



NEWSLETTER

OCTOBER 1968

INTRODUCTION

An important and definable part of the overall problem of the evaluation, storage, and retrieval of scientific information is the compilation of critically selected numerical and other quantitative scientific data. In order to promote international co-operation and effort in this field, a Committee on Data for Science and Technology, or CODATA, was established in 1966 by the International Council of Scientific Unions (ICSU).

This first edition of the CODATA Newsletter is intended to provide background information on the origin and organization of CODATA, and to define its tasks and objectives, within the context of world-wide activity on the compilation, evaluation, and dissemination of numerical data for science and technology. A general dissertation, by Prof. F.D. Rossini, the President of CODATA, on the history, present status, and possible future developments on an international basis, of the evaluation of scientific and technological data, is followed by descriptions of the organization and activities of CODATA, and of the First International CODATA Conference, by Dr. Guy Waddington, the former Executive Director of CODATA.

Future issues of the Newsletter will not only present news of planned or established national and international data programmes, but will also serve as a forum for the discussion of topics of interest to both the individual data evaluator and the user of the data. Special attention will be given to data activities within the International Scientific Unions, and to new developments and recommendations regarding scientific units, standards and symbols.

The Newsletter will, in addition, announce newly published or forthcoming data compilations, which may subsequently be used to up-date the „International Compendium of Numerical Data Projects“. Reports will be given of the results and recommendations of the Annual and Bureau Meetings of CODATA, together with news of the CODATA Task Groups, and of the International CODATA Conferences.

The staff of the CODATA Central Office will endeavour to cover the important aspects of the compilation and evaluation of numerical data for science and technology. The response of the reader is, however, essential to the effective exchange of information, and suggestions, comments and criticisms regarding the content of the Newsletter are welcome.

It is hoped that with better communication among them, compilers everywhere will develop a sense of belonging to a special community of scientists, who have a vital role to play in the fuller and more effective utilization of scientific knowledge.

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President of ICSU CODATA

Mr. Chairman and Members of the Conference:

With your indulgence, I would like to go back into history to begin my report on „Data for Science and Technology - from the Past into the Future“.

In the early days, the individual scientist was expert in nearly all areas of known science. He worked alone and, with his own hands, did everything that needed to be done. He built his own apparatus and maintained his own records. He occasionally communicated orally or in writing with a fellow scientist in his own, or another country. As the scope of science increased, he became aware of the need to know what his fellow scientists were doing, and the volume of communication on scientific matters increased. Then came scientific societies for oral communication, and journals for publishing scientific papers. As time went on, individual scientists were obliged to specialize more and more, and to reduce their range of interests to smaller and smaller areas of science in order to be able to keep abreast of the knowledge being generated.

At this stage, the individual scientist was still able to be in direct personal contact with substantially all of the original published papers in his then restricted field. But, with the further passage of time and the continued expansion in scientific output, the individual scientist found it extremely difficult to know about all the papers in his field that were appearing in all journals. Then came abstract journals to keep the individual scientist informed of the location of the original scientific papers in his area of interest.

The quantity of scientific information is increasing at an enormous rate, said to be doubling every eight to ten years. About 150 years ago, there were in the world about 50 scientific journals; 100 years ago, about 500; 50 years ago, about 5,000; and, today, of the order of 50,000. The number of persons in the world who are engaged in generating and publishing scientific information has increased enormously. We are told that 90 to 95 percent of all the scientists who have ever lived are living today. It is estimated that more than one million scientific and technical papers now appear each year in journals, bulletins, reports, and related media.

Now, with all this, the working time of a scientist has not increased. In fact, his effective time has decreased, because of the proliferation of administrative procedures and accounting methods required in our modern operations. The scientist today has reached the point where nearly all his working time would be required to read and properly digest all of the original published papers in his field. We are facing a serious problem. The scientist can, of course, further subdivide his field of interest, and hold his own that way. But there is a limit to this continued splintering of science - learning more and more about less and less.

Something different must be done to make it possible for the scientist today to assimilate fully the new knowledge being generated in his field. In principle, the solution is simple: We can interpose between the original literature and the end-using scientist a system of review and appraisal by qualified experts of all the original scientific information in given fields. Such reviews and appraisals would be performed for each area of science, with the results being made available through appropriate media.

This idea of having the original papers in the scientific literature reviewed and appraised for the end-using scientist is not new. In some measure, it has been going on for years in the form of review articles covering specialized areas in given sciences. But, looked at on a global basis, these efforts at review and appraisal of the original scientific literature have in large part in the past been carried on sporadically. Where such works have been of significant magnitude, they have generally been carried on independently and without much coordination.

The review and appraisal of scientific information constitutes an intellectual task of high order. Though the work can be aided and expedited by machines, automatic devices, and high-speed computers, it can be performed effectively and efficiently only by having skilled scientists appropriately involved.

Further, because of the enormous size of the task, and because the product has utility for scientists the world over, the work needs international as well as national coordination and guidance. In the long run, the world can cope with the explosion of scientific information only if more scientists will dedicate themselves to the work of critically reviewing and appraising the original scientific literature. To bring this about, we must see that the scientists engaged in this type of work are given appropriate high status in the scientific community of the world, with corresponding compensation.

Critical reviews and appraisals of scientific information are needed in every field. But the prime field for development in this regard is the area of numerical data for science and technology.

The numerical data which are to be reviewed and appraised for the benefit of science and technology are generated by observation and measurement, which operations constitute the backbone of science. The better and more accurately we can observe and measure, the better and more rapidly can we develop theories to explain the natural state of things, and to guide ourselves to more fruitful observation and measurements.

Measurements in science have come a long way in the past four centuries. For example, from a German publication of the year 1536, showing the 16th century „rute“, or rod, for measuring pastures, fields, vineyards, and fruit gardens, we read as follows: „To find the length of a measuring rod the right way, and as it is common in the craft....take sixteen men, short men and tall ones, as they leave Church, and let each of them put one shoe after the other and the length thus obtained shall be a just and common measuring rod to survey the land with“.

Next, let us simply look at the present day definition of the unit of length, which is the meter, m, which is equal exactly to 1,650,763.73 wavelengths of light in vacuo produced by the unperturbed transition $2p_{10} - 5d_5$ in the pure nuclid Krypton-86. This is the orange-red radiation of Krypton.

