Table VI. Publications of Compiled Data on Atomic and Molecular Properties Sponsored by the National Standard Reference Data System

Selected Tables of Atomic Spectra, Si II, Si III, Si IV
NSRDS-NBS 3 Section 1

Atomic Transition Probabilities, Hydrogen Through Neon
NSRDS-NBS 4, Volume I

The Band Spectrum of Carbon Monoxide
NSRDS-NBS 5

Tables of Molecular Vibrational Frequencies
NSRDS-NBS 6 (in press)

Electron Impact Ionization Cross-Section Data for Atoms, Atomic Ions, and Diatomic Molecules
I. Experimental Data, Kieffer and Dunn, *Revs. Modern Phys.* 38, 1 (1966).

Table VII. Nondata Publications on Atomic and Molecular Properties Sponsored by the National Standard Reference Data System

Bibliography on Atomic Transition Probabilities
NBS Misc. Pub. 278

Bibliography of Flame Spectroscopy,
NBS Misc. Pub. 281 (in press)

Bibliography of Atomic and Molecular Processes for 1963,
ORNL-AMPIC - 1

Bibliography of Atomic and Molecular Processes for 1964,
ORNL-AMPIC - 3

Directory of International Workers in the Field of Atomic and Molecular Collisions, ORNL-AMPIC - 2

Bibliography of Electron Cross-Section Data,
Joint Institute for Laboratory Astrophysics Report No. 34

NSRDS Status Report, April 1966, NBS Tech. Note 289

tion projects. It is logical that a careful bibliographic research job is an essential first step in compilation of numerical data. In some cases there is no justification for publishing the bibliography, since the primary need is for the actual tables. However, in other cases the bibliography is important enough and of interest to a large enough number of people so that publication as a separate volume is justified, especially since the publication can usually precede the appearance of the tables themselves. A number of bibliographies which have resulted from projects under the cognizance of the Office of Standard Reference Data are shown in Table VII.

It is hoped that increasing numbers of scientists will turn to the Office of Standard Reference Data and to the National Standard Reference Data System as an information resource, both at the present time and in the future, as the output of tables increases. The National Standard Reference Data System is intended to be a primary nationwide source of reliable numerical reference data in the physical sciences. In the pursuit of this goal, we invite the cooperation of all scientists to take part in the compilation work which is the essential aspect of this effort, so that the system can grow to its maximum utility.

The Development of the United Kingdom Data Program

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Current data projects in Britain in x-ray crystallography, interatomic distances, mass spectrometry, and thermodynamic properties of gases are briefly summarized.

In recent decades the work of collection and compilation of data has been confined to certain areas where there is a clear interest among potential users and a group of scientists keen on undertaking the work. The difficulty in moving toward a more systematic procedure has been to decide which areas can most profitably be tackled first and which organizations in which countries are best fitted to tackle particular sections of the work. It has been generally recognized that no one country can afford to do the whole job itself. Therefore, several countries are assessing, extending, and coordinating their national data programs prior to active participation in a truly international program.

The USA took the lead in 1963 when the National Bureau of Standards announced a National Standard Reference Data Program–a broad and systematic attack on the problem. The importance of this development was immediately recognized in Britain, and in 1964 the Department of Scientific and Industrial Research (D.S.I.R.) took steps to establish a smaller-scale equivalent British program. This involved identifying current British data activities, deciding which of them was appropriate to build up or extend as part of the British contribution, and stimulating the necessary expansion of effort with financial support wherever appropriate. In all this activity close contact has been maintained with the National Bureau of Standards.

Not long after the D.S.I.R. decision, the International

Council of Scientific Unions (ICSU) drew attention to the need for organized international cooperation on data activities and set up a working party to examine the problem. At that time there was no British National Committee on Data for Science and Technology. Therefore, following informal discussions between D.S.I.R. and the Royal Society, the two bodies set up an *ad hoc* committee with Sir Gordon Sutherland (the British representative on the ICSU working party) in the Chair. This *ad hoc* committee was formed to advise Sir Gordon for his ICSU working party meetings. It afterwards went on to consider possible areas of work for data activities in the U. K.

