The National Standard Reference Data System Program in Atomic and Molecular Properties*

S. A. ROSSMASSLER
Office of Standard Reference Data, National Bureau of Standards, Washington, D. C. 20234

Received November 17, 1966

This paper reports in some detail how the program for one of the technical areas in the National Standard Reference System—that of Atomic and Molecular Properties—developed, what projects are active as part of this program, and what products have appeared so far.

Defining the scope of a general technical area involves a meeting of many minds, and when starting from scratch, it is a matter of successive approximations. The staff of the Office of Standard Reference Data made a first assumption that Atomic and Molecular Properties would be taken to mean properties primarily characteristic of the individual atoms or molecules rather than of any state of aggregation or system of particles. With that premise, a preliminary and tentative list of specific properties was assembled. The list was circulated to members of the National Bureau of Standards for their comments, additions, and deletions. Some outside scientists were asked to criticize the list as well. The tentative list of properties was modified by combining all of the comments, so that when the Office convened an advisory panel of scientists in this area, we were able to supply them with a well-analyzed tentative list.

ADVISORY PANEL MEETING

The advisory panel first met in May 1965 under the chairmanship of Prof. E. U. Condon of the University of Colorado. One of the first items considered was the development of a reasonably firm, comprehensive list of properties comprising the scope of this area. The panel agreed on 63 specific items under 15 major headings shown in Table I.

It is appropriate to comment at this point that the exact scope of any one of the technical areas primarily is a matter of internal concern. The Office of Standard Reference Data has set up a number of partitions for convenience and to permit division of responsibilities, but so far as the outside user is concerned, these partitions have little functional meaning. For the user, the only matter of real importance is that no significant property or group of properties be left out inadvertently or forgotten. Thus, atomic and molecular x-ray spectral data are defined as part of the atomic and molecular properties area, whereas x-ray crystallographic data are considered to be solid state properties. Collision cross-sections are considered to be atomic and molecular properties while reaction rates are considered to be chemical kinetic data.

Table I. Atomic and Molecular Properties

A. Fundamental constants and properties
B. Atomic energy levels
C. Atomic spectral data
D. Atomic and molecular x-ray spectral data
E. Atomic and molecular collision data
F. Particle-surface interactions
G. Plasma properties
H. Direct spectral data
I. Information on molecular energy levels derived from spectral data–diatomic molecules
J. Information on molecular energy levels derived from spectral data–polyatomic molecules
K. Other well-defined properties of atoms and molecules
L. Transition probabilities
M. Descriptive chemical and analytical data
N. Nonobservable computed functions
O. Interatomic and intermolecular forces

As the list of properties was agreed on, priorities were assigned to each specific topic, taking account of the importance to science and technology, the available scientific manpower competent to do compiling work on the specific topic, and the amount of data reported in the scientific literature which would provide a suitable reservoir of information for the compiler. Twenty-eight topics were given a high level of priority according to these criteria. These high level topics are shown in Table II.

The advisory panel which assembled this list also made recommendations to the Office of Standard Reference Data on sources of information on data compilation projects already active in specific areas, lists of possible future compilers who might wish to share in the work, and pitfalls which might be encountered in establishing new projects.

EXISTING DATA REFERENCE RESOURCES

In planning the program it was important to take account of existing compilations of numerical data pertinent to the selected topics. With limited resources, it was obviously essential to concentrate on areas where

* 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 need was greatest. In some cases an existing compilation was recognized as being able to satisfy needs of users fairly well. In other areas, even though there were several active compilation projects going on, additional effort was recommended for one or more reasons. Table III lists a few of the already published general compilations which contain atomic and molecular data. This list is not intended to be exhaustive, and many other titles could be added. In addition to compilations of general scope, there are many volumes containing data on specialized topics, some of which are shown in Table IV. This table does not include any of the large number of reference sources dealing with molecular spectral data, some of which are presented in Table V.