From these two examples, we see the enormous increase in the past 450 years of man's capabilities for measuring length. Today, much of the numerical data appearing in the literature of the world is of very high accuracy and precision. In reviewing and appraising such data, it is important that all of the accuracy and precision be preserved in the transition from the original record to the final compilation. Further, where discord exists among data on the same properties, the appraiser must be able to derive from the detailed context of all the measurements that weighted value which is most likely to be near the true value.

* A report presented at the opening of the First International CODATA Conference on the „Generation, Collection, Evaluation, and Dissemination of Numerical Data for Science and Technology“, at Arnoldshain, near Frankfurt/Main, Germany-BRD, June 30 to July 5, 1968.

As we said earlier, it is no longer possible for each individual scientist to review and appraise all of the numerical data in his field of interest appearing in original papers in the literature. He will not be able to review all of the relevant literature because of its magnitude; and he will usually not possess the expertise necessary to reduce and appraise the enormous amount of data to some understandable and useful meaning.

With critical tables of reference data produced by competent experts, we can have efficient utilization of our scientific manpower. The end-using scientists in educational, governmental, and industrial organizations can then pursue the work of their respective missions, fortified with the knowledge that they have at their disposal essentially all of the existing numerical data in the literature reduced to some useable form of reference data. The number of man-days of scientific time that could be saved thereby in our laboratories would be enormous. But what is equally important, the numerical values available would be of much higher quality than could be produced by the sporadic effort of scientists primarily interested in other problems. This latter point is very important for our technology and industry today, where the precise control of temperature, pressure, and other variables makes possible the conduct of industrial processes heretofore considered impossible.

Let us now review briefly some of the international efforts on the compilation of data for science and technology.

The Landolt-Börnstein Tables, headquartered in Germany, first appeared in 1883, with an edition of 281 pages. In 1894, came the second edition of 575 pages; in 1905, the third edition of 877 pages; and in 1912, the fourth edition of 1,330 pages. In the years 1923 to 1936, came the fifth edition, in 8 volumes of 7,457 pages. In the years 1950 to 1969, came the sixth edition of 26 volumes of about 20,000 pages. Because it is no longer practical for them to cover simultaneously all areas of science, the Landolt-Börnstein Tables have a new series of volumes, on specialized topics. These include nuclear physics and technology, magnetic properties, astronomy and astrophysics, atomic and molecular properties, crystal and solid-state physics, geophysics, etc.

The „Tables Annuelles de Constantes et Données Numériques“, headquartered in France, had ten volumes appear over the years 1910 to 1930. From 1936 to 1945, there were 40 installments, which covered the literature to 1939. Then a new title was given to this work, „Tables de Constantes Sélectionnées“ (Tables of Selected Constants), to cover specialized topics. These include nuclear physics, spectroscopy, oxidation-reduction potentials, optical rotatory power, semi-conductors, and terpenoids.

The Kaye and Laby Tables of Physical and Chemical Constants, headquartered in England at the National Physical Laboratory, have appeared in one volume, running through 13 editions from 1911 to 1966.

The International Critical Tables, headquartered in the U.S.A., at the National Academy of Sciences, came out in the years 1926 to 1933, as one edition of eight volumes in 3,819 pages. Contributions to this work came from 408 scientists in 18 countries. The organization of the International Critical Tables was established in 1919 by the International Union of Pure and Applied Chemistry, with the National Academy of Sciences of the U.S.A. being assigned the financial and editorial responsibility for the work. In 1923, the International Research Council, which was the predecessor of our present International Council of Scientific Unions (ICSU), gave its blessing to the project. It was hoped that the International Critical Tables would become a continuing operation, with revisions from time to time, but, unfortunately, the Editor-in-Chief, Edward W. Washburn, died in 1934, and this continuity never came to pass. The importance of the International Critical Tables to the science and technology of the world is evident from the fact that a significant number of sets of these tables are being sold today, 42 years after their original issue.

In the years 1938 to 1957, other data-compiling projects, operating on a continuing basis, came into existence in the U.S.A. These projects together involved total expenditures approaching one million dollars per year, and included the following:

The American Petroleum Institute Research Project 44 on physical, thermodynamic, and spectral properties of hydrocarbons and related compounds; the Manufacturing Chemists Association Research Project on physical, thermodynamic, and spectral properties of chemical compounds; the U. S. Atomic Energy Commission Project on nuclear data; the U. S. Bureau of Mines Project on thermodynamic data on metallurgical compounds; the Purdue University Center on thermophysical properties; the Dow Chemical Company Project on thermodynamic properties of selected compounds; and several National Bureau of Standards Projects on thermodynamic, thermochemical, atomic, and other properties of a large variety of compounds. With some change in sponsorship, all these projects are still operating.

In 1955, the National Academy of Sciences reviewed the situation in the U.S.A., decided that a new plan should be provided for coordinating and encouraging data-compiling activities, and, in 1957, established an Office of Critical Tables, with the following responsibilities: (1) To survey the needs of science and industry for critical tables of numerical data; (2) To stimulate and encourage existing continuing data-compiling projects; (3) To promote uniform editorial policy and procedures, with the use of internationally approved constants, units, and symbols; (4) To provide a directory-survey of continuing data-compiling projects; (5) To assist in establishing needed data-compiling projects for new scientific areas with financial support.

In its now ten years of existence, the Office of Critical Tables in the U.S.A., under the direction of Dr. Guy Waddington, has made significant progress on its objectives. The most difficult one, the fifth in the list, involving funds, came about in 1963 with the establishment, by the United States Government, of a National Standard Reference Data Program, operated by the National Bureau of Standards. This Program is under the direction of Dr. Edward L. Brady, and has close liaison with the Office of Critical Tables.

In the U.S.A., the Office of Critical Tables of the National Academy of Sciences functions in an advisory capacity to stimulate and encourage work on continuing data-compiling projects in all sectors of the scientific and technical community of the U.S.A., including both government and non-government areas. Also, the Office of Critical Tables serves as the link between the U.S.A. and other countries and the International Unions, through the International Council of Scientific Unions. The Executive Committee of the Office of Critical Tables, of which the Director of the National Bureau of Standards is a Member ex-officio, serves as the Advisory Committee for the National Standard Reference Data Program and also as the United States National Committee for CODATA.

