

The programme will involve 5 sessions: The demand for a global plant species information system, botanical decision-making and data collection strategies, data structures and logical designs, system configuration--machines and communications, as well as management, ownership, and funding.

Each session will involve formal presentations as well as organized group discussions. There will also be demonstrations and poster sessions.

Further details from co-organizers: George F. Russell, Botany Department, NHB-166, Smithsonian Institution, Washington, DC 20560, U.S.A. or Frank A. Bisby, Biology Department, Building 44, University of Southampton, Southampton, U.K. SO9 5NH.

Ernst Meyer -- 1990 Herman Skolnik Award

Dr. Ernst Meyer, formerly of BASF-AG of the Federal Republic of Germany, has been named to receive the 1990 Herman Skolnik Award of the Division of Chemical Information of the American Chemical Society (ACS). The award was established in 1976 at the ACS Centennial Meeting in New York to recognize outstanding contributions to and achievements in the theory and practice of chemical information science, and was named after its first recipient. It will be presented to Dr. Meyer at the 200th ACS National Meeting in Washington, D.C. on 28 August 1990 at which time a special symposium in Dr. Meyer's honor will also be held.

Dr. Meyer has played a major pioneering role in revolutionizing chemical information handling through the use of computer methodology since the late 1950s. In particular, he was a leader in the development of input and searching techniques for topological and fragment representations of chemical substances, including generic or Markush representations, intended to be used for large-scale operations. In recent years, Dr. Meyer has broadened his area of research into that of structure-activity correlations.

Brief Report of "National CODATA Conference-1990" in India

CODATA activity in India has been gaining importance in the last few years. To take stock of data activity in various areas of science and technology, the National Committee of CODATA requested Prof. A. S. Kolaskar of the University of Poona to organize the national meeting. This meeting was held at Pune from 5-7 February 1990 on the campus of the University of Poona. During this meeting, papers were presented in the areas of meteorology, astrophysics, space science, materials science, oceanography, environmental science, toxicology, biotechnology, crystallography, animal husbandry, and agricultural sciences. These papers were of two types: (1) by database creators and managers, and (2) by database users on their scientific work. Computer scientists in the area of parallel computing, distributors of intelligent networking, and policy makers in the area of informatics for science and technology were not only present--but gave review talks. About 55 participants from all over the country participated in the meetings.

The papers presented during the meeting were of very high quality and brought out quite clearly that several large, medium, and specialized small data banks in various areas of science and technology exist in India. The software generally used is produced in-house. In biotechnology--due to special efforts of the Government of India, Department of Biotechnology, the progress has been quite substantial, and most of the major international data banks are now available in the country. A network of computers through NICNET (National Informatics Center Network) is available for biotechnologists in India. These scientists can also interact with each other through another network called INDONET. In fact, during this meeting on-line data search capability at NYCRY (Cambridge crystallographic data at University of Madras, Madras) was demonstrated. Similarly through NICNET, scientists at Pune, Bangalore, Madurai, and New Delhi are connected. These networks have the facility to tap international networks using VSNL (Videsh Sanchar Nigam Network). More scientists soon be on the network.

The last session of the conference was a round table discussion. Several suggestions were made during this session to make CODATA activity visible. Some of these suggestions which the National Committee has endorsed are:

- publish *Proceedings* of the conference
- disseminate *CODATA Newsletters* not only to scientists but also to libraries of major universities and institutes
- bring out a directory of data banks in India
- respond to the need for new data banks on properties of biomaterials such as proteins, nucleic acids for biosensors, for software on parallel computers, and on laboratory animals, environmental science, Ayurvedic medicines, etc.

--Prof. A. S. Kolaskar, University of Poona
(Secretary, Indian National Committee for CODATA)

Evaluated Thermochemical Data

The new volume—*Thermochemical Data for Reactor Materials and Fission Products*, by Cordfunke and Konings, provides critically assessed thermophysical and thermochemical data for reactor materials and compounds of fission product elements. The choice of substances studied include those which must be considered in the analysis of the release of radionuclides in event of nuclear reactor excursions and/or faults. This important gap in prior publication series produced in the UK, USA, USSR, and at IAEA (Vienna) deals particularly with oxides, hydroxides, and iodides of barium, cesium, ruthenium, strontium, tellurium, and lanthanide elements—in short, reaction products of the prominent fission products with the fuel itself, the cladding and eventually with the concrete pit, etc. The work is not limited to the computer-aided evaluation and—where necessary estimation—but, indeed, to the assessment and documentation of the basic experimental determinations.