The *ad hoc* committee received from D.S.I.R. a preliminary survey of current British activities and provisionally recommended that four areas—crystal data, interatomic distances, thermodynamic properties of gases, and possibly certain types of spectral data—were suitable areas for development in Britain. This view was subsequently endorsed by the ICSU Working Party.

At first the responsibility for stimulating and coordinating activities lay with the National Physical Laboratory, the British equivalent of the National Bureau of Standards. However, in 1965 the Government agencies in civil science were reorganized and D.S.I.R.'s functions were split. With the emergence of a major ICSU interest it was decided that the Office for Scientific and Technical Information (OSTI) should take over the functions in relation to the international data programs. OSTI is part of the Department of Education and Science and is in the same Branch as the Division which deals with International Scientific Relations.

LISTING OF PROJECTS IN BRITAIN

To assist informed policy making in the field of data generally, OSTI surveyed data projects in progress in Britain at the end of 1965. OSTI intends to revise this publication annually and is contributing it to the ICSU worldwide survey. Generally appreciative comments have shown that such surveys are of use in bringing relevant work to other researchers' notice, quite apart from their value in policy making.

Current work in the four fields of interest mentioned before is briefly summarized below. These descriptions are not exhaustive and are certainly not intended to be read as a complete list of data projects in Britain or even as a complete list of those supported by OSTI.

AREAS OF CURRENT ACTIVITY

X-ray Crystallography. Commencing in 1963, D.S.I.R. (now OSTI) supported work directed by Professor J. D. Bernal at Birkbeck College, London. The last stages of this work were incorporated in a new and broader approach at the Chemistry Department of Cambridge University financially supported by OSTI. This is the first stage in the development of a crystal data center. Besides the center's primary task of collecting, organizing, and disseminating data, consideration is being given to a measurement service to scientists and to research on measurement methods.

The work is presently confined to data activities and particularly to the data on organic single crystals. There is full participation in current international arrangements whereby experimental and compilation work in Britain and the USA is brought together in the National Bureau of Standards for the printing of reference handbooks by computer methods. The tapes produced in this way will be available to the British center for retrieval purposes. This informal link-up should work well and should enable valuable experience to be gained about the operation of mechanized data centers in this way. It could well provide a broad pattern for the international organization of data activities in other subject fields.

Interatomic Distances. The Chemical Society has published several editions of its handbook containing these data. In recent years the proportion of these data which are derived from x-ray crystallography has risen steeply and accordingly it is intended that a future edition, for which much work has already been done, will appear under the aegis of the x-ray crystallography center at Cambridge.

Mass Spectrometry. D.S.I.R. was approached by mass spectrometry users about a data center in this field. After public discussion of possibilities, an expert advisory committee was established. A study aimed at outlining the possible scope of a data center in mass spectrometry was commissioned by OSTI from the Atomic Weapons Research Establishment, Aldermaston. This establishment was chosen since it houses one of the principal mass spectrometry groups in Britain. This report was evaluated by the expert advisory committee. A pilot scheme was established at Aldermaston in November 1965, with OSTI financial support. Among its other activities the data center is investigating and evaluating methods of comparing mass spectrometry data on a computer-assisted basis. A comprehensively indexed, computer-searchable list of references, both of mass spectrometry work and of work relevant to mass spectrometry, is being constructed. A computer-ordered bulletin, containing much of this material, has recently started publication. International discussions took place before the final methods of indexing were decided upon.

It is intended to provide a worldwide critical service in mass spectrometry from this center. It will be the U.K. repository for computer data tapes on allied subjects. Thus the NBS ionization data are available at the Aldermaston Mass Spectrometry Data Center.

Thermodynamic Properties of Gases. This project differs from the others in that it has been internationally funded from the outset. It was designed by the International Union of Pure and Applied Chemistry (IUPAC), funded by national contributions through IUPAC, and controlled at working level by an IUPAC committee. Coordination of national programs is undertaken by a scientific center, presently established at Imperial College, London, which is also responsible for collecting, compiling, and disseminating national contributions. Almost every country in the world is prepared to submit data to the center and to undertake experimental work. This experimental work is funded nationally and not through the IUPAC center. OSTI contributes to the cost of the center.

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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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.