With this background, let us now review briefly how CODATA was established. In the spring of 1964, when it was abundantly clear that the problem of data for science and technology was an international one, it was suggested that ICSU take the lead in providing international coordination and guidance in this field. In June, 1964, ICSU established a Working Group, under Professor Harrison Brown, to examine the problem. This Working Group met late in 1964 and formulated a recommendation that ICSU should establish a Committee in this field. In April, 1965, the recommendation was approved and the Working Group was requested to prepare a constitution and seek nomination for membership from unions and countries. In January, 1966, the General Assembly of ICSU, under Professor Sir Harold Thompson, approved the establishment of a Committee on Data for Science and Technology, or CODATA, with a constitution and initial membership.

CODATA has the following assignments on a world-wide basis: (1) To ascertain, through the Unions and appropriate National Bodies, what data-compiling work is going on and what the needs are; (2) To achieve coordination among, and provide guidance for, data-compiling projects; (3) To encourage support for data-compiling projects by appropriate private, governmental, and intergovernmental agencies; (4) To encourage the use of internationally approved constants, units, and symbols, and, when desirable, uniform editorial policy and procedures; (5) To produce a compendium-directory-survey of continuing data-compiling projects and related work; (6)

To encourage and coordinate research on new forms for preparing and distributing critically evaluated numerical data.

CODATA has held three annual meetings: In 1966, at Paris; in 1967, at Moscow; and in 1968, at Frankfurt. The Bureau of CODATA has held six meetings in its three years of existence: One each in Paris, Moscow, London, and Enumclaw, Washington, U.S.A., and two in Frankfurt. For its first two years, CODATA had its Central Office in Washington, D. C., U.S.A., with Dr. Guy Waddington as Director. Beginning July 1, 1968, the Central Office of CODATA moves to Frankfurt, Germany, with Dr. Christoph Schäfer as Director.

Looking now into the future, I feel that CODATA must move sharply forward to discharge its responsibility in the area of critically evaluated numerical data for the scientific and technical community of the world. Broadly taken, the basic objectives of CODATA are to have compilations of critically evaluated numerical data for science and technology available in suitable forms on a world-wide basis, with the compilations satisfying the following requirements:

1. Covering all substances and all properties of interest to all sectors of the scientific and technical community.
2. Being fully self-consistent with all physical relations and with the internationally approved constants, units, symbols, and nomenclature.
3. Having an accepted standard order of arrangement, understood and useable at the bench by scientists in all countries.
4. Being produced in forms needed by the several sectors of the scientific and technical community, at the various levels.
5. Being produced by scientists of high capabilities, adequately compensated.
6. Being maintained up-to-date by revision at appropriate intervals.
7. Being adequately supported from governmental and private industrial sources.
8. Being readily available at reasonable cost in any part of the world scientific community.

In order to achieve these objectives, CODATA must provide the needed guidance according to a plan that will be freely

acceptable to workers in various fields and in different countries. We can envision a whole array of World Centers of Numerical Data for Science and Technology, covering each area of science and appropriately tying in to the Central Office of CODATA as a hub. Hopefully, these World Centers of Numerical Data should be reasonably well distributed over the scientific community of the world, with each country sharing appropriately in carrying on the responsibility for providing numerical data for science and technology.

With these Centers of Numerical Data established, one for each area of data, the Central Office of CODATA, working closely with each Center, could become a central repository for one set of all the data, in whatever form the data were compiled. The Central Office of CODATA could, through its Compendium-Directory-Survey, inform scientists the world over as to the nature, location, product, etc., of each data-compiling Project and each Center of Numerical Data. CODATA could perhaps serve as a central clearing house for orders for data from any of the Centers or from any listed data-compiling Project. The Central Office of CODATA need not maintain an inventory of sets of the data from each Center and each Project, but could simply process orders and have shipments made direct to the purchaser from the original suppliers of the data.

As a central repository, and with the approval of the suppliers of the data, CODATA could, if desired, prepare, by automatic means, collections of numerical data in various combinations to suit „bench“ scientists and engineers engaged in work in special fields. The form of presentation of the data could be in a whole host of ways: bound volumes; loose-leaf sheets; punch cards; tapes; direct retrieval by teletype-computer systems; etc.

One can see that, in the area of numerical data for science and technology, CODATA could become an integral part of the total international network of centers of scientific information, the feasibility of which is under consideration by an ICSU-UNESCO Committee.

CODATA - ORGANIZATION AND ACTIVITIES

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In 1964 the Executive Committee of ICSU considered a proposal that it establish a mechanism for encouraging and informally coordinating worldwide efforts to evaluate, consolidate and compress the quantitative property values of science. ICSU is the ideal organization to accommodate such an activity because it brings together many disciplines of science through its 15 member Unions. The Executive Committee of ICSU was receptive to the proposal and established a Working Group to consider the problem in detail and to develop a plan for action. The Working Group had the following composition: Professor Harrison Brown (U.S.A., Convenor), Academician V.A. Kirillin (U.S.S.R.), Professor W. Klemm (Germany-BRD), Professor F.D. Rossini (U.S.A.), Sir Gordon Sutherland (U.K.), and Professor B. Vodar (France). The Working Group met several times. At its first meeting in Washington, D.C., in December 1964, it formulated a recommendation that ICSU establish a Committee on Data for Science and Technology, and defined its purposes and work. Then, at the request of the Executive Committee, it prepared a constitution for the proposed new committee and made recommendations concerning its preliminary make-up. The recommendations of the Working Group were presented to the General Assembly of ICSU in Bombay, India, in January 1966, and were approved. Thus, the legal basis of the ICSU Committee on Data for Science and Technology was established. Subsequently the acronym, CODATA, came into general use.

The terms of reference of CODATA as developed by the Wor-

king Group were incorporated with very little modification into the Constitution and read as follows:

„The general purpose of the Committee is to promote and encourage on a worldwide basis, the production and distribution of compendia and other forms of collections of critically selected numerical and other quantitatively expressed values of properties of substances of importance and interest to science and technology. To do this, the Committee should include the following points in its mission:

- (a) to increase awareness among all scientists of the importance of the problem, and, in particular, to encourage young scientists to appreciate and participate in compilation work;
- (b) to point out the need for improved status, salaries, working conditions, and facilities for compilers;
- (c) to point out that evaluation and publication of numerical and other quantitative data is inherently expensive and that subsidies from various sources may be required to promote both their production and fullest utilization;
- (d) to increase personal contacts among workers in this area by encouraging and arranging periodic meetings of specialists in the various fields and exchange visits between related compilation centers; and
- (e) to encourage programs of precise experimental determination to fill in gaps in knowledge and to extend and complete compilations in important areas.