It has been achieved with great care and attention to important details, for example, by the determination of new experimental values to fill gaps or to enhance data in regions where problems appear.

These new critical assessments will prove invaluable for reactor safety evaluation—a concern of inevitably increasing international significance as well as in the modelling of multiphase, multicomponent systems generally.

It is a tribute to the achievement of what can still be done by several individuals thoroughly devoted to their task. In this instance the publisher seems to have collaborated in producing an appropriate and excellent printing and binding endeavor thereby creating a truly landmark tool for the chemical thermodynamicist and the reactor engineer.

Thermochemical Data for Reactor Materials and Fission Products, by E. H. P. Cordfunke & R. J. M. Konings, Editors, North Holland, Amsterdam (1990). 696 pp. ISBN 0-444-88485-8. \$192. --An Editor (EFW)

Focus on: Global Change

The Institute for Scientific Information (ISI) this month launched a new multidisciplinary current awareness product available on diskette called FOCUS ON: GLOBAL CHANGE. International in scope and multidisciplinary, this biweekly research tool provides bibliographic information from thousands of science and social science journals, as well as from the business and popular environmental press. It covers:

- Current research on the physical, chemical and biological processes that affect the earth as a system
- Public policy developments, proposed and existing government regulations, legal issues, health issues, and other social, economic, and political factors that are affected by environmental change

The product is available on IBM PC and compatible, Macintosh, and NEC computers. Charter subscription to FOCUS ON: GLOBAL CHANGE is being offered for a limited time at the rate of \$245 for 26 issues. Risk-free trial-review basis offered by Institute for Scientific Information, 3501 Market Street, Philadelphia, PA 19104. Tel. 1-800-336-4474 or, from outside the U.S. and Canada, 1-215-386-0100, ext. 1483.

CODATA Publications

Columbus Conference Abstracts, *CODATA Bulletin* 22-1. (a)

The Provision of Materials Property Data via Computerized Systems, A CODATA Symposium held at the Institute of Inorganic Chemistry of the Siberian Division of the USSR Academy of Sciences, Novosibirsk, 6th and 7th September, 1989, *CODATA Bulletin* 22-2. (b).

Survey of Data Activities in East-Asian Countries, A CODATA Task Group Symposium held in Kyoto, Japan, 1-3 March, 1990, *CODATA Bulletin* 22-3, edited by Y. Hu and E. F. Westrum, Jr. (c)

Proceedings of the 11th Annual CODATA Conference on Scientific and Technical Data in a New Era, edited by P. Glaeser. (d)

CODATA Referral Database (CRD). (e)

(a) Hemisphere Publishing Corporation, New York, 1990, 147 pp., \$33.

(b) Hemisphere Publishing Corporation, New York, 1990, 118 pp., \$33.

(c) Hemisphere Publishing Corporation, New York, (Expected July 1990), ca. 208 pp., \$33.

(d) Hemisphere Publishing Corporation, New York, 1990, 370 pp., \$70. ISBN 0891169318.

(e) Produced on various diskettes with manual and simple search software. Available (see order form on page 3) \$175, Version 1, April 1990. (Update available early 1991 for nominal fee to purchasers of Version 1.)

CODATA Calendar

1990

June

15 CODATA Fundamental Constants Task Group. Ottawa, Canada

July

15 CODATA Hybridoma Data Bank Task Group. Columbus, OH, U.S.A.

15 CODATA Microbial Strain Data Network Task Group. Columbus, OH, U.S.A.

15-19 12th International CODATA Conference, "Data for Discovery," Columbus, Ohio, U.S.A.

20-21 17th CODATA General Assembly, Columbus, Ohio, U.S.A.

(Notice also the Calendar in *MDN*, pp. 7,8)

On the Definition of Data

C. Jaschek

Centre de Données Stellaires, Strasbourg, France

During a recent CODATA meeting I found out with a certain surprise that the experts present--who represented more than one dozen different sciences--did not agree on a definition of data. The following lines are an effort to clarify the issue.

Informaticians accept as definition of data "any input for computers." Such a wide definition puts on the same level a mathematical value like $\sin 45^\circ$, a predicted value of the thermal conductivity of a new polymer, the observed magnitude of a star, and the critical value of the gravitational constant. In fact, the very broadness of the definition conspires against its usefulness.

"Data are parameters deduced from observations and/or experiments by means of a model or theory."