Table II. High Priority Projects

NBS[a]	Atomic energy levels
NBS	Atomic ionization potentials and electron affinities
	Atomic absorption coefficients
NBS	Atomic oscillator strengths
NBS	Laser emission lines
NBS	Multiplet wave lengths, intensities
NBS	X-ray spectral wave length data
	Atomic and molecular collision data
NBS	Heavy particle–heavy particle interactions
NBS	Electron–heavy particle interactions
	Plasma collision frequencies
	Direct spectral data
NBS-O[b]	Infrared spectra
NBS	Microwave spectra
O	Visible and ultraviolet absorption spectra
O	NMR spectra
	ESR spectra
NBS-O	Mass spectra
	Molecular energy level data derived from spectra
O	Diatomic tables of electronic levels, symmetries, vibrational constants, dissociation energies
	Diatomic potential curves
	Polyatomic electronic energy levels
NBS	Vibrational fundamentals and levels
	Rotational constants
	Chemical shifts and coupling constants
NBS	Ionization potentials, appearance potentials, electron affinities
	Refractive indexes (spectral response)
NBS	Dielectric constants (and dipole moments)
O	Interatomic distances and angles
	Interatomic and intermolecular forces
O	Nonobservable computed functions

[a] NBS, project supported by the National Standard Reference Data System. [b] O, project with other support.

Table III. Existing General Compilations

International Critical Tables
National Research Council, McGraw Hill, New York, N. Y.

Landolt-Börnstein Tabellen
Springer-Verlag, Berlin

Tables de Constantes et Données Numériques
G. Charlat, Pergamon Press, New York, 1958

Multivolume "Handbooks," Beilstein, Gmelin, Mellor

Handbook of Chemistry and Physics
Chemical Rubber Company, Cleveland, Ohio, 46th ed., 1965

Handbook of Chemistry
N. A. Lange, Ed., McGraw Hill, New York, N. Y.

American Institute of Physics Handbook
McGraw Hill, New York, N. Y., 2nd ed.

The Merck Index of Chemicals and Drugs
Merck & Co., Inc., Rahway, N. J., 7th ed. 1960

Smithsonian Physical Tables
W. E. Forsythe, Smithsonian Institution, 1959

Tables of Physical and Chemical Constants
G. W. C. Kaye and T. H. Laby, John Wiley & Sons, New York, N. Y., 1959

Table IV. Existing Specialized Compilations

X-Ray Wavelengths for Spectrometer
General Electric Co., 3rd ed., 1964

MIT Wavelength Tables
G. R. Harrison, MIT Press

Tables of Interatomic Distances
L. E. Sutton, Chem. Soc. of London, England, 1958

X-Ray Wavelengths
J. A. Bearden, Clearinghouse for Federal and Scientific Information, 1964

Atomic and Molecular Collision Cross Sections
C. F. Barnett, J. A. Ray, J. C. Thompson, ORNL Sigma Center, 1964

Tables of Experimental Dipole Moments
A. L. McClellan, Freeman, 1963

Atomic Energy Levels
J. A. Bearden and A. F. Burr, Clearinghouse for Federal and Scientific Information, 1965

Atomic Energy Levels, NBS Circular **467**
C. E. Moore (Sitterley), National Bureau of Standards

An Ultraviolet Multiplet Table, NBS Circular **488**
C. E. Moore (Sitterley), National Bureau of Standards

Table V. Existing Compilations and Reference Sources of Molecular Spectral Data

American Petroleum Institute, RP44
Infrared, Raman, Ultraviolet, NMR, Mass

Manufacturing Chemists Association Research Project
Infrared, Raman, Ultraviolet, NMR, Mass

Sadtler Research Laboratories Spectra

Coblentz Society Spectra

Documentation for Molecular Spectroscopy
Infrared, UV, NMR, EPR

Organic Electronic Spectral Data, Inc., UV and Visible Spectra
Volume IV, Interscience Publishers, 1958–59

Microwave Spectral Tables, NBS Monograph 70, Vols. I & II
P. F. Wacker & M. R. Pratto, 1964

Molecular Spectra and Molecular Structure
G. Herzberg, Van Nostrand Books, 1950

The Identification of Molecular Spectra
R. W. B. Pearse and A. G. Gaydon, John Wiley & Sons, 1963

ASTM Spectral Data Indexes
Infrared, Far Infrared, Visible, UV, Mass

Hershenson's Indexes, Infrared, NMR, ESR
Academic Press, 1964–65

ACTIVATION OF A&M PROGRAM

With this the background, the Office of Standard Reference Data began to identify existing compilation work, encourage people to continue their past valuable contributions, and establish new projects where the available competence, interest, and time coincided with the priority list and limited financial resources. Table II shows topics for which a program is now actively working, under either NBS or other sponsorship, to compile, evaluate, and distribute useful numerical data. Many of the originally recognized high priority topics are being at least partially covered. This does not mean that the level of coverage is adequate, because in most cases substantial expansion of these existing projects is vitally needed. In addition, in some cases an individual project is actively covering only a very small fraction of the total possible material.