To accomplish the foregoing general aims the Committee is instructed to give its attention to the following tasks:

* Executive Director of the Central Office of CODATA in Washington, D.C., U.S.A. from January 1966 through June 1968.

- (a) to ascertain on a worldwide basis through the appropriate Unions and national bodies,
 - (i) what work on critical compilation of evaluated numerical data is being carried on in each country;
 - (ii) what work is being sponsored by each Scientific Union or by other international groups; and
 - (iii) what the needs of science and industry are for additional compilations of evaluated data;
- (b) to achieve coordination among, and strengthening of, existing programs in such a way as to maximize their effectiveness, to minimize unintentional or undesirable overlap, and to recommend new compilation programs when necessary;
- (c) to encourage the support of needed work by appropriate private, governmental and intergovernmental agencies; and to encourage needed experimental work;
- (d) to encourage the use of nomenclature, symbols, and constants advocated by the responsible Unions; and, when desirable, uniform editorial policy and procedures for presentation of information;
- (e) on a worldwide basis
 - (i) to stimulate wider distribution of compilations of high quality;
 - (ii) to maintain and distribute a directory of continuing data compilation projects and related publications; and
 - (iii) to encourage adequate indexing of the substances and properties covered by all such compendia;
- (f) to encourage and coordinate research on new methods for the preparation and dissemination of critically evaluated tables generally expressed in numerical form".

Membership

It was foreseen that CODATA, to accomplish its purposes, would require the kinds of contact with the worldwide scientific community that could be provided by the Member Unions of ICSU, but would also need the resources of both finance and manpower that can be generated within the major technologically involved nations. The initial membership of CODATA included members from eleven international unions and six major countries. The Constitution also provides for liaison representatives from other international organizations, from other parts of ICSU, and co-opted experts as appropriate. The current status of membership is shown on page 11. In addition to the original six, several other countries have been invited to nominate members, and Canada now is a full member. Italy is in the process of becoming a member. The full Committee meets once each year to review policy matters. A six-man Bureau of the Committee supervises the program and meets twice each year.

A Central Office staffed by an Executive Director and supporting technical and secretarial personnel carries out the program of work recommended by the Committee. For the first two years the Central Office was situated in the National Academy of Sciences in Washington, D.C., under the direction of Dr. Guy Waddington. Beginning on July 1, 1968, the office began to function according to plan in quarters supplied by the German Institute for Documentation in Frankfurt/Main, Germany, under the direction of Dr. Christoph Schäfer, who had spent the prior 1 1/2 years in Washington, D.C.

Financial Support

The following general principles govern the financial support of the Committee and its Central Office: Union Members and additional members shall meet expenses of attendance at meetings from the resources of their sponsoring organizations. The expenses of Bureau Members have been supplied by ICSU. The expenses of the Central Office are covered by dues from Member countries in amounts roughly proportionate to the scientific activities within these countries. A more precise dues structure is under study by the Committee.

The Compendium

A major assignment of the Central Office of CODATA is to determine on a worldwide basis, what work on critical compilation of evaluated numerical data is being carried on in each country and in each Union. Accordingly, the Central Office has undertaken a survey of compilation work and by questionnaire and other appropriate means has collected in-

formation which is now being sifted, analyzed and grouped. The resulting material will be published in book form as "The International Compendium of Numerical Data Projects". This book will be a valuable source for those seeking compilations of evaluated data in various fields, but its prime purpose is to provide an overview of worldwide activity to provide a basis for coordination of current critical tables programs in all countries and all international organizations and to identify those areas receiving inadequate or no attention. The stress in the Compendium will be on centers that systematically and on a continuing basis keep abreast of numerical data for particular fields or categories of substances. Only activities of this type can provide compilations that are up-to-date. Many new centers are being established and will be described even though they do not yet have significant output. Also, some small areas of science have been periodically covered by an individual compiler in book form with long time gaps between editions. These, too, will be included. For each entry in the Compendium there will be given brief information about the organization conducting the work, the coverage of substances and properties, an analysis of special features of the work, and information permitting ordering or purchase of the books, cards or other forms of publication. It is expected that the first edition of the Compendium will be completed in 1968 with revisions to appear in future years. The distribution will be from the Central Office in Frankfurt/Main, Germany.

Conferences

Another less tangible mission of CODATA is to stimulate and improve communications between compilers of the world and various groups having responsibilities in the critical tables area. A direct method of accomplishing this end is to sponsor formal conferences. The First International CODATA Conference held at Arnoldshain, Germany, on June 30 - July 5, 1968, is an example. This conference is described in considerable detail elsewhere in this Newsletter. Other conferences of this kind are planned for the future - probably at about two - year intervals. Also, National Members of CODATA, to promote understanding and communications within their countries have organized conferences at the national level. In June 1967, a one-day meeting was held at the Royal Society, London, with attendance preponderantly from the U.K., but with invited speakers from other countries. A similar but smaller meeting was organized by Professor Kotani in Japan. CODATA has also associated itself informally with the U.S. Gordon Conference on Critical Tables which met in 1966 and will meet again in 1969.

Task Groups

CODATA has encountered a number of special tasks and will undoubtedly meet more such in the future. Under its Constitution it may establish ad hoc task groups to undertake such tasks. Two Task Groups are already functioning and another is under consideration:

1. The Task Group on Computer Use

At the organizational meeting of CODATA in Paris, June 1966, the following resolution was passed:

"It is recognized that in the generation, evaluation, storage, retrieval, and dissemination of quantitative data, increasing use will be made of computers and other aids. Paralleling this development will be the need for the associated software to accomplish such tasks as coding, indexing, correlating, storing, and transmission of numerical data. To assure the orderly development of the foregoing matters on a worldwide basis, it is recommended that the Committee establish a small Task Group composed of experts of the highest competence from different countries and disciplines to seek ways of achieving maximum exchange of information about the methodology of handling data, including software, and to stimulate new work in this field".

The current Membership of the Task Group is given on page 11. The Group, as an initial step, is currently working on a report on the status of automated techniques used in data centers in various countries. The Group has met in Paris in June 1967 and again in Washington, D.C., in May 1968. Reports on its activities will appear in future issues of the Newsletter.

