INTERNATIONAL ASPECTS AND THE FUTURE

OSTI's investigations led it to classify data activities in four ways:

(a) Fields where working scientists recognize the need for organized data and where data activities are well advanced. (Crystallographic, nuclear, and thermodynamic data are prime examples).

(b) Fields where working scientists recognize the need for organized data but where individual workers are discouraged by the sheer volume of data or of specialized effort required. (Mass spectrometry is a good example).

(c) Fields where data have been too fragmented or of insufficiently high quality for satisfactory data projects to be started, but where recent instrumental advances have suddenly changed the picture—*e.g.*, cartographical data since the advent of computer-controlled map making machines.

(d) Fields where systematic data activities are still impossible, or where scientific workers are unaware of, or apathetic about, the value of organized data.

The future usefulness of central offices, such as OSTI, lies, we feel sure, in upgrading types (b), (c), and (d) to type (a). Much of this work is, and will continue to be, education rather than promotion and it is here that international coordination, such as the ICSU interest, can have such beneficial results. Experience and intergovernmental exchanges have tended to show that activities, such as described in x-ray crystallography or mass spectrometry, may well be the best method of mobilizing national contributions to an agreed international program. The results of these national activities are then made internationally available by publication, by the provision of an international service, or increasingly by the interchange of computer memory tapes. OSTI welcomes the present opportunity for the international promotion of data awareness among scientists and for the possibility of international scientific agreement on worthwhile data projects.

A World System of Evaluated Numerical Data for Science and Technology*

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Received November 16, 1966

Voluntary international coordination of programs for production of critical tables of standard reference data will be the aim of the Committee on Data for Science and Technology (CODATA), recently established by the International Council of Scientific Unions (ICSU). CODATA will have initial representation from 10 to 12 of the constituent unions of ICSU and six major countries (France, Germany, Japan, U. K., U. S. A., and U. S. S. R.). A central staff office will be located initially in Washington, D. C.

A half century ago it was quite feasible to plan systematically for the collection, evaluation, and publication of all or nearly all of the useful data in the scientific literature in one single coordinated effort. The publication of the "International Critical Tables of Numerical Data: Physics, Chemistry and Technology" (ICT) (*1*) between 1926 and 1933 was the result of such an effort. The "Tables de Constantes et Données Numériques" (*2*), founded by Charles Marie of Paris in 1909 was similar in its approach, though less critical in its quality and less comprehensive in its coverage. The "Landolt-Börnstein Tabellen" (*3*), started in 1883 in Germany, is now in the final phase of producing the sixth and last comprehensive edition. In each of the six editions an effort was made to cover all fields of the physical sciences.

What is the status of the foregoing three publications today? The ICT was never revised for a variety of reasons. The untimely death of its editor-in-chief in 1934, the lack of a sufficiently bold and well-funded plan for providing continuity, and an unsettled period of world affairs all contributed. The French and German comprehensive programs have continued until the present time but in modified form. Some years ago it became plain to the editors of both that in future the effort should be limited to monographs on selected topics of current importance and interest.

The day of the coverage of all of science by a single centralized editorial effort has passed. The problem has become too large for any one group. But somehow mechanisms must be devised for extracting, evaluating, and publishing numerical property values in convenient form, on a continuing basis for all of the sciences; otherwise, data determined with accuracy, at great expense, will be lost in the morass of the primary literature.

* Presented before the Division of Chemical Literature, Symposium on Compilations of Data on Chemical and Physical Properties of Substances, 152nd National Meeting of the American Chemical Society, New York, N. Y., Sept. 12, 1966.

The breakdown of coordinated mechanisms for extracting, evaluating, and publishing numerical data was apparent a decade or more ago. In 1957 the National Academy of Sciences–National Research Council of the U. S. A. started the Office of Critical Tables (OCT) which formulated a plan and began to grapple with various aspects of the problem. The primary concept was that the total task of evaluating and compiling the numerical data of science should be decentralized and that the numerical data for each significant area of science should be evaluated by experts located in appropriate scientific centers.