Analysis of this program indicates that reasonable current coverage of the high priority topics within the area of atomic and molecular properties would require that the number of existing data compilation activities be at least doubled. To cover these same areas plus a number of related topics of only slightly lower priority, existing efforts should be multiplied by at least three. Such expansion of the effort would take care of only the existing literature. It makes no allowance for any expansion as the near future brings the inevitable increase in the rate of appearance of scientific articles, nor does it provide flexibility for the more distant future which will surely reveal whole new areas of important scientific experiment, including measurement techniques not now known.

FEATURES OF CURRENT PROJECTS

Most of the projects in Table II were started with the understanding that a continuing effort would be needed to search the past literature, cover the current literature, and continue to provide up-to-date coverage in the future. Five of these projects are performing data center or information center functions at least to some degree. The NBS supports data centers dealing with atomic energy levels, atomic oscillator strengths, and collision data for electron–heavy particle interactions. The Atomic Energy Commission jointly with the National Standard Reference Data System is supporting an information center on heavy particle–heavy particle interactions, although this center is at present confining most of its information activities to in-house services. In addition, there is a mass spectrometric information center in the Bureau of Standards which supplies bibliographic information on request from the public, and which is working with the investigators of a project on ionization potentials and appearance potentials, supplying background and current bibliographic information so that the compilers can concentrate on the scientific aspects of their work.

Participation of Non-Federal Organizations. Private organizations, technical associations, and interested individuals have long been active in several scientific areas, providing important reference resources in specialized topics. Infrared spectroscopy, visible and ultraviolet absorption spectra, NMR, mass spectroscopy, molecular energy level data for diatomic molecules, interatomic distances and angles, and nonobservable computed functions are some of the topics covered in this way. These activities include projects in Canada, Great Britain, and Germany as well as the United States.

Interest in Other Compilation Projects. The Office of Critical Tables of the National Academy of Sciences–National Research Council is working with the Office of Standard Reference Data in a continuing effort to develop current information about data compilation projects throughout the world. Nevertheless, it is highly probable that there are a number of important projects of which the Office of Standard Reference Data has no knowledge. Some of these gaps are probably due to the lack of publicity about the projects. Scientific communication, even with the best of intentions, is not without its blind spots.

The comments of Dr. Weisman elsewhere in this symposium have indicated some of the ways in which we have sought to identify existing compilation projects which we might otherwise have overlooked. The Office of Standard Reference Data welcomes information on all compilation projects in the physical sciences and will attempt in every case to define a basis of cooperation, with the goal of providing reliable numerical information for the public.

CONSIDERATIONS OF CRITICALITY

These remarks have omitted any detailed mention of the level of criticality needed for compilation. As has already been indicated, we feel that measurements reported in the original scientific literature should be subjected to the highest possible level of scrutiny and critical analysis in preparation of the tables of data which appear as a result of our efforts. However, we cannot divorce ourselves from the day-to-day needs of the scientific and technological community for tables of numbers which will serve their needs where no tables now exist. To that end, we encourage compilation workers in each of the individual projects to set their standards as high as possible while maintaining compatibility with some reasonable level of output. We encourage them further to make every effort to upgrade their standards as rapidly as possible.

We are coming more and more to recognize that an important aspect of the compilation of numerical data in any particular scientific area is a clear definition and statement of the quality considerations involved. In many cases the statement of such standards requires setting up of two or three categories of qualities of compilation.

PRODUCTS

Preparation of tables of data takes a great deal of time. Therefore, it is encouraging that a substantial number of the projects associated with the National Standard Reference Data System have already produced tables and are making them available to the public. Several other compilations of data are in manuscript form and will be appearing soon. Table VI lists these compilations.

In addition, a number of bibliographies have been published as the initial output of one or more of the compila-

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

R. M. S. HALL
Office for Scientific and Technical Information, State House, High Holborn, London, W.C.1., England

Received January 13, 1967

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