2. The Task Group on Key Values for Thermodynamics

The function of this Task Group will be to compile, and recommend for general use, a relatively short list of values of important thermodynamic quantities of selected special substances which are used repetitively by compilers in many different centers, and also by experimenters, in publishing data of the type that is included in thermodynamic compilations. For example, the standard heats of formation of water and carbon dioxide, and standard entropies at 25°C of selected elements, have a role in thermodynamic calculations on a par with numerical values of relative atomic masses and of the fundamental constants. The Membership of the Task Group is given on page 11. The Group met in Arnoldshain on June 30, July 1 and 2, 1968, and formulated its task and the procedures for implementing that task. A report embodying these conclusions is given on page 8.

3. The Task Group on Fundamental Physical Constants

It is foreseen that within a relatively few years a new internationally agreed set of internally consistent fundamental constants will be needed by compilers. The formation of a Task Group to deal with this problem has been authorized. The membership of this group and the manner in which it will seek the cooperation and assistance of other organizations is being studied by the Bureau of CODATA.

National Links to CODATA

The following type of extension of the organization of CODATA has been extremely helpful in fostering its aims. Each National Member has organized or will organize within his country, a National Committee for CODATA attached to the ICSU adhering body. Already functioning effectively are: the Japanese National Committee for CODATA attached to the Science Council of Japan, the German National Committee for CODATA attached to the Deutsche Forschungsgemeinschaft, the U.K. National Committee for CODATA attached to the Royal Society, the U.S.A. National Committee for CODATA attached to the National Academy of Sciences, and the U.S.S.R. National Committee for CODATA attached to the Akademia Nauk of the U.S.S.R.

Still another type of organizational link, intentionally kept informal, is between governmental groups and CODATA. In the U.K., U.S.A. and U.S.S.R., there now exist governmentally sponsored programs for the funding and management of data compilation activities. These are a part of the governmental structure. The leaders of these groups have been brought into informal contact with one another and also when they so desire, receive advice and guidance from the National Committees of their countries.

In the foregoing pages it is seen that a substantial number of people and committees are directly or indirectly involved in the work of CODATA. It is intended that all of these people will be fully informed of plans and programs through the CODATA Newsletter.

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FIRST INTERNATIONAL CODATA CONFERENCE

on

Generation, Collection, Evaluation and Dissemination of Numerical Data for Science and Technology.

GUY WADDINGTON

Office of Critical Tables, National Academy of Sciences, Washington, D.C., U.S.A.

CODATA held its first international conference in the Taunus hills about 20 miles north of Frankfurt/Main, Germany, from June 30 to July 5, 1968. Prof. W. Klemm, Member of the Bureau of CODATA, and Chairman of the German National Committee for CODATA, was the General Chairman of the Conference. Dr. Guy Waddington, past Executive Director of the Central Office of CODATA, served as Program Chairman and Dr. Christoph Schäfer, new Executive Director of the Central Office, now located in Frankfurt/Main, was responsible for all local arrangements.

The Conferees were housed and the sessions held in the Evangelische Akademie Arnoldshain. The facilities were excellent in all respects for the informal „Gordon-type“ conference which drew about 90 experts from 12 countries. Among these experts were: directors and compilers from data centers, representatives of international unions, of national academies of many countries, of governmental funding and management programs, and of publishers of scientific data. Also present were several hand-picked groups of specialists in compilation areas in which international coordination is needed, e.g. chemical thermodynamics and spectroscopy.

An analysis of the Conference Program (see pages 9 and 10) reveals a studied effort on the part of the program committee to stimulate coordination among compilers from different countries; to examine common problems requiring solutions; to standardize in areas where standardization is useful; and to seek ways for CODATA to advance its aims as quickly and effectively as possible.

Speakers from the three major governmental funding programs for data compilation (U.K., U.S.A., and U.S.S.R.) of the world revealed similarities in general objectives of their respective programs, but some differences too. The U.S. program, described by Dr. E. L. Brady of the National Bureau of Standards, is decentralized and confines itself to projects dealing with well-defined physical properties of well-characterized substances. The U.K. program, represented by Dr. R. E. Fairbairn of the Office of Scientific and Technical Information, and C.G. Giles of the Ministry of Technology, has objectives similar to the U.S. program, but in addition emphasizes properties of engineering materials. The program of the U.S.S.R., which is centered in the State Service of Standard and Reference Data, but with substantial input from the Academy of Sciences of the U.S.S.R., as revealed by Academician M.A. Styrikovich, has the same general functions as the U.K. and U.S.A. programs, but is also responsible for establishment of quantitative legal specifications for the properties of industrial materials.

It was clear from reports given that the national standardizing laboratories (NBS, NPL, etc.) of the three foregoing countries and also of Canada, France, Germany, and Japan, will play an increasingly important role in compiling reference data. Germany for the first time, through the Physikalisch-Technische Bundesanstalt (PTB) is embarking on a program of data compilation analysis. It was reported by G. Denègre that France, in which metrology was spread over a certain number of laboratories, is beginning to reorganize its activity, and is setting up a national metrological laboratory. Japanese governmental laboratories participate in collecting infrared data and gas chromatographic data.

It was generally agreed that industry, as well as government, should contribute to the support of compilation work. Prof. A. Bylicki of Poland made a strong plea for producing data useful to industry.

Discussion was initiated on a number of relatively large specialized compilation projects of different types which are conducted in various countries. Prof. Hellwege, Editor-in-Chief of the Landolt-Börnstein Tabellen, reviewed the workings of this long-established project, which supports itself by sale of its publications. Noteworthy is the new policy of no longer providing general coverage of all fields of science, but only monographs on areas of great current interest. An index of all Landolt-Börnstein volumes now in preparation will be most welcome. Prof. B. Vodar reviewed the status of the "Tables de Constantes et Données Numériques", which operates on a smaller scale than the preceding project, but also confines itself to monographs. This program has supported itself by contributions from industry, from sales of publications, and to some extent by governmental funds. Its future support and direction is being re-evaluated.

The IUPAC Centre on Thermodynamic Properties of Fluids at Imperial College, directed by Dr. S. Angus, is interesting in that the initiative for its formation came from the International Union of Pure and Applied Chemistry, an international union; its funding, though partly international, is guaranteed by the British Government; and the expertise for conducting its program is by panels of experts from many countries.