After several years it became apparent in the United States that substantial sums of money and a strong management team were necessary to make an impact on the task of starting new centers or strengthening established ones. Accordingly, in recognition of the great importance of the problem to the United States, the Office of Science and Technology in the Executive Office of the President of the U. S. A. issued a directive in 1963 that there be established at the National Bureau of Standards an Office of Standard Reference Data to administer a National Standard Reference Data Program (NSRDP). This program under Dr. E. L. Brady is now very actively stimulating projects for compilation of evaluated numerical physical and chemical properties of well-characterized substances for the main areas of the physical sciences.

But this active and excellent program at the National Bureau of Standards obviously poses a dilemma for the U. S. and for other countries. Science is international and data compilations contain the fruits of research in all countries. All countries need compilations of data to nourish their research and industry. Thus it is very clear that the production of compilations of evaluated numerical property values must be thought of as a world problem. No one country should supply all of the needed financial resources; even more important, no one country can supply the expert manpower needed for the task. Other countries besides the U. S. sharing this realization include France, Germany, Great Britain, Japan, and the U. S. S. R.

Some sort of international collaboration is required as it was 40 years ago when the preparation of the ICT was undertaken. The initial incentive for production of the ICT came from the International Union of Pure and Applied Chemistry and the plan of action was endorsed by the International Research Council which later became the International Council of Scientific Unions (ICSU). And now, a half century later, organized international science has seen the problem and has recommended actions to be described below .

In June 1964 a proposal, originating in the National Academy of Sciences of the United States, was placed before the Executive Committee of ICSU, that an international committee be formed to facilitate international coordination in matters pertaining to evaluation and compilation of numerical data. The Executive Committee of ICSU responded favorably to this proposal. The following events then ensued:

(1) A Working Group was named by H. W. Thompson, then President of ICSU, to formulate the terms of reference, the program, the make-up of the committee, and the organization required to implement the program recommended by the committee. The composition of the Working Group was: Harrison Brown, Convenor (U. S. A.); V. A. Kirillin (U. S. S. R.); W. Klemm (Germany); F. D. Rossini (U. S. A.); Gordon Sutherland (U. K.); and B. Vodar (France).

(2) The Working Group at meetings in Washington, D. C., and Frankfurt, Germany, and by correspondence, carried out its assigned duties. A formal report embodying its recommendations was prepared for submittal to the January 1966 meeting of the General Assembly of ICSU in Bombay, India.

(3) The General Assembly endorsed unanimously the recommendations of the Working Group. It approved a constitution for the committee, the tentative membership, and a grant from ICSU of $10,000 to assist the committee to get started in its work.

The general purpose and direction which the committee will take are well stated in a Resolution prepared by the Working Group and presented to the General Assembly of ICSU at Bombay. It reads:

> "As a part of the larger problem of the evaluation, storage, and retrieval of scientific information, the compilation of critically evaluated numerical data emerges as a definable and important aspect. It was agreed that ICSU, as a leading international scientific organization, should take steps: (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 call attention to the need for improved status, salaries, working conditions, and facilities for compilers; (c) to point out that evaluation and publication of numerical data are inherently expensive and that subsidies should be provided to compilers to keep book prices low, and to libraries to make possible regular purchase of major collections of data; (d) to increase personal contacts among workers in this area by periodic meetings of specialists in the various fields and exchange visits between related compilation centres; and (e) to encourage programmes of precise experimental determinations to fill in gaps in knowledge and to extend and complete compilations in important areas.
>
> "Even partial success in accomplishing the foregoing aims will do much to establish a favourable climate for implementing the international plan inherent in the following Resolution:
>
> '1. The International Council of Scientific Unions should establish a Committee on Data for Science and Technology, consisting of representatives from the interested Unions and National Representatives from countries having substantial programmes in this area.
>
> '2. The Committee on Data for Science and Technology should direct its attention to the following tasks:
>
> (a) to ascertain on a world-wide basis through the Unions and appropriate national bodies (i) what work on evaluation and publication of 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 programmes in such a way as to minimize unintentional or undesirable overlap, and to recommend new compilation programmes 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 world-wide basis, (i) to stimulate wider distribution of compilations of high quality; (ii) to maintain and distribute a directory of continuing data compilations 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 tables of numerical data.