In a recent book (*Data in Astronomy*, Cambridge University Press, 1989) I have given a definition of astronomical data as "any parameter which can be deduced from observation by means of a model or theory." Data are thus based upon observations. In order to make this definition applicable to natural sciences in general, it should be modified to read "data are parameters deduced from observations and/or experiments by means of a model or theory."

I think that for data handling such a definition has the merit of producing a neat separation of what we are talking about. In the first place it separates mathematical figures from physically meaningful results. I think that no one would object that we distinguish between the value of π and that of the fusion point of gold.

In the second place, it separates neatly values based upon observation from those based upon a prediction from models. I also think that no one would disagree on the convenience of distinguishing these two items. If this is not done carefully in data banks from the start, we will end up compiling (and averaging) expectations and realities. What does a "range" or an "average" mean under such conditions? It is irresponsible not to inform data users of such a mixture, but the best policy is to keep these two things quite separate, because despite all precautions, if they are kept together, confusion will occur sooner or later.

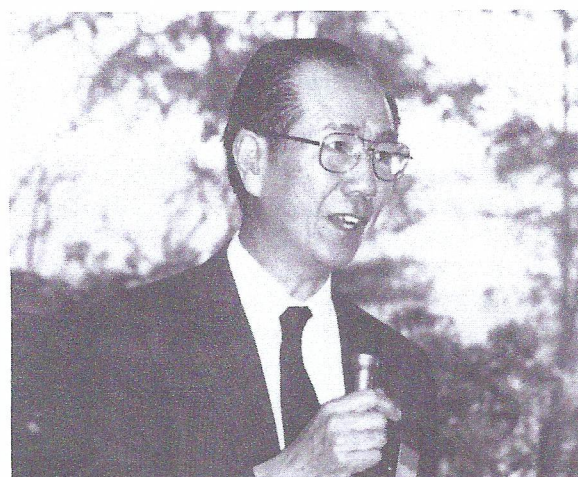
The definition also provides a clear footing for "critical data." These are refined data, that is, data from experiments compared and discussed in detail. If we were to use the term "critical" in connection with the informaticians' definition of data, we would have no clear understanding of its meaning, since obviously a critical value of π does not exist.

I think all of us can only benefit by using clear definitions of our basic concepts.

Comments anyone?

Survey of East-Asian Data Sources

(continued from p. 3)



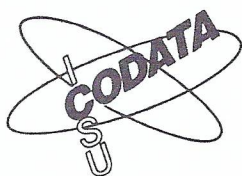
Professor Kazuo Takayanagi, Chairman of the Scientific Organizing Committee addresses the symposium.

nations. The collection of these papers has been edited by Yaru Hu and Edgar Westrum and published together with résumés of the participants as *CODATA Directory 22-3* (1990). Significant progress since the production of the *Directory of East-Asian Data Sources* (*CODATA BULLETIN 21-3*, 1989) was noted and, indeed, there was evidence that the TG activities were providing a catalytic awareness and a stimulus for enhanced database activities even in some of the countries not previously involved in the TG. (See for instance the article on India, page 4.)

At the Third Meeting, there was a session for discussing future activities of this Task Group. The new Chairman of the TG, Professor Mitsuo Tasumi, emphasized the importance of the continuation and expansion of the scope of the Task Group. The participants unanimously supported the application by Professor Tasumi to the CODATA Executive Committee for the renewal of this Task Group for another two-year term, 1991-1992. At the same time, it was agreed to alter the title of this Task Group to "Survey of Data Sources in Asian-Oceanic Countries" to include countries such as Australia, India, and Pakistan.

The present members of the Task Group (from China, Japan, and Korea) confirmed their plan to prepare the revision and update of the above-mentioned *Directory* as a main target of the Task Group activities. In fact, the further survey of the data sources has been started in China and Korea, and will start soon in Japan. Participants from other countries basically gave consent of intent to cooperate with the Task Group and investigate the possibility of similar surveys in their respective countries. Some of them agreed to serve as Task Group members.

The next (Fourth) Task Group Meeting will be held in Seoul, Korea, in early 1991, with Professor Mu Shik Jhon as the Chairman of the Local Organizing Committee.