The Thermophysical Properties Research Center, in which experimental and theoretical research, and documentation, are carried out, in addition to compilation of physical properties, was described by Prof. Y.S. Touloukian. This center provides an example of a compilation program narrow in scope as to properties, but having very wide coverage.

Dr. L. Hjärne of the International Atomic Energy Agency (IAEA), Dr. J. J. Schmidt of the Kernforschungszentrum Karlsruhe, Germany-BRD, and Dr. N. B. Gove of the Oak Ridge National Laboratory revealed the extremely effective cooperation among nuclear data compilers in major countries which results in effective collection and dissemination of various types of nuclear data. Large centers in France, the U.K., the U.S.A. and the IAEA in Vienna, with cooperation from many other countries constitute a coordinated international network for data collection and exchange.

An effort was made to have several panels and task groups explore the possibility of worldwide cooperation in selected areas. A panel on infrared spectra, chaired by Dr. R. N. Jones of Ottawa, arrived at a consensus in general terms as to what is needed in the consolidation and distribution of infrared spectra at the national and international level. An informal summary of the conclusions of this panel is given on the next page. A similar panel on data for chemical thermodynamics, chaired by Dr. O. Kubaschewski of NPL, agreed that the subdivision of work among existing centers provides a convenient basis for cooperation among them. A panel report from this group will be studied by CODATA.

The Task Group on Key Values for Thermodynamics, as a result of several afternoon meetings, identified their terms of reference and planned for proceeding toward a list of recommended key values for use by compilers and others. This statement is given on the next page.

The Task Group on Computer Use sponsored a half-day symposium, chaired by Prof. G. Black of the U.K. Computer Centre at Manchester, on applications of computers to processing, generation, and storage and retrieval, of thermodynamic, crystallographic, nuclear, and spectral data. The operation of the JANAF data project at the Dow Chemical Company in Midland, Michigan, U.S.A., discussed by Dr. D. R. Stull, while still using "human" evaluation, makes very extensive use of computers in generating and updating numerical property values. Also, the utilization of computers for storage of spectral data, described by Dr. R.N. Jones, obviously has a great potential for future use.

It is clear that CODATA Task Groups and the less formal panels, whose contributions to the Conference were marked,

constitute efficient mechanisms for obtaining consideration of international problems and for generating recommendations regarding standardization and compatibility.

The Friday morning session entitled "A Discussion of CODATA" moderated by Sir Gordon Sutherland, brought forth a diversity of comments and suggestions. A particularly challenging proposal submitted by Academician V. N. Kondratiev of the U.S.S.R. and presented to the Conference by Dr. V. Medvedev, asked for the formation of a broad program to consolidate, evaluate and publish the data of chemical kinetics. There was agreement both on the importance, and difficulty, of the suggested program, which the Bureau of CODATA will consider at its next meeting.

The general problem of links between operating projects, international unions, focal points in countries, between unions and other unions, and so on, was brought out in different ways by four or five experts. It was agreed that CODATA must continue to seek development of improved means of communication between centers, sponsors, international unions and concerned organizations.

The problem of coordination of centers was covered in a comprehensive report by Prof. F. D. Rossini, who outlined a tentative plan on how a world system of centers might be brought into being. This plan was brought forward purely as a basis for discussion and for further consideration by CODATA. Several nuclear scientists present commented that in their field there already existed a world center with subcenters in four different countries which, taken together, may be considered as a world center.

Two sessions in particular epitomize the important reasons for holding the Conference, namely, to identify problems within the terms of reference of CODATA which it can solve, or help to solve. The Thursday morning session on "Special Topics" revealed many problems and challenges relating mostly to needed coordination among compilers. Among these are the needs for definition of commonly used terms such as data, standard reference data, etc; the need for better indexing; and the need for improved efficiency in utilizing the primary literature. The Friday session sought to single out high priority problems for the attention of CODATA.

Lack of space prevents the presentation of the results of the above discussions. CODATA in its planning, with a recording of the discussions at its disposal, will take cognizance of the many useful ideas put forth. One suggestion in particular endorsed by a large majority of the participants is that CODATA should have the Second International CODATA Conference on Numerical Data for Science and Technology in 1970 at a suitable place in Western Europe.

Informal Letter Report to the Panel on Infrared Spectra at the First International CODATA Conference from

Dr. R. N. JONES, Panel Chairman

Panel Members:

F. F. Bentley	D. R. Lide, jr.	D. J. Shields
I. Eliezer	W. M. Linfield	T. Shimanouchi
L. V. Gurvich	E. R. Lippincott	R. G. Simard
R. N. Jones	Y. Mashiko	M. K. Wilson
H. Kaiser	S. A. Rossmassler	B. Vodar
K. G. Heyden	P. Sadtler	B. J. Zwolinski

As you know, this was an informal conference, conducted in the spirit of the Gordon Research Conferences. The results of our deliberations therefore have no official status with respect to future plans of CODATA, nor are they to be regarded as formal directives to other organizations that might have interest in this subject.

Nevertheless, the conference provided a unique opportunity to bring together representatives of most of the widely scattered groups that are actively involved in the generation, collection, evaluation and dissemination of infrared spectral data. Many of us came to the conference with diverse views about the future of infrared documentation, and I think it is fair to say that our discussions led us towards some common accord.

At Arnoldshain several of you asked me to supply copies of my notes for the Thursday morning report, and I am therefore circulating this letter as an „aide-memoire“ to the panel participants.

In the first place, we recognized that there is a strong need for more infrared spectra for the identification of organic and inorganic compounds, and it was our consensus that independent projects, both governmental and private, should continue to take the main responsibility for this work. We agreed that improved quality of data leads to increased utility of the information derivable from the reference spectra. Such improvement can come, in the first place, from better authentication of the compound structure, and secondly from more effective use of the performance capabilities of the available instruments.

We noted also that the application of infrared spectrophotometry in several important areas of science is restricted by the limitations of existing instrumentation and techniques. Among these areas are the interchange of quantitative data among laboratories; the more detailed interpretation of molecular structure; more accurate kinetic and equilibrium studies (particularly of the liquid state); and the calculation of thermodynamic functions.