'3. To assist the Committee in implementing the proposed plan or modifications thereof, the ICSU may wish to establish a central office which is adequately funded.'

"The Committee to be appointed should be free to organize itself for the practical achievement of these goals."

The committee has now been established and has been assigned the acronym CODATA. It has provision for three kinds of members:

(a) Members representing international scientific unions; (b) members representing scientific communities of countries with substantial programs in numerical data compilation; and (c) members coopted because of their special competence in the area.

The initial number of members will be not more than 18. An effort will be made to achieve a reasonable balance among the scientific disciplines represented on the committee.

Each international scientific union federated in ICSU, which expresses an interest in the numerical data program and a desire to participate in the work of the committee, may designate a representative. Each Union representative should avail himself of advisory help from the appropriate groups or individuals in his Union.

Each country in which there exists a substantial program for evaluating numerical and other quantitative data may have a national representative on the committee. The nomination of such representatives shall be made by the national body adhering to ICSU. The national representative should avail himself of advisory help from the appropriate groups or individual experts in his country.

Other international organizations, not a part of ICSU, which are interested in numerical data compilation work, may be invited to nominate liaison representatives. Special and scientific committees of ICSU may send representatives to meetings of the committee. Also, persons expert in various disciplines, whose presence may from time to time be of special benefit to the activities of the committee, may be invited to act as consultants.

During periods between meetings of the committee, its business will be conducted by a Bureau consisting of a President, two Vice-Presidents, and a Secretary-Treasurer. This group will meet at least twice a year and will be supported by a central office.

The initial make-up of the Committee is as follows:

National Representatives

France:	Prof. B. Vodar
Germany:	Prof. Dr. W. Klemm
Japan:	Prof. Dr. M. Kotani
U. K.:	Sir Gordon Sutherland
U. S.:	Prof. F. D. Rossini
U. S. S. R.:	Academician M. A. Styrikovich

Unions Represented

International Astronomical Union (IAU)
International Union of Geodesy and Geophysics (IUGG)
International Union of Pure and Applied Chemistry (IUPAC)
International Scientific Radio Union (URSI)
International Union of Pure and Applied Physics (IUPAP)
International Geographical Union (IGU)
International Union of Crystallography (IUCr)
International Union of Theoretical and Applied Mechanics (IUTAM)
International Union of Physiological Sciences (IUPS)
International Union of Geological Sciences (IUGS)
International Union of Pure and Applied Biophysics (IUPAB)

Other ICSU Representation

ICSU Abstracting Board (IAB)
Federation of Astronomical and Geophysical Services (FAGS)

The Bureau, elected by the Committee, has membership as follows:

President:	Prof. F. D. Rossini
Vice-President:	Prof. Dr. W. Klemm
Vice-President:	Prof. B. Vodar
Secretary-Treasurer:	Sir Gordon Sutherland

The Central Office, which will carry out policies and programs formulated by the committee, will be located in Washington, D. C., for the first two years. Later it will be moved to an appropriate site in Western Europe. The initial staff will consist of an Executive Director, Assistant Director, and Technical Assistant, plus supporting secretarial services. These individuals, to the greatest extent possible, will be from different countries. The first Executive Director is the author of this paper. Recruitment of competent people for the other positions is well in hand.