Task Group on Materials Database Management

Materials Database Newsletter

April 1990, Number 10

NETWORKS

In two separate, though related actions, the American Chemical Society (ACS) and the MPD Network have signed protocols with the intent to cooperate in the worldwide distribution of USSR numeric scientific and technical information. ACS, through its Chemical Abstracts Service, signed an agreement with the USSR Academy of Sciences. A first step in this cooperative activity will be the establishment of STN International demonstration centres in Moscow and Novosibirsk. MPD Network and VNITs MV, the Soviet Research Centre on Materials Problems of USSR Gosstandart, reached an accord on the distribution of databases on the properties of materials. Through this collaboration, it is expected that a number of USSR industrial materials databases will be distributed within the USSR and to Western countries via MPD Network. FURTHER INFORMATION: J. G. Kaufman, MPD Network, 2540 Olentangy River Road, P. O. Box 02224, Columbus, Ohio 43202, USA.

DATABASES

Information on the mechanical and physical characteristics of all grades of ductile and malleable iron is now available in BCIRA's Mastercaster range of microcomputer programs for foundries under the title *Design Data - Cast Iron*. The program will calculate and display tensile, compressive, torsional, and shear properties as well as hardness ranges, moduli of elasticity and rigidity, Poissons ratio, and fatigue limits. Also covered are thermal expansion, heat capacity, density, as well as principal electrical and magnetic properties. It will also compare UK, international, and other national specifications. The program runs under MS-DOS on IBM PC or compatibles. A grey iron database will be available in the near future. Further details and a free demonstration disk are available from: Geoff Franklin, BCIRA, Alvechurch, Birmingham, UK, B48 7QB.

STANDARDS

To support exchange of data among different engineering functions in a manufacturing environment, the International Standards Organization (ISO) has a standards activity called STEP - Standard for the Exchange of Product Data. This work is under the auspices of ISO Committee TC184/SG4/WG1. The primary focus of this work is to facilitate the interchange of information among the planning, design, analysis, drafting, processing, and manufacturing steps of an industrial process. Materials information is considered an important type of data to exchange, and a Materials Committee exists. During the past few months, a general materials model has been developed. Its initial emphasis will be on materials data used for finite element analysis; however, other uses such as materials testing, development of design allowables, and quality control will be considered in the near future. The materials model will be of great importance in future materials data standards, and it is essential that a full review be made by all interested parties at an early stage. The next STEP meetings will be held 23-27 April 1990 in Reston, VA, USA, and 25-29 June 1990 in Gothenberg, Sweden. In addition, a draft document will become available between these two meetings. FURTHER INFORMATION: John Rumble, NIST, A323 Physics Building, Gaithersburg, MD 20899, USA. Tel: +1 (301) 975-2203.

CALENDAR

23-27 April 1990, Las Vegas, NV, USA

CORROSION/90 Symposium topics will include the application and impact of computers in corrosion control, measurement, information exchange and design and calculations. CONTACT: NACE Conference Manager, P. O. Box 218340, Houston, TX 77218, USA,

21-23 May 1990, San Francisco, CA, USA

Technical Committee Meetings of ASTM E49 on **COMPUTERIZATION OF MATERIALS PROPERTY DATA**

21-22 June 1990, Petten, NETHERLANDS

CERAMICS CLASSIFICATION Workshop. CONTACT: Mr. S. Schneider, NIST, Gaithersburg, MD 20899, USA. Tel: +1 (301) 975-5657. FAX: +1 (3-1) 926-8349.

28-31 August 1990, Tokyo, JAPAN

COMPUTER AIDED INNOVATION OF NEW MATERIALS, International Conference and Exhibition on Computer Applications to Materials Science and Engineering. CONTACT: Professor M. Doyama, CAMSE '90, c/o Nikkan Kogyo Shimbun Ltd., Business Bureau, 8-10 Kudan Kita, 1-chome, Chiyoda-ku, Tokyo 102, Japan.

November 1990, Petten, NETHERLANDS

CEC/CODATA Workshop on MATERIALS DATA FOR COMPUTER AIDED ENGINEERING. CONTACT: Mr. H. Kröckel, JRC Petten, P. O. Box 2, 1755 ZG, Petten, The Netherlands.

11-15 November 1990, San Antonio, TX, USA

Fall Meeting of ASTM Committee E49 on **COMPUTERIZATION OF MATERIALS PROPERTY DATA**

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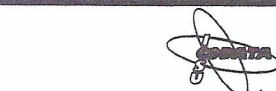
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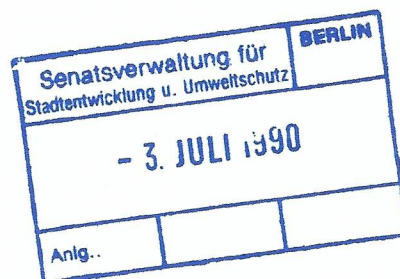
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CODATA / NEWSLETTER

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