We agreed that certain aspects of the problems associated with the efficient storage and retrieval of infrared spectral data need emphasis. The efficient use of infrared spectral data for all applications requires the maintenance of general indexes covering all the reference collections in addition to the indexes to the various individual spectra collections. It is also important that appropriate storage and retrieval systems, including those using computers and other automated searching devices, be developed and maintained to serve the variety of user needs.

Finally, we expressed the view that at, or in association with, the next CODATA Conference an opportunity should be provided to explore the common use of various kinds of reference data relating to molecular structural analysis. The techniques we had in mind included infrared, ultraviolet, Raman and microwave spectrometry, nuclear magnetic resonance spectrometry, mass spectrometry and x-ray crystallography. Concurrent, but separate consideration might also be given to the spectrographic techniques that relate more directly to atomic properties.

Though not spelled out specifically at our Panel Discussion, it became evident, during the Arnoldshain Conference (and particularly at the Friday morning closing session) that a clear distinction must be maintained between „evaluated“ and „non-evaluated“ numerical scientific data. In the field of infrared documentation there is a need to clarify the concept of „evaluated“ data and the manner in which it can be implemented both at national and international levels.

Report of the CODATA Task Group on Key Values for Thermodynamics *

The Task Group met during the First International CODATA Conference at Arnoldshain/Germany, and approved the following report:

1. Certain compounds and certain properties shall be designated as key compounds and key properties with respect to thermodynamic tabulations.
2. The properties at this particular time so designated are ΔH_f° , S° and H° at 298.15 K.
3. The key substances shall include all the elements in their standard reference states and standard monatomic gaseous states; and such additional compounds as the Task Group may determine.
4. The Task Group proposes to recommend a list of key property values for the key substances for consideration by the scientific community over a one year period. This may be accomplished by publication in the Bulletin of Thermodynamics and Thermochemistry and in other appropriate journals.
Submission of this list to the public provides an opportunity for comments from the scientific community to the Task Group.
5. After the lapse of the prescribed period, the Task Group will proceed to recommend final values for the properties involved. The final approval rests on CODATA. The recommended values will be published according to the procedures laid down by CODATA.
6. After the final publication of the first list of approved key values the Task Group will from time to time make additions to the list and such revisions as are deemed necessary.

*) The membership of the Task Group is designated by CODATA and includes representation from important compilation projects that make major use of the defined key values, such as the National Bureau of Standards, Washington, D. C., and the Institute of High Temperatures, Academy of Sciences of the U.S.S.R., Moscow. The current membership of the Task Group is given on page 11.

PROGRAMME
FIRST INTERNATIONAL CODATA CONFERENCE

on

Generation, Collection, Evaluation and Dissemination of Numerical Data
for Science and Technology.

Evangelische Akademie
Arnoldshain, near Frankfurt/Main, Germany-BRD
June 30 - July 5, 1968

Monday, July 1, 1968

Opening of Conference:

Prof. W. Klemm, Institute of Inorganic Chemistry, University Münster, Münster, Germany-BRD

Morning Session - Chairman: Prof. W. Klemm

Data for Science and Technology - from the Past into the Future
Prof. F. D. Rossini, University of Notre Dame, Notre Dame, Ind., U.S.A.

An International Network of Information Centres, and the Role of CODATA - panel discussion
Moderator: Prof. H. Kaiser, Institute of Spectrochemistry, Dortmund, Germany - BRD

Established National Data Systems:

- (a) The National Standard Reference Data Project of the U.S.A.
Dr. E. L. Brady, National Bureau of Standards, Washington, D.C., U.S.A.
- (b) The National Numerical Data Programme of the U.S.S.R.
Academician M. A. Styrikovich, Academy of Sciences of the U.S.S.R., Moscow, U.S.S.R.
- (c) The National Numerical Data Programme of the U.K.
Dr. R. E. Fairbairn, Office for Scientific and Technical Information, London, U.K.

Announcements regarding Panels, Task Groups and Working Groups

Dr. Guy Waddington, CODATA, Washington, D. C., U.S.A.

Evening Session - Moderator: Sir Gordon Sutherland, Emmanuel College, Cambridge, U. K.

Panel discussion on developing National Programmes:

France: Prof. B. Vodar, High Pressure Laboratory of CNRS, Bellevue, France
Germany-BRD: Dr. H. Stussig, Association of Industrial Research Institutes, Cologne, Germany-BRD
Japan: Prof. M. Kotani, Department of Physics, Osaka University, Osaka, Japan
Canada: Dr. R. N. Jones, National Research Council, Ottawa, Canada
Poland: Prof. A. Bylicki, Institute of Physical Chemistry of the Polish Academy of Sciences, Warsaw, Poland
Israel: Prof. A. S. Kertes, Department of Inorganic Chemistry, Hebrew University of Jerusalem, Jerusalem, Israel

Panel discussion on the role of the International Unions:

IAU: Dr. Charlotte Sitterley, National Bureau of Standards, Washington, D. C., U.S.A.
IUPAC: Dr. Guy Waddington, CODATA, Washington, D. C., U.S.A.
IUCr: Dr. Olga Kennard, University Chemical Laboratory, Cambridge, U. K.
IUPAP: Prof. B. Vodar, High Pressure Laboratory of CNRS, Bellevue, France
IUPAB: Prof. J. T. Edsall, Biological Laboratories, Harvard University, Cambridge, Mass., U.S.A.

Tuesday, July 2, 1968

Morning Session - Chairman: Academician M. A. Styrikovich, Academy of Sciences of the U.S.S.R., Moscow, U.S.S.R.

Special problems of the Tables de Constantes et Données Numériques

Prof. B. Vodar, High Pressure Laboratory of CNRS, Bellevue, France

The IUPAC Centre on Thermodynamic Properties of Fluids

Dr. S. Angus, IUPAC Thermodynamic Tables Project Centre, Imperial College, London, U. K.

Special problems of the Landolt-Börnstein Tables

Prof. K. H. Hellwege, Institute of Technical Physics, Technical University, Darmstadt, Germany-BRD

The Gmelin Institute

Dr. K. C. Buschbeck, Gmelin Institute, Frankfurt/Main, Germany-BRD

The TPRC Center for Measurement, Documentation and Compilation of Thermophysical Properties

Prof. Y. S. Touloukian, Purdue University, Lafayette, Ind., U.S.A.