It should be made clear that CODATA and its Central Office are in no way competitive or overlapping with existing national programs such as the National Standard Reference Data Program in the U. S. and its counterpart in the U. K. These provide funding and management for compilation programs primarily within countries, whereas the functions of the ICSU Committee will be largely coordinational, advisory, and stimulative, and will be world-wide.

Since the mere existence of a committee and office does not assure useful action and results, it is in order to ask what sort of benefits will flow from the ICSU activity. The nature of these are implicit in the stated terms of reference of CODATA. However, a more tangible expression of these is expressed in the following plans and expectations:

(a) Surveys will be made immediately, through each National Representative, of the pertinent activities in each country. These will include identification of continuing numerical data centers and their publications, centers in formation, single or occasional books of tables of acceptable quality, and other relevant matters.

(b) Similar surveys will be made, through each Union Representative, of the activities, capabilities, and needs of each Union.

(c) The results of (a) and (b) will be reported in a Directory to be publicly available and to be revised at intervals.

(d) It is expected that the acts of carrying out steps (a) and (b) will result in the establishment in each country and each union of committees to provide support to the national and union representatives, respectively. (Such committees have already been established in the U. S. National Academy of Sciences and the U. K. Royal Society.)

(e) When appropriate, informal links will be established with governmental and intergovernmental groups concerned with critical tables or reference data projects.

(f) Subcommittees will be established to provide international communications on special relevant topics. (For example, a Task Group is in process of formation for exchange of information of computer applications to numerical data handling.)

(g) Plans have been initiated for a "Gordon-type conference" to be held in Western Europe in 1968 to be cosponsored by the ICSU Committee and a suitable European organization.

The above list is not exhaustive but indicates the variety of ways in which the CODATA can be helpful.

The title of this paper, "A World System of Evaluated Numerical Data for Science and Technology," expresses a hope and a need—not a neat blueprint. The system, if it can be created, will be the sum of numerous publications produced in many countries in many different ways. The funding of the efforts leading to the publications may be by governments, societies, trade associations and other industrial groups, and by private publishers. A leading and probably dominant role in supplying material for the integrated world system will be played by organized national efforts such as the National Standard Reference Data Program in the U. S. If communications can be established among compilers of the world, then standards of excellence can be agreed on and adhered to, undesirable overlap can be avoided, and a planned coverage of all areas of science can be maintained. Achievement of such international cooperation will require a willingness of all participants in the program to work together for the benefit of science and industry in all countries. The ICSU Committee on Data for Science and Technology will do all it can to bring about this needed world-wide cooperation.

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Organizing Physical Molecular Data for Qualitative Chemical Analysis*

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Received October 20, 1966

The American Society for Testing and Materials Committee E-13 on Molecular Spectroscopy has been active for 15 years in the area of indexing and searching infrared, ultraviolet, and visible absorption data. Committee E-14 has made significant contributions in its field and, although the data concerned do not fall in the category of molecular data, the contributions of Committee E-19 on Gas Chromatography and the Joint Committee on X-ray Powder Diffraction deal with the same kinds of problems for the same end results. Of recent years, the National Standard Reference Data Program of the National Bureau of Standards has provided added impetus and support in some of these areas. General descriptions of these activities are given, including recent advances made through ASTM and the Coblentz Society via NSRDP support.

In a simple interpretation of the process of using physical molecular data for qualitative chemical analysis, such data have been likened to fingerprints of compounds, and the analogy of making identifications by comparison of unknown data with files of data obtained from known materials is made. Further, it would appear obvious that the larger the number of different known fingerprints in the files, the better the prospects of identifying any given unknown. Also, as with human fingerprints, most molecular data are rather complex and require mechanized indexing and searching procedures for maximum efficiency in utilization. However, the analogy soon begins to break down, for although there are 10 different fingerprints per

* Presented before the Division of Chemical Literature, Symposium on Compilations of Data on Chemical and Physical Properties of Substances, 152nd National Meeting of the American Chemical Society, New York, N. Y., Sept. 12, 1966.