Experiences from Nuclear Data Compilers

Dr. J. J. Schmidt, Nuclear Research Centre, Karlsruhe, Germany-BRD

Evening Session - Chairman: Prof. B. Vodar, High Pressure Laboratory of CNRS, Bellevue, France

Common Problems of Thermodynamic Compilation Centres - short report and panel discussion

Moderator: Dr. O. Kubaschewski, National Physical Laboratory, Teddington, U. K.

Common Problems of Infrared Compilers - short report and panel discussion

Moderator: Dr. R. N. Jones, National Research Council, Ottawa, Canada, with

Dr. S. A. Rossmassler, National Bureau of Standards, Washington, D. C., U. S. A.

Wednesday, July 3, 1968

Morning Session - Chairman: Prof. Gordon Black, National Computer Centre, Manchester, U. K.

CODATA Task Group on Computer Use

Introduction: Mr. R. Bernhardt, Centre for Mechanization in Documentation, Frankfurt/Main, Germany-BRD

The Programme of the Task Group on Computer Use

Prof. Gordon Black, National Computer Centre, Manchester, U.K.

Automation of Data in Special Areas

(a) Thermodynamic Data - Dr. D. R. Stull, Dow Chemical Company, Midland, Mich., U.S.A.

(b) Crystallographic Data - Dr. Olga Kennard, University Chemical Laboratory, Cambridge, U. K.

(c) Nuclear Data - Dr. N. B. Gove, Oak Ridge National Laboratory, Oak Ridge, Tenn., U.S.A.

Dr. L. Hjärne, International Atomic Energy Agency, Vienna, Austria

(d) Spectral Data - Dr. R. N. Jones, National Research Council, Ottawa, Canada

Prof. Y. Mashiko, Japanese Government Chemical Industrial Research Institute, Tokyo, Japan

Evening Session - Chairman: Prof. M. Kotani, Department of Physics, Osaka University, Osaka, Japan

The Roles of National Laboratories and Institutes

The Concept of a National Standard Reference Data System in the U.S.A.

Dr. M. B. Wallenstein, National Bureau of Standards, Washington, D.C., U.S.A.

(presented by Dr. E. L. Brady, after the news of the sad loss of Dr. M. B. Wallenstein)

Discussion on the Role of National Laboratories and Institutes

U.K.: Dr. E. F. G. Herington, National Physical Laboratory, Teddington, U. K.

Mr. C. G. Giles, Ministry of Technology, London, U. K.

Germany-BRD: Prof. U. Schley, Institute of Metrology of Germany-BRD (Physikalisch-Technische-Bundesanstalt), Braunschweig, Germany-BRD

Canada: Dr. R. N. Jones, National Research Council, Ottawa, Canada

Japan: Prof. Y. Mashiko, Japanese Government Chemical Industrial Research Institute, Tokyo, Japan

France: Mr. G. Denègre, National Bureau of Metrology, Paris, France

U.S.S.R.: Prof. L. V. Gurvich, Institute of High Temperature, Academy of Sciences of U.S.S.R., Moscow

The New Chemical Kinetics Data Programme of the Academy of Sciences of U.S.S.R.

Academician V.N. Kondratiev, Institute of Chemical Physics, Academy of Sciences of U.S.S.R., Moscow

(presented by Dr. V. Medvedev, Institute of High Temperature, Academy of Sciences of U.S.S.R., Moscow)

Thursday, July 4, 1968

Morning Session - Chairman: Dr. Guy Waddington, CODATA, Washington, D. C., U.S.A.

Discussion of Reports of Working Groups and Panels

(a) Panel on Thermodynamic Data (evaluation of data, co-ordination of centres, computer use)

Moderator: Dr. O. Kubaschewski, National Physical Laboratory, Teddington, U. K.

Report from the Chairman of the CODATA Task Group on Key Values for Thermodynamics,

Prof. Stig Sunner, Thermochemistry Laboratory, Lund University, Lund, Sweden

(b) Panel on Infrared Spectroscopy (evaluation of standards, co-ordination of centres, symbols and units, and digitizing of spectra)

Moderator: Dr. R. N. Jones, National Research Council, Ottawa, Canada

(c) Panels on Special Topics

Area I Definitions and Terminology

Moderator: Dr. S. Angus, IUPAC Thermodynamic Tables Project Centre, Imperial College, London, U. K.

Area II Indexing, Classification and Ordering

Moderator: Prof. K. H. Hellwege Institute of Technical Physics, Technical University, Darmstadt, Germany-BRD

Area III Efficient Use of Literature

Moderator: Dr. O. Kubaschewski, National Physical Laboratory, Teddington, U. K.

Prof. Y. S. Touloukian, Thermophysical Properties Research Center, Purdue University, Lafayette, Ind., U.S.A.

Prof. B. J. Zwolinski, Thermodynamics Research Center, Texas A&M University, College Station, Texas, U.S.A.

Mr. D. D. Wagman, National Bureau of Standards, Washington, D.C., U.S.A.

Area IV Handbooks

Moderator: Prof. Y. S. Touloukian, Thermophysical Properties Research Center, Purdue University, Lafayette, Ind., U.S.A.

A User looks at Numerical Data Evaluation

Dr. H. A. Skinner, Department of Chemistry, University of Manchester, Manchester, U.K.

Evening Session - Chairman: Prof. W. Klemm, Institute of Inorganic Chemistry, University Münster, Münster, Germany-BRD

Social Evening with Chamber Music

Friday, July 5, 1968

Morning Session - Chairman: Prof. F. D. Rossini, University of Notre Dame, Notre Dame, Ind., U.S.A.

Remarks on the New Central Office of CODATA

Dr. Christoph Schäfer, CODATA, Frankfurt/Main, Germany-BRD

A Discussion of CODATA

Moderator: Sir Gordon Sutherland, Emmanuel College, Cambridge, U. K.

Closing Remarks

Prof. F. D. Rossini, University of Notre Dame, Notre Dame, Ind., U.S.A.

ISCU CODATA

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Vice President	Prof. B. Vodar (France)
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	Mr. J. d'Olier (France)
	Mr. F. Schulte-Tigges (Germany-BRD)
	Dr. R. L. Wigington (U.S.A.)
	The appointment of a member from the U.S.S.R. is pending.
Ex officio member	Dr. Christoph Schäfer (Germany-BRD)

2. Task Group on Key Values for Thermodynamics

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	Prof. L. V. Gurvich (U.S.S.R.)
	Prof. D. M. Newitt (U. K.)
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October 